



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2014 – 07:05 PM BST

PDB ID : 4V5Y  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with paromomycin and ribosome recycling factor (RRF).  
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.  
Deposited on : 2007-06-19  
Resolution : 4.45 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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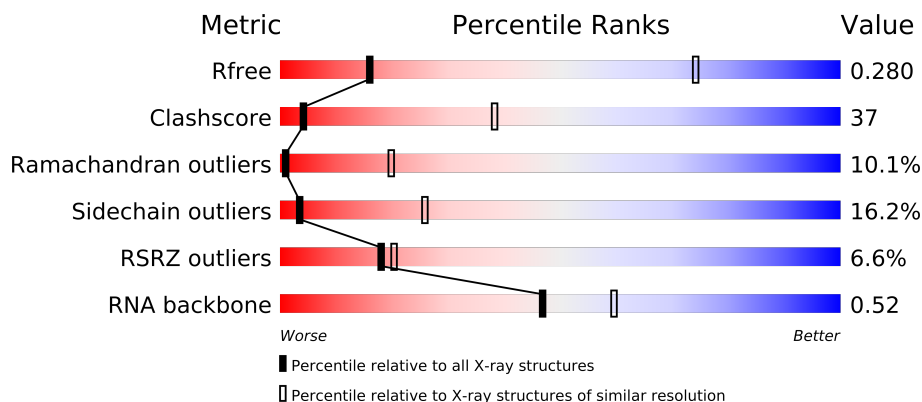
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 4.45 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1020 (5.30-3.50)                                      |
| Clashscore            | 79885                       | 1285 (5.30-3.50)                                      |
| Ramachandran outliers | 78287                       | 1214 (5.26-3.50)                                      |
| Sidechain outliers    | 78261                       | 1195 (5.26-3.50)                                      |
| RSRZ outliers         | 66119                       | 1020 (5.30-3.50)                                      |
| RNA backbone          | 1838                        | 1030 (6.00-2.80)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AA    | 1542   |                  |
| 1   | CA    | 1542   |                  |
| 2   | AC    | 232    |                  |
| 2   | CC    | 232    |                  |
| 3   | AD    | 205    |                  |
| 3   | CD    | 205    |                  |
| 4   | AE    | 166    |                  |
| 4   | CE    | 166    |                  |
| 5   | AF    | 135    |                  |
| 5   | CF    | 135    |                  |
| 6   | AG    | 178    |                  |
| 6   | CG    | 178    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 7   | AH    | 129    |                  |
| 7   | CH    | 129    |                  |
| 8   | AI    | 129    |                  |
| 8   | CI    | 129    |                  |
| 9   | AJ    | 103    |                  |
| 9   | CJ    | 103    |                  |
| 10  | AK    | 128    |                  |
| 10  | CK    | 128    |                  |
| 11  | AL    | 123    |                  |
| 11  | CL    | 123    |                  |
| 12  | AM    | 117    |                  |
| 12  | CM    | 117    |                  |
| 13  | AN    | 100    |                  |
| 13  | CN    | 100    |                  |
| 14  | AO    | 89     |                  |
| 14  | CO    | 89     |                  |
| 15  | AP    | 82     |                  |
| 15  | CP    | 82     |                  |
| 16  | AQ    | 83     |                  |
| 16  | CQ    | 83     |                  |
| 17  | AR    | 74     |                  |
| 17  | CR    | 74     |                  |
| 18  | AS    | 91     |                  |
| 18  | CS    | 91     |                  |
| 19  | AT    | 86     |                  |
| 19  | CT    | 86     |                  |
| 20  | AB    | 240    |                  |
| 20  | CB    | 240    |                  |
| 21  | AU    | 70     |                  |
| 21  | CU    | 70     |                  |
| 22  | BA    | 120    |                  |
| 22  | DA    | 120    |                  |
| 23  | BB    | 2904   |                  |
| 23  | DB    | 2904   |                  |
| 24  | BI    | 141    |                  |
| 24  | DI    | 141    |                  |
| 25  | BC    | 272    |                  |
| 25  | DC    | 272    |                  |
| 26  | BD    | 209    |                  |
| 26  | DD    | 209    |                  |
| 27  | BK    | 123    |                  |
| 27  | DK    | 123    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BP    | 114    |                  |
| 28  | DP    | 114    |                  |
| 29  | BE    | 201    |                  |
| 29  | DE    | 201    |                  |
| 30  | BY    | 58     |                  |
| 30  | DY    | 58     |                  |
| 31  | B0    | 56     |                  |
| 31  | D0    | 56     |                  |
| 32  | B4    | 38     |                  |
| 32  | D4    | 38     |                  |
| 33  | B1    | 54     |                  |
| 33  | D1    | 54     |                  |
| 34  | B3    | 64     |                  |
| 34  | D3    | 64     |                  |
| 35  | BV    | 94     |                  |
| 35  | DV    | 94     |                  |
| 36  | B2    | 46     |                  |
| 36  | D2    | 46     |                  |
| 37  | BL    | 144    |                  |
| 37  | DL    | 144    |                  |
| 38  | BM    | 136    |                  |
| 38  | DM    | 136    |                  |
| 39  | BX    | 63     |                  |
| 39  | DX    | 63     |                  |
| 40  | BH    | 149    |                  |
| 40  | DH    | 149    |                  |
| 41  | BJ    | 142    |                  |
| 41  | DJ    | 142    |                  |
| 42  | BN    | 127    |                  |
| 42  | DN    | 127    |                  |
| 43  | BO    | 117    |                  |
| 43  | DO    | 117    |                  |
| 44  | BQ    | 117    |                  |
| 44  | DQ    | 117    |                  |
| 45  | BS    | 110    |                  |
| 45  | DS    | 110    |                  |
| 46  | BU    | 103    |                  |
| 46  | DU    | 103    |                  |
| 47  | BF    | 178    |                  |
| 47  | DF    | 178    |                  |
| 48  | BG    | 176    |                  |
| 48  | DG    | 176    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 49  | BR    | 103    |                  |
| 49  | DR    | 103    |                  |
| 50  | BT    | 100    |                  |
| 50  | DT    | 100    |                  |
| 51  | BZ    | 78     |                  |
| 51  | DZ    | 78     |                  |
| 52  | BW    | 84     |                  |
| 52  | DW    | 84     |                  |
| 53  | B6    | 185    |                  |
| 53  | D6    | 185    |                  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 54  | MG   | AA    | 1608 | -        | X                |
| 54  | MG   | AA    | 1614 | -        | X                |
| 54  | MG   | AA    | 1617 | -        | X                |
| 54  | MG   | AA    | 1619 | -        | X                |
| 54  | MG   | AA    | 1621 | -        | X                |
| 54  | MG   | AA    | 1622 | -        | X                |
| 54  | MG   | AA    | 1623 | -        | X                |
| 54  | MG   | AA    | 1624 | -        | X                |
| 54  | MG   | AA    | 1625 | -        | X                |
| 54  | MG   | AA    | 1626 | -        | X                |
| 54  | MG   | AA    | 1627 | -        | X                |
| 54  | MG   | AA    | 1632 | -        | X                |
| 54  | MG   | AA    | 1633 | -        | X                |
| 54  | MG   | AA    | 1637 | -        | X                |
| 54  | MG   | AA    | 1639 | -        | X                |
| 54  | MG   | AA    | 1647 | -        | X                |
| 54  | MG   | AA    | 1651 | -        | X                |
| 54  | MG   | AA    | 1652 | -        | X                |
| 54  | MG   | AA    | 1656 | -        | X                |
| 54  | MG   | AA    | 1657 | -        | X                |
| 54  | MG   | AA    | 1658 | -        | X                |
| 54  | MG   | AA    | 1659 | -        | X                |
| 54  | MG   | BB    | 3017 | -        | X                |
| 54  | MG   | BB    | 3018 | -        | X                |
| 54  | MG   | BB    | 3020 | -        | X                |
| 54  | MG   | BB    | 3028 | -        | X                |
| 54  | MG   | BB    | 3033 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 54  | MG   | BB    | 3036 | -        | X                |
| 54  | MG   | BB    | 3047 | -        | X                |
| 54  | MG   | BB    | 3051 | -        | X                |
| 54  | MG   | BB    | 3055 | -        | X                |
| 54  | MG   | BB    | 3057 | -        | X                |
| 54  | MG   | BB    | 3059 | -        | X                |
| 54  | MG   | BB    | 3064 | -        | X                |
| 54  | MG   | BB    | 3078 | -        | X                |
| 54  | MG   | BB    | 3080 | -        | X                |
| 54  | MG   | BB    | 3093 | -        | X                |
| 54  | MG   | BB    | 3097 | -        | X                |
| 54  | MG   | BB    | 3100 | -        | X                |
| 54  | MG   | BB    | 3108 | -        | X                |
| 54  | MG   | CA    | 1608 | -        | X                |
| 54  | MG   | CA    | 1615 | -        | X                |
| 54  | MG   | CA    | 1620 | -        | X                |
| 54  | MG   | CA    | 1621 | -        | X                |
| 54  | MG   | CA    | 1623 | -        | X                |
| 54  | MG   | CA    | 1625 | -        | X                |
| 54  | MG   | CA    | 1626 | -        | X                |
| 54  | MG   | CA    | 1627 | -        | X                |
| 54  | MG   | CA    | 1628 | -        | X                |
| 54  | MG   | CA    | 1641 | -        | X                |
| 54  | MG   | CA    | 1646 | -        | X                |
| 54  | MG   | CA    | 1657 | -        | X                |
| 54  | MG   | CA    | 1658 | -        | X                |
| 54  | MG   | CE    | 201  | -        | X                |
| 54  | MG   | DB    | 3028 | -        | X                |
| 54  | MG   | DB    | 3030 | -        | X                |
| 54  | MG   | DB    | 3036 | -        | X                |
| 54  | MG   | DB    | 3052 | -        | X                |
| 54  | MG   | DB    | 3058 | -        | X                |
| 54  | MG   | DB    | 3065 | -        | X                |
| 54  | MG   | DB    | 3068 | -        | X                |
| 54  | MG   | DB    | 3083 | -        | X                |
| 54  | MG   | DB    | 3086 | -        | X                |
| 54  | MG   | DB    | 3101 | -        | X                |
| 54  | MG   | DB    | 3108 | -        | X                |
| 54  | MG   | DB    | 3111 | -        | X                |
| 55  | PAR  | BB    | 3111 | -        | X                |
| 55  | PAR  | DB    | 3112 | -        | X                |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287128 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1530     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |         |       |
| 1   | CA    | 1530     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |         |       |
| 2   | CC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |
| 3   | CD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |         |       |
| 4   | CE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |         |       |
| 5   | CF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AG    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1174  | 730 | 226 | 214 | 4 |         |         |       |
| 6   | CG    | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1196  | 745 | 230 | 217 | 4 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |
| 7   | CH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |
| 8   | CI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |         |       |
| 9   | CJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |
| 11  | CL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |         |       |
| 12  | CM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 876   | 541 | 177 | 155 | 3 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |
| 13  | CN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |
| 14  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |
| 15  | CP    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 400 | 126 | 111 | 1 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |         |       |
| 16  | CQ    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 657   | 417 | 122 | 115 | 3 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | AR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |         |       |
| 17  | CR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |         |       |
| 18  | CS    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 644   | 413 | 121 | 108 | 2 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |
| 19  | CT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 20  | AB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |         |       |
| 20  | CB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21  | AU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |         |       |
| 21  | CU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |         |       |

- Molecule 22 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 22  | BA    | 117      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2507  | 1116 | 459 | 815 | 117 |         |         |       |
| 22  | DA    | 117      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2507  | 1116 | 459 | 815 | 117 |         |         |       |

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

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 23  | BB    | 2841     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60995 | 27210 | 11229 | 19715 | 2841 |         |         |       |
| 23  | DB    | 2841     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60995 | 27210 | 11229 | 19715 | 2841 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |
| 24  | DI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25  | BC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |         |       |
| 25  | DC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | DD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BK    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 930   | 582 | 179 | 164 | 5 |         |         |       |
| 27  | DK    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 930   | 582 | 179 | 164 | 5 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |
| 28  | DP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |
| 29  | DE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | BY    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |
| 30  | DY    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | B0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |
| 31  | D0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |
| 32  | D4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 33  | B1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |         |       |
| 33  | D1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 34  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |
| 34  | D3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |
| 35  | DV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 36  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |
| 36  | D2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |
| 37  | DL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |
| 38  | DM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 39  | BX    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |
| 39  | DX    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |         |       |
| 40  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |
| 41  | DJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | DN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 43  | BO    | 116      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |         |       |
| 43  | DO    | 116      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 44  | BQ    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |         |       |
| 44  | DQ    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |
| 45  | DS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 46  | BU    | 102      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |         |       |
| 46  | DU    | 102      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BF    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |         |       |
| 47  | DF    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | BG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |
| 48  | DG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |
| 49  | DR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | BT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |         |       |
| 50  | DT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | BZ    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |
| 51  | DZ    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | BW    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 596   | 367 | 120 | 108 | 1 |         |         |       |
| 52  | DW    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 596   | 367 | 120 | 108 | 1 |         |         |       |

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

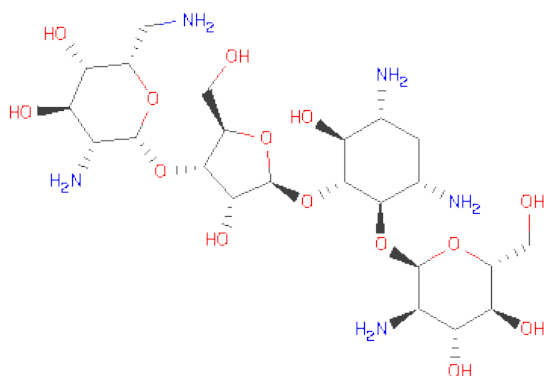


| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | B6    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1478  | 924 | 270 | 282 | 2 |         |         |       |
| 53  | D6    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1478  | 924 | 270 | 282 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54  | DB    | 111      | Total | Mg  | 0       | 0       |
|     |       |          | 111   | 111 |         |         |
| 54  | BB    | 110      | Total | Mg  | 0       | 0       |
|     |       |          | 110   | 110 |         |         |
| 54  | AA    | 60       | Total | Mg  | 0       | 0       |
|     |       |          | 60    | 60  |         |         |
| 54  | CA    | 61       | Total | Mg  | 0       | 0       |
|     |       |          | 61    | 61  |         |         |
| 54  | CE    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 55 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 55  | AA    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |
| 55  | BB    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |
| 55  | CA    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 55  | DB    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

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

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

- Molecule 57 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | AA    | 291      | Total | O   | 0       | 0       |
|     |       |          | 291   | 291 |         |         |
| 57  | AL    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 57  | AN    | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 57  | AT    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 57  | BB    | 495      | Total | O   | 0       | 0       |
|     |       |          | 495   | 495 |         |         |
| 57  | BC    | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 57  | BD    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | BE    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 57  | BL    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | BT    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | CA    | 296      | Total | O   | 0       | 0       |
|     |       |          | 296   | 296 |         |         |
| 57  | CE    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 57  | CL    | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 57  | CN    | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |

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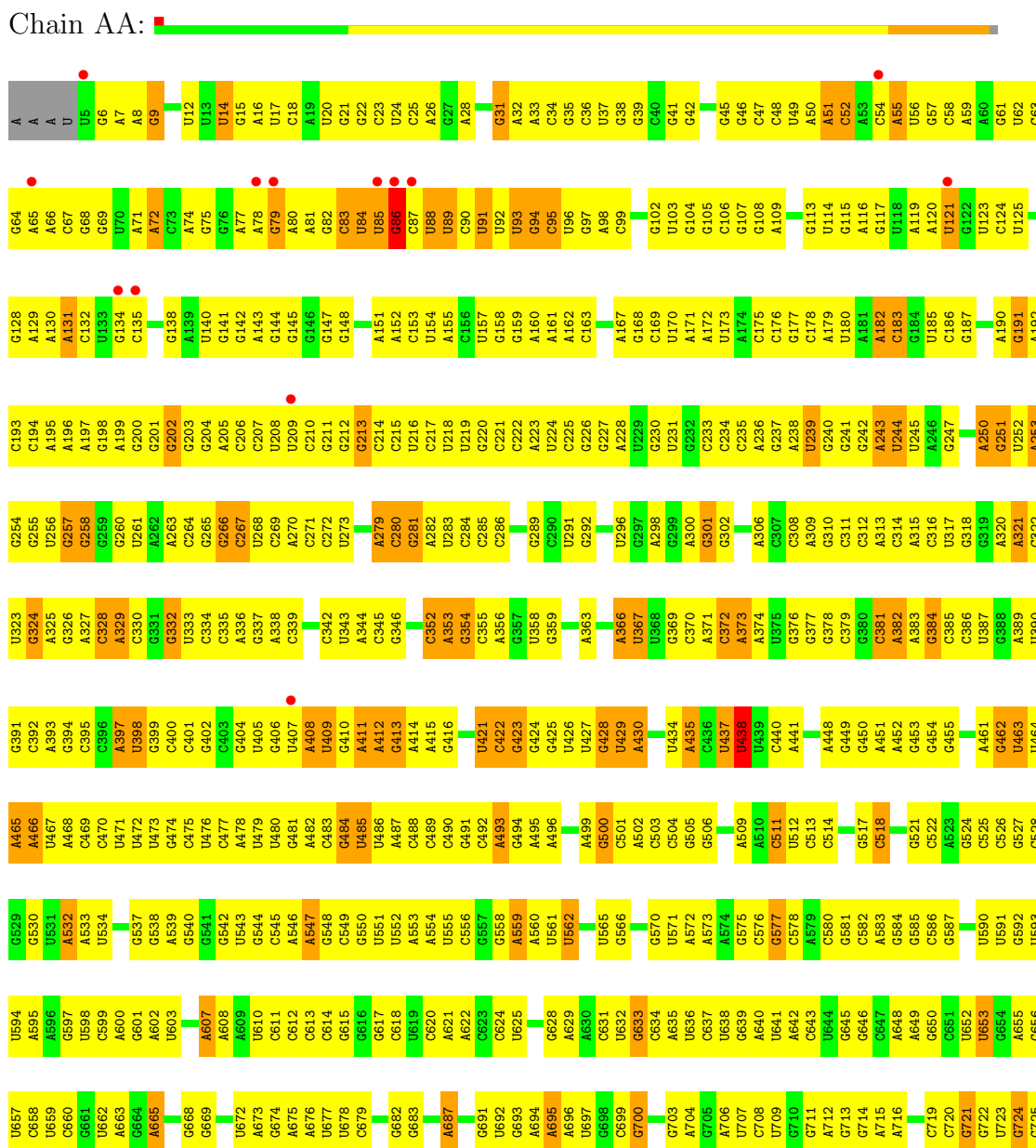
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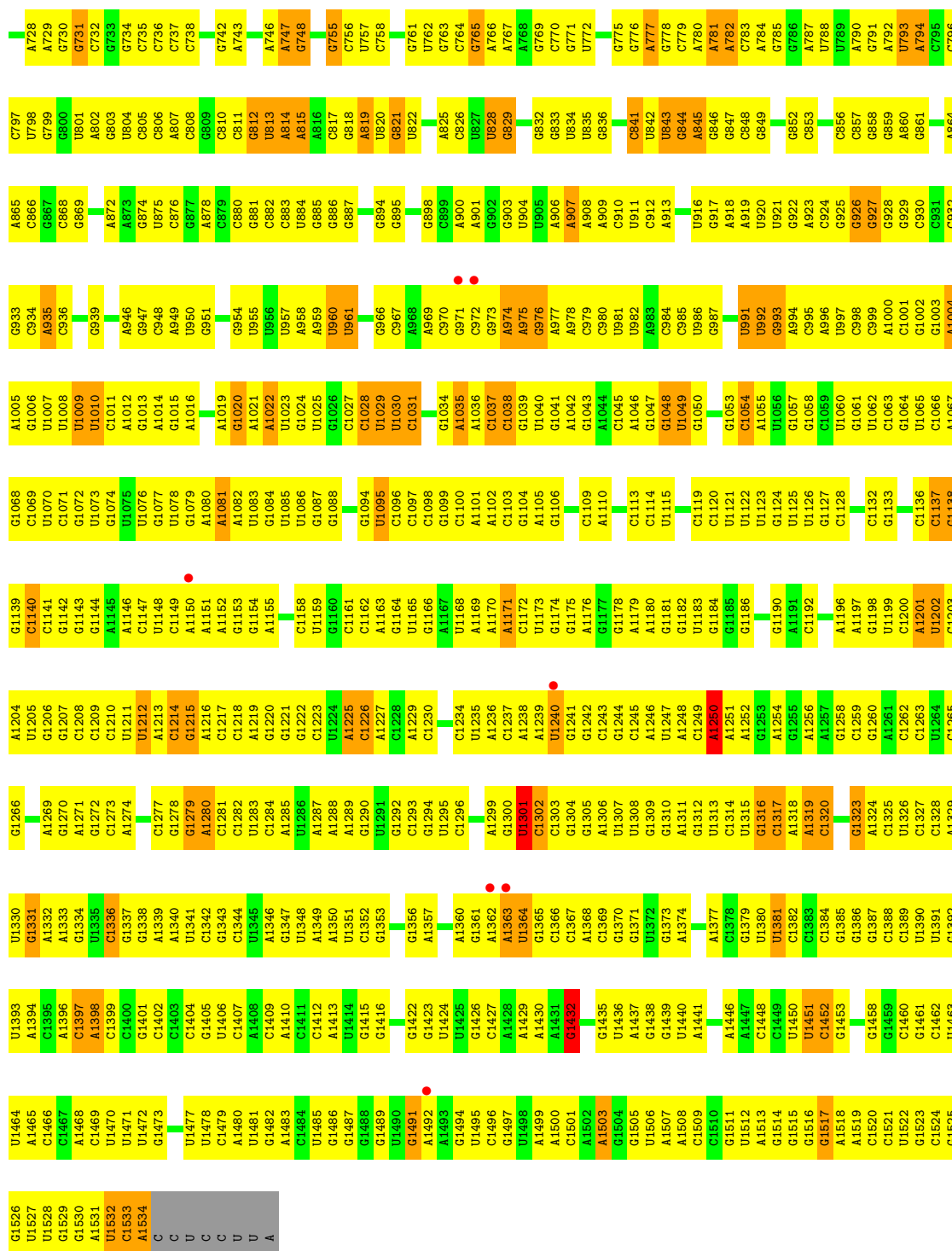
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 57  | CP    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | CT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DB    | 502      | Total<br>502 | O<br>502 | 0       | 0       |
| 57  | DC    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 57  | DD    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DE    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DL    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | DQ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DR    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

### 3 Residue-property plots

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

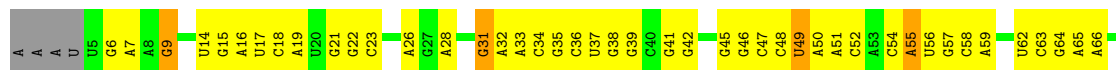
#### • Molecule 1: 16S rRNA



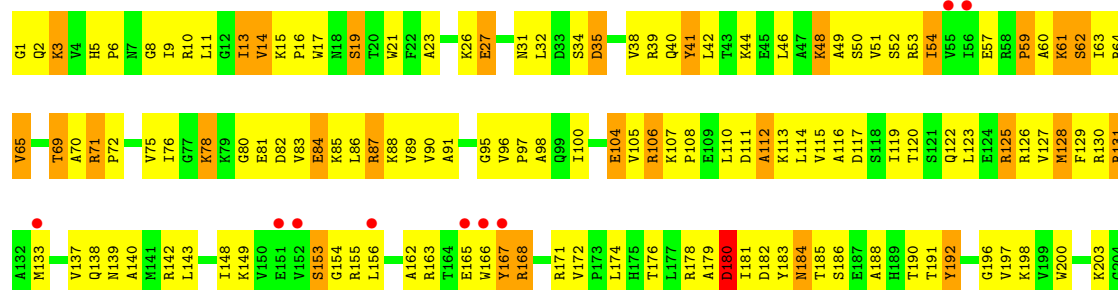


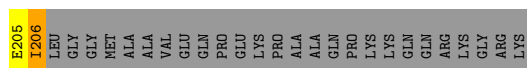
• Molecule 1: 16S rRNA

Chain CA:



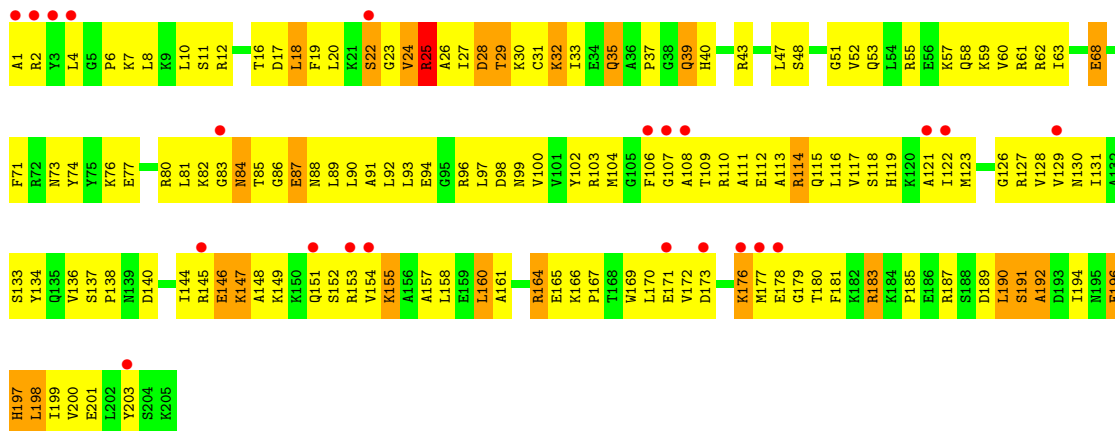






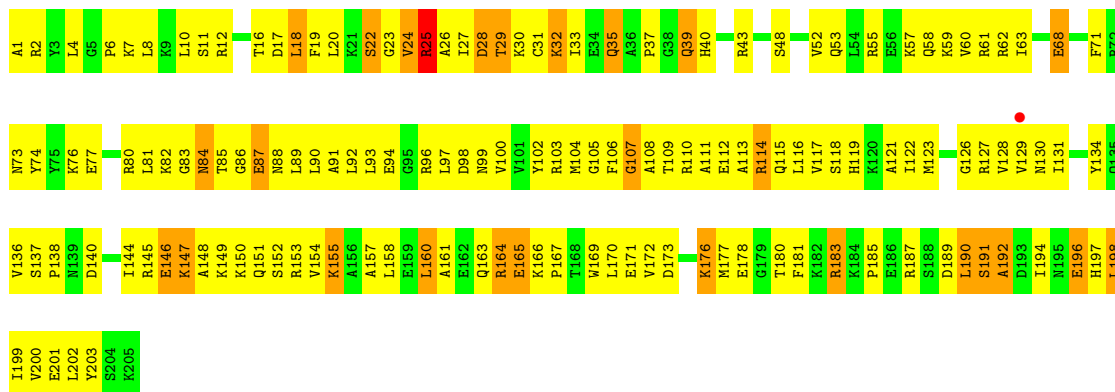
• Molecule 3: 30S ribosomal protein S4

Chain AD:



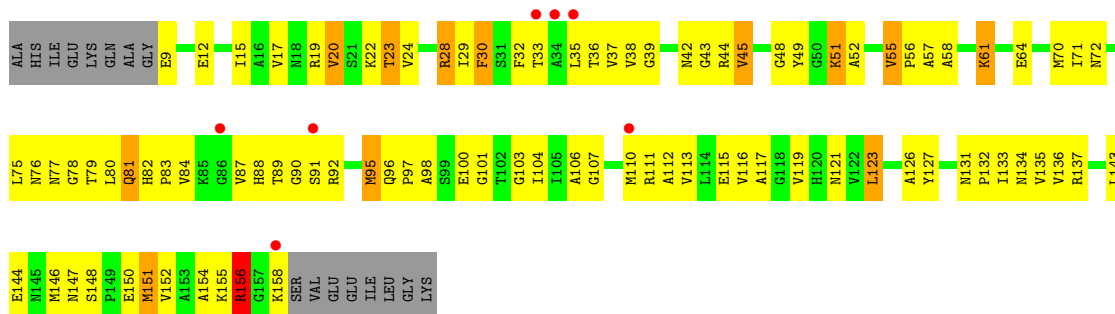
• Molecule 3: 30S ribosomal protein S4

Chain CD:



• Molecule 4: 30S ribosomal protein S5

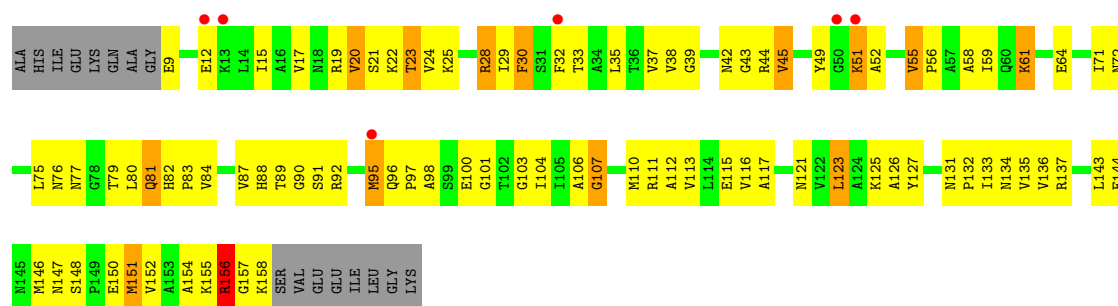
Chain AE:



• Molecule 4: 30S ribosomal protein S5

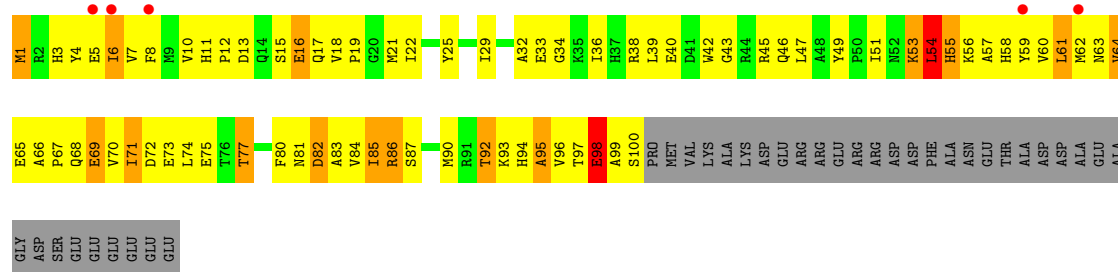
Chain CE:





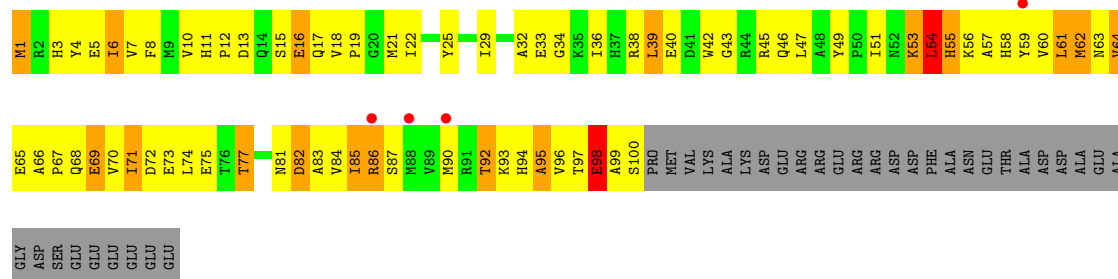
• Molecule 5: 30S ribosomal protein S6

Chain AF:



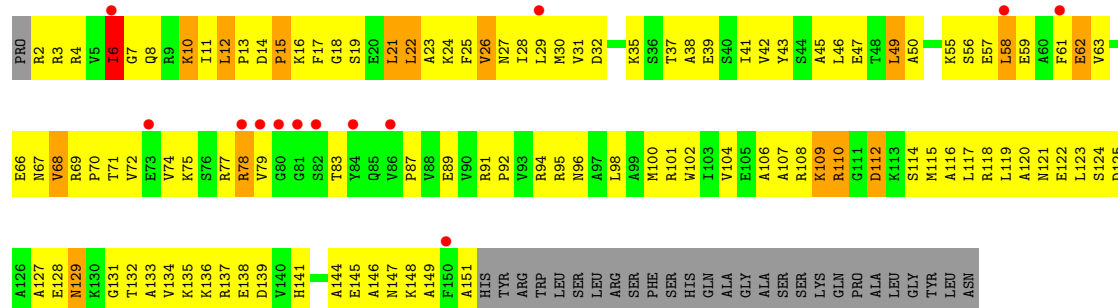
• Molecule 5: 30S ribosomal protein S6

Chain CF:



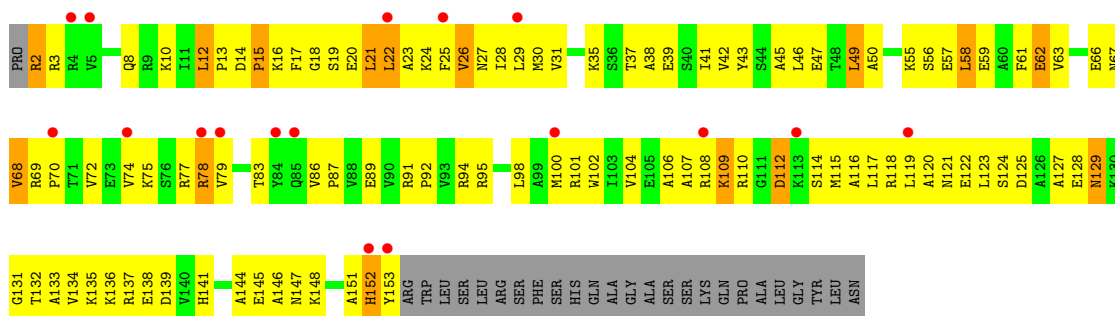
• Molecule 6: 30S ribosomal protein S7

Chain AG:



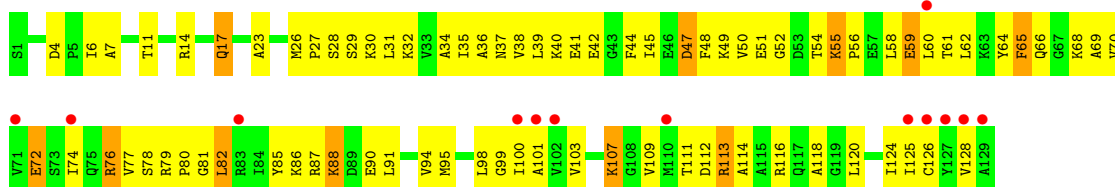
• Molecule 6: 30S ribosomal protein S7

Chain CG:



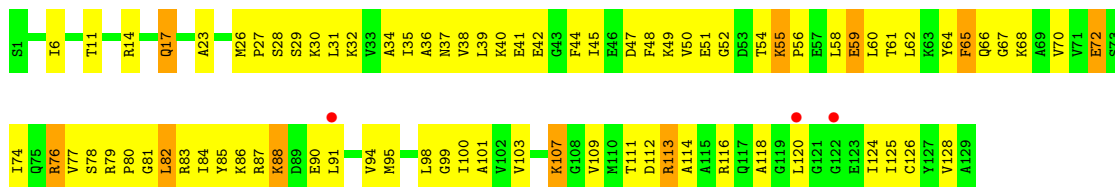
- Molecule 7: 30S ribosomal protein S8

Chain AH:



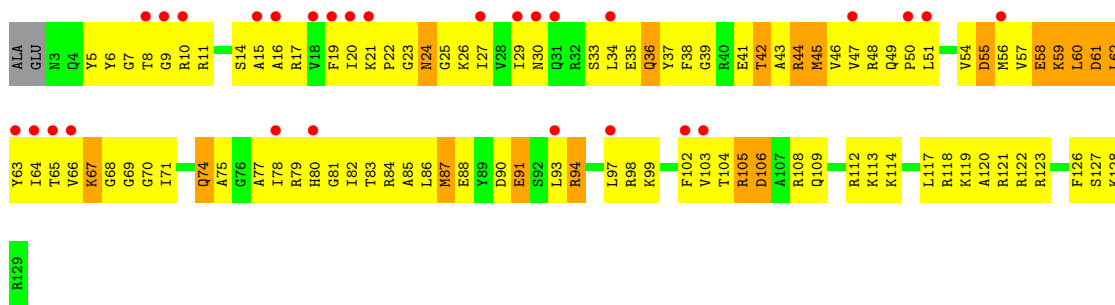
- Molecule 7: 30S ribosomal protein S8

Chain CH:



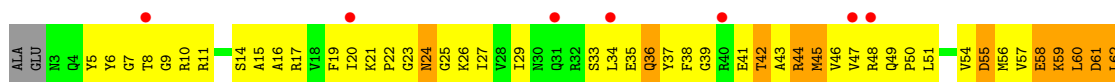
- Molecule 8: 30S ribosomal protein S9

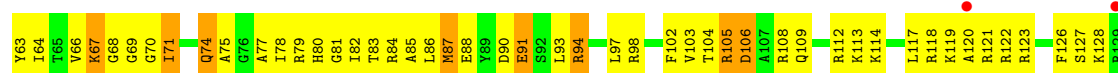
Chain AI:



- Molecule 8: 30S ribosomal protein S9

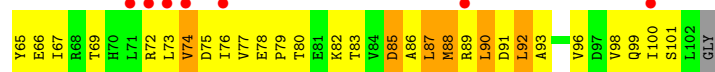
Chain CI:





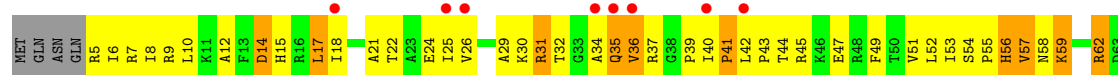
- Molecule 9: 30S ribosomal protein S10

Chain AJ:



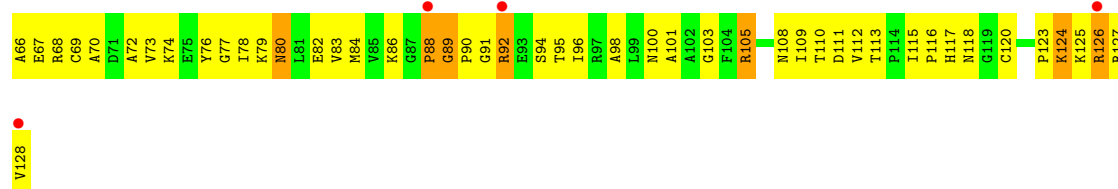
- Molecule 9: 30S ribosomal protein S10

Chain CJ:



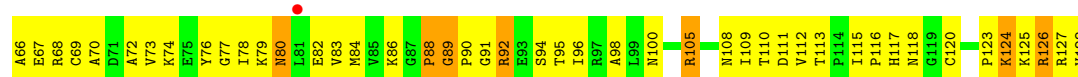
- Molecule 10: 30S ribosomal protein S11

Chain AK:



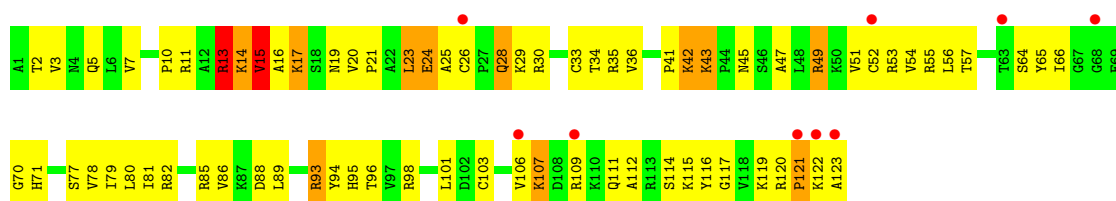
- Molecule 10: 30S ribosomal protein S11

Chain CK:



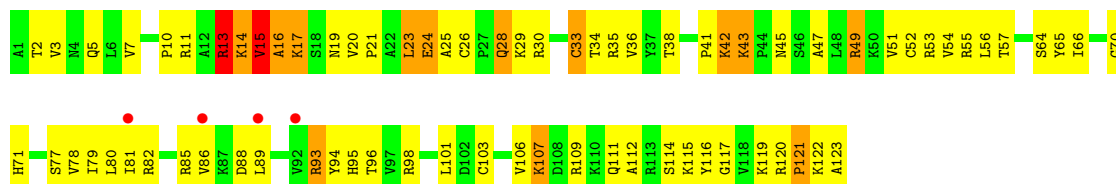
- Molecule 11: 30S ribosomal protein S12

Chain AL:



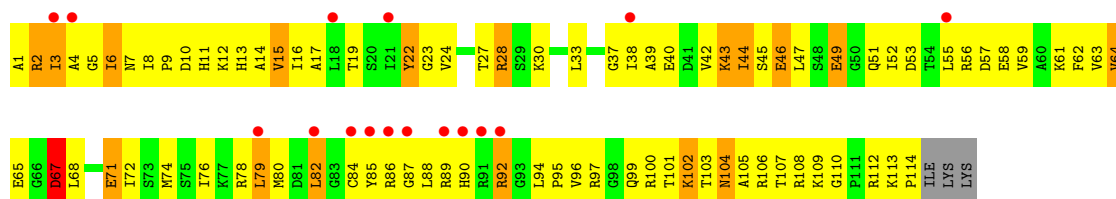
- Molecule 11: 30S ribosomal protein S12

Chain CL:



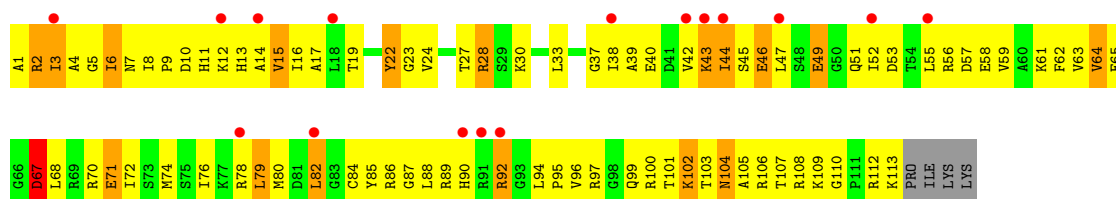
- Molecule 12: 30S ribosomal protein S13

Chain AM:



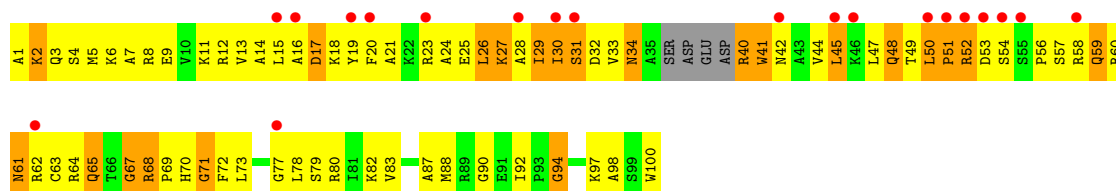
- Molecule 12: 30S ribosomal protein S13

Chain CM:



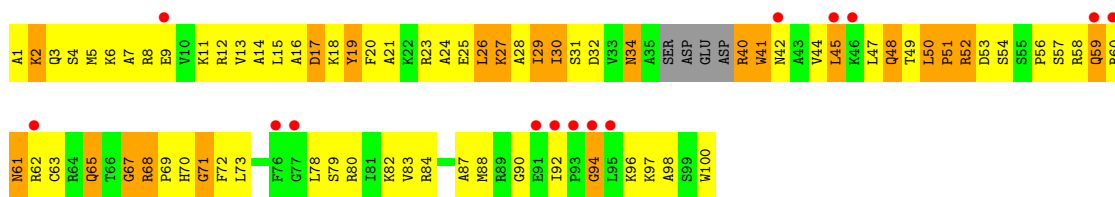
- Molecule 13: 30S ribosomal protein S14

Chain AN:



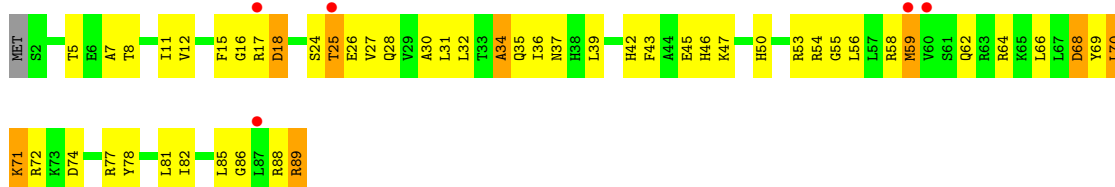
- Molecule 13: 30S ribosomal protein S14

Chain CN:



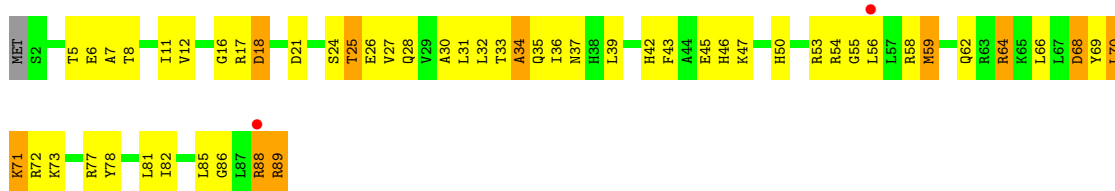
• Molecule 14: 30S ribosomal protein S15

Chain AO:



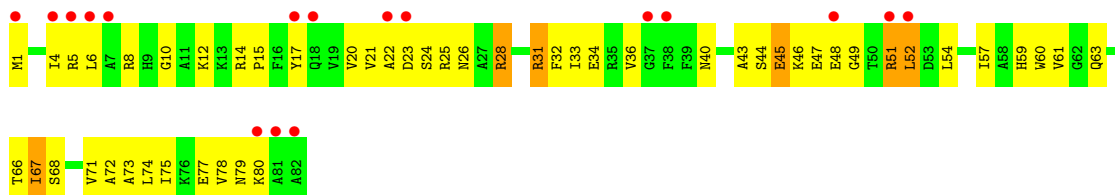
• Molecule 14: 30S ribosomal protein S15

Chain CO:



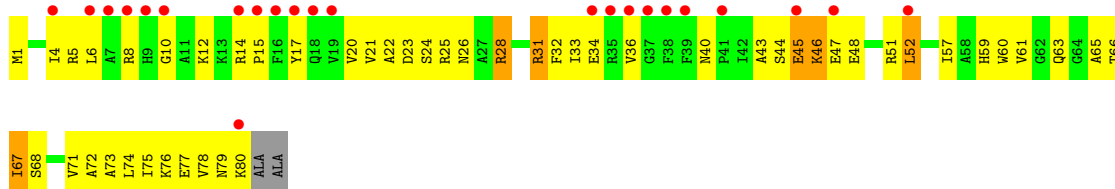
• Molecule 15: 30S ribosomal protein S16

Chain AP:



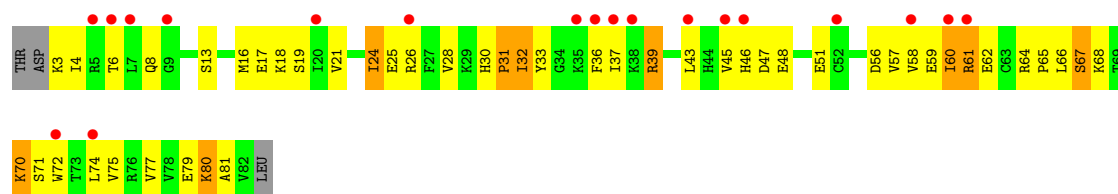
• Molecule 15: 30S ribosomal protein S16

Chain CP:



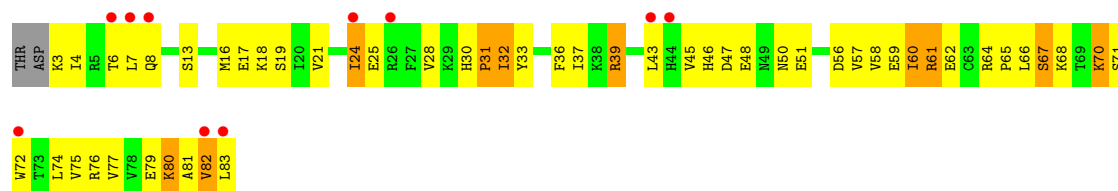
• Molecule 16: 30S ribosomal protein S17

Chain AQ:



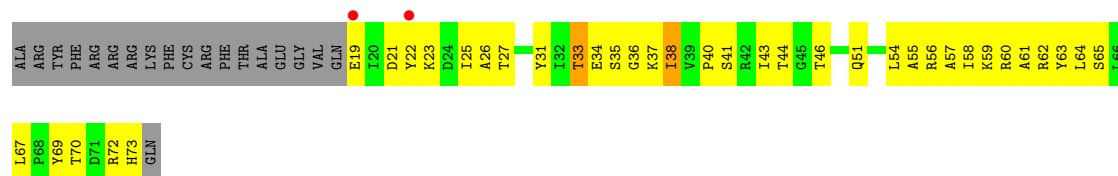
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



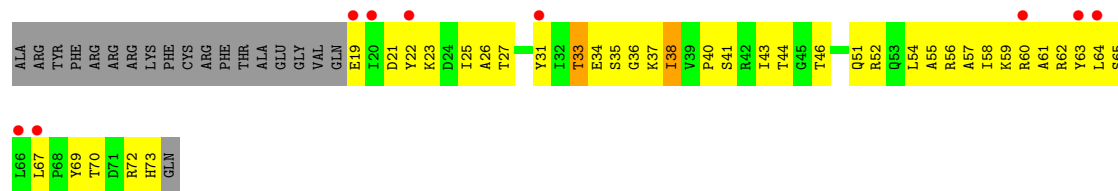
- Molecule 17: 30S ribosomal protein S18

Chain AR:



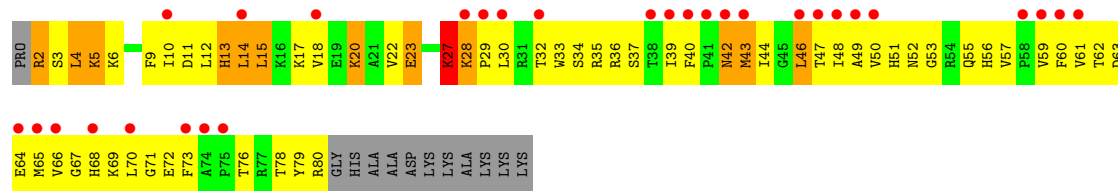
- Molecule 17: 30S ribosomal protein S18

Chain CR:



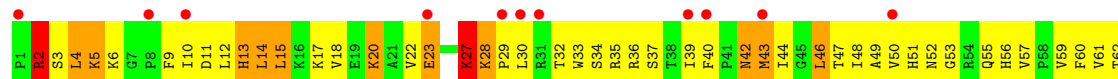
- Molecule 18: 30S ribosomal protein S19

Chain AS:



- Molecule 18: 30S ribosomal protein S19

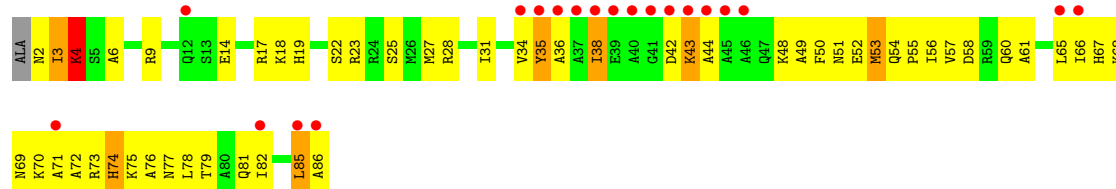
Chain CS:





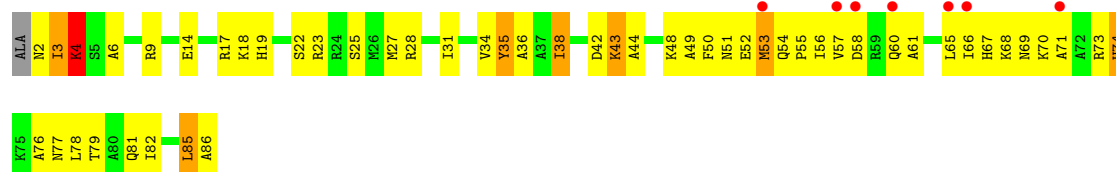
• Molecule 19: 30S ribosomal protein S20

Chain AT:



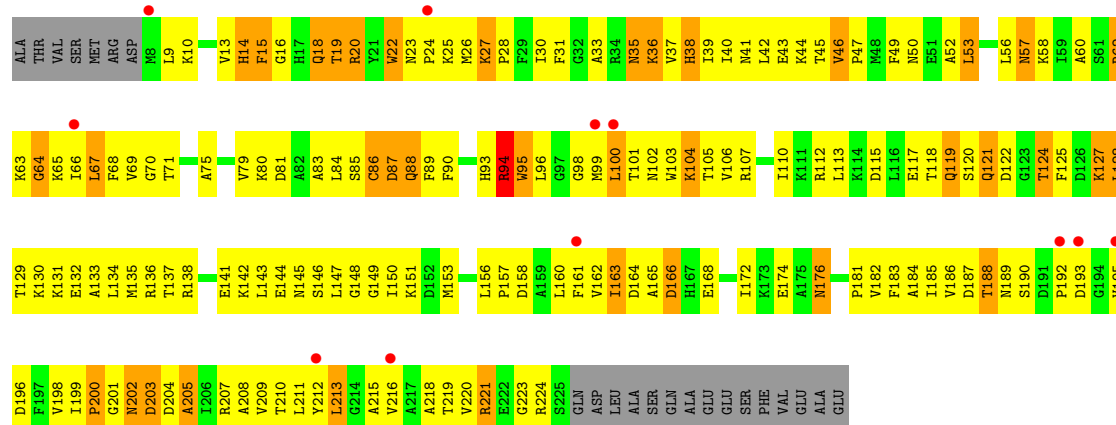
• Molecule 19: 30S ribosomal protein S20

Chain CT:



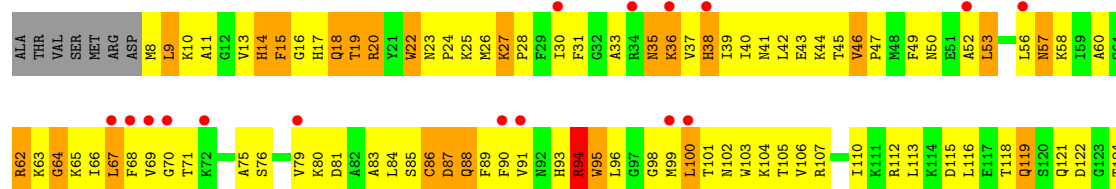
• Molecule 20: 30S ribosomal protein S2

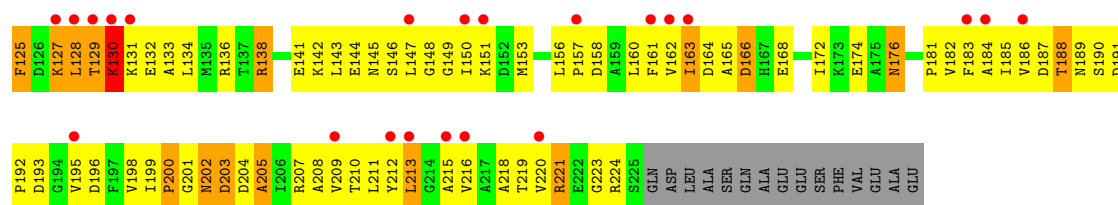
Chain AB:



• Molecule 20: 30S ribosomal protein S2

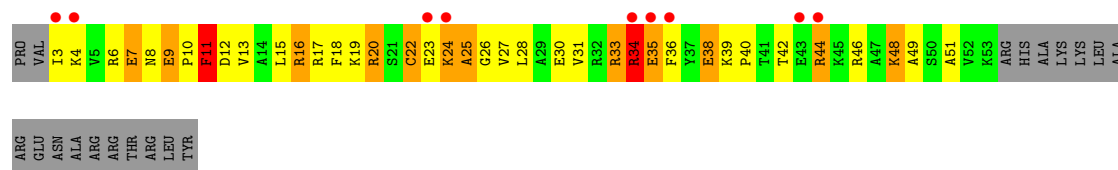
Chain CB:





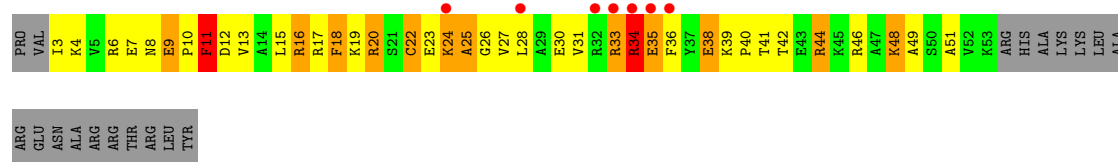
• Molecule 21: 30S ribosomal protein S21

Chain AU:



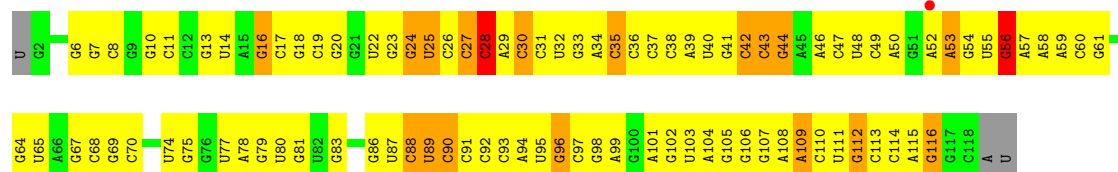
• Molecule 21: 30S ribosomal protein S21

Chain CU:



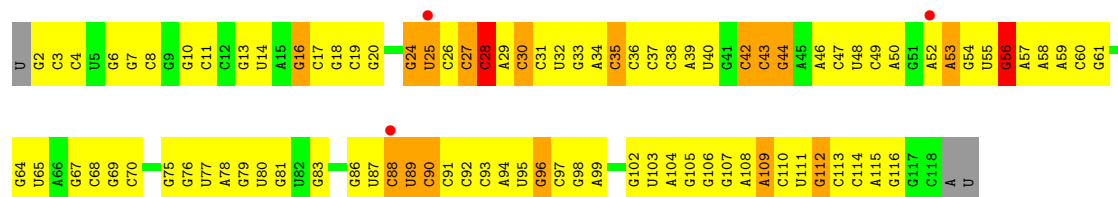
• Molecule 22: 5S rRNA

Chain BA:



• Molecule 22: 5S rRNA

Chain DA:



• Molecule 23: 23S rRNA

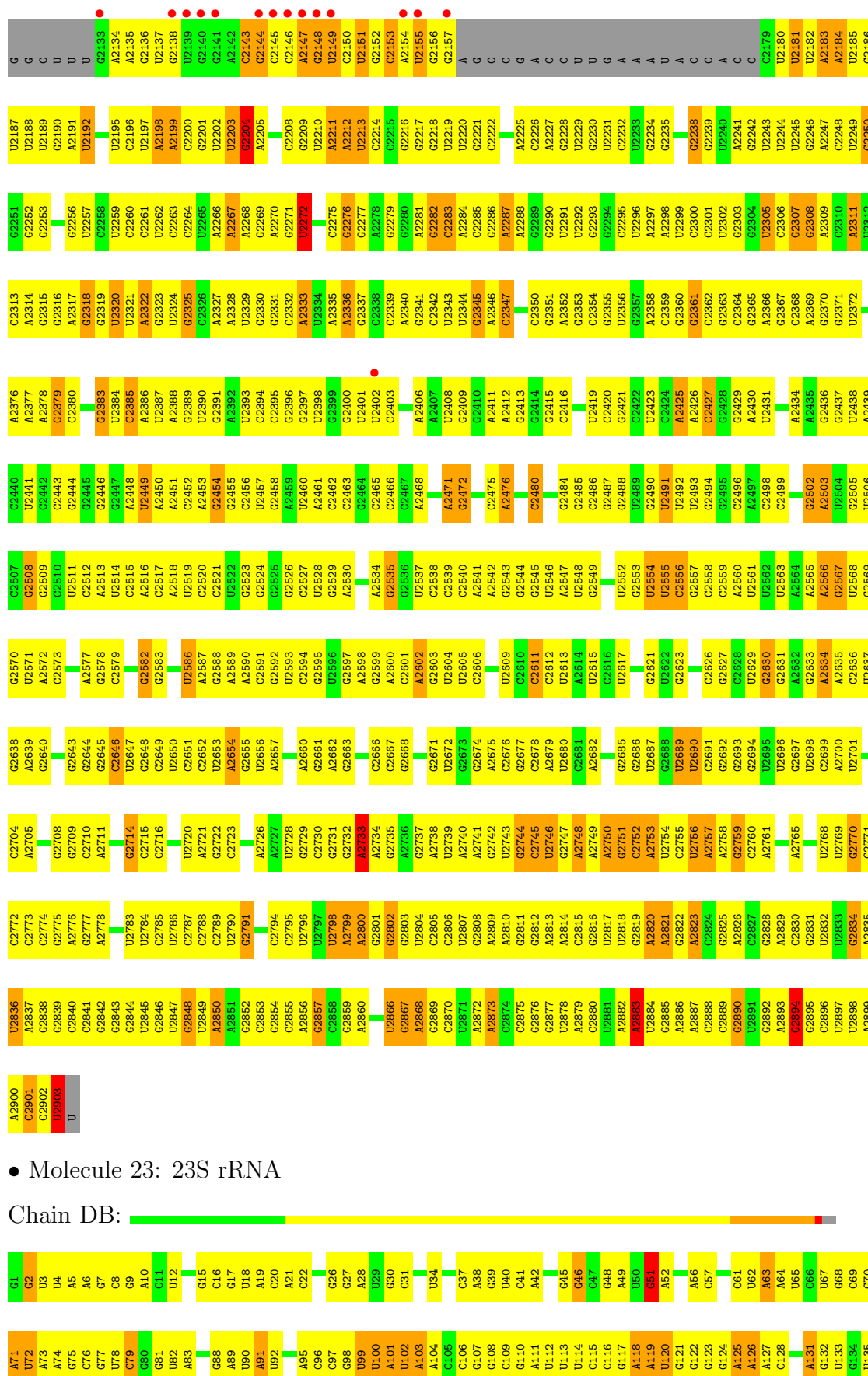
Chain BB:





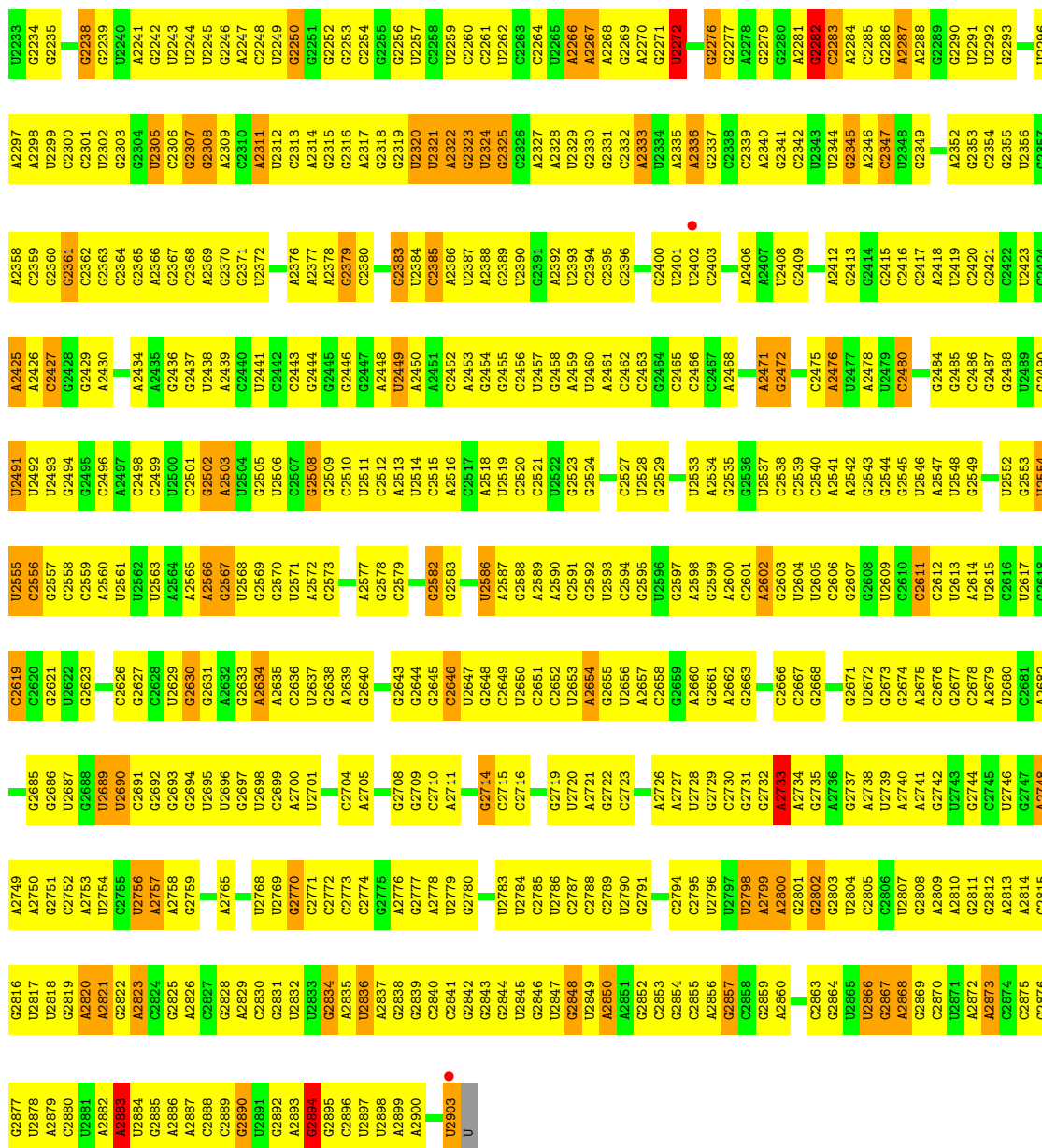
|       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |     |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| C1064 | A1001 | C935  | C873 | U811 | A739 | C678 | A614 | G548 | A480 | G408 | C337 | C269 | U200 | U139 | A74 |
| U1065 | G1002 | A936  | G874 | C812 | C740 | C679 | U615 | G549 | G481 | G409 | G338 | A270 | U200 | C140 | G75 |
| G1068 | C1007 | C937  | G875 | U813 | U741 | C680 | A616 | G550 | A492 | G410 | U339 | G271 | A203 | G76  |     |
| A1069 | A1008 | G938  | C876 | C814 | A742 | G681 | G617 | G551 | A483 | G411 | A340 | G272 | A204 | G77  |     |
| A1070 | A1009 | A941  | A877 | C815 | A743 | G682 | G618 | U552 | C485 | C412 | C341 | G273 | G205 | U78  |     |
| G1071 | A1010 | G942  | A878 | C816 | A744 | U683 | G619 | G553 | C486 | C413 | C341 | G274 | C208 | C79  |     |
| C1072 | G1011 | G943  | G    | C817 | G745 | G684 | G620 | U554 |      | C414 | A345 | C275 | C209 | G80  |     |
|       | U1012 | G944  | G    | G818 | U746 | A685 | A621 |      | C490 | A415 | A346 | U276 | C210 | G81  |     |
| C1077 | A1013 | G945  | G    | G819 | U747 | U686 | G622 |      | G491 | U416 |      | G277 | C211 | U82  |     |
| A1076 | C1014 | C946  | G    | A820 | A753 | C687 | C623 |      | A492 | C417 | U349 | A278 | U148 | A83  |     |
|       | U1015 | A947  | U    | G822 | U754 | U688 | G624 |      | G493 | C418 | G359 | A279 | A149 |      |     |
| A1080 | G1016 | C948  | C    | C823 | U755 | A689 | G625 |      | G494 | U419 | C351 | U280 | U150 | G88  |     |
| U1081 | G1017 | G949  | A    | U824 | A756 | C691 | A627 |      | G495 | C420 | C352 | A282 | G215 | A89  |     |
| U1082 | U1018 | G950  | U    | A825 | G757 | C692 | G628 |      | G496 |      | C353 | A283 | A216 | U90  |     |
| U1083 | C951  | U     | C    | U826 | G758 | A693 | G629 |      |      |      | U354 | U284 | A217 | A91  |     |
| A1084 | A1020 | G952  | C    | U827 | U759 | U694 | C564 |      |      |      | G356 | U285 | A218 | U92  |     |
|       | U1021 |       | C    | U828 | A764 | G695 | A631 |      | U499 | G425 | G359 | U286 | G215 | C151 |     |
| A1085 | G1022 | U955  | G    | A829 | C765 | G696 | A632 |      | A501 | U427 | U360 | U287 | A219 | A152 |     |
| A1086 | U1023 | G956  | A    | G830 | U766 | C697 | A633 |      | A502 | A428 | U361 | U288 | A220 | U93  |     |
| G1087 | G1024 | C957  | C    | U831 |      | C698 | C634 |      | A503 |      | U362 | U289 | A221 | A94  |     |
| A1088 | U1025 | U958  | U    | U832 | U769 | A699 | G635 |      | A504 | A430 | G363 | U290 | A222 | A95  |     |
| A1089 | G1026 |       | U    | A833 | G770 | G700 | G636 |      | A505 | U431 | U364 |      | A223 | C96  |     |
| A1090 | U1027 | C961  | A    | C834 | G771 | U701 | A637 |      | A506 | A432 | U365 | U296 | A224 | U98  |     |
| G1091 | A1028 | U962  | C    | C835 | G772 | U702 | G638 |      | A507 |      | U366 | U297 | A225 | U99  |     |
| C1092 | A1029 | U963  |      | G836 | U773 | U703 | U639 |      | A508 |      | C366 | U298 | A226 | A100 |     |
|       | U1030 | C964  |      | C837 | G774 | G704 | C640 |      | A509 | C435 |      |      | A227 | A101 |     |
|       | G1031 |       |      | U838 | U775 | A705 | U641 |      | C510 | U437 | U369 |      | A228 | U102 |     |
|       | U1032 | U967  |      | U839 | G776 | U706 | U642 |      | A511 | G438 | G370 |      | A229 | A103 |     |
| A1098 | U1033 | C968  |      | C840 | U777 | G707 | A643 |      | U512 | A439 | G371 |      | A230 | A104 |     |
| G1099 | G1034 | G969  |      | G841 | U779 | G708 | A644 |      | A513 |      | G372 |      | A231 | A105 |     |
| C1100 | U1035 | U970  |      | U842 | U780 | U709 | C645 |      | A514 | U441 | U373 |      | A232 | C106 |     |
| U1101 | G1036 | G971  |      | G843 | A781 | U710 | U646 |      | A515 | G442 |      |      | A233 | G107 |     |
| A1102 | U1037 | A972  |      | A844 | U782 |      | G647 |      | C516 | A443 | G377 |      | U234 | G108 |     |
| C1104 | G1038 | A973  |      | U845 | A783 |      | G648 |      | C517 | G444 | G378 |      | U235 | U11  |     |
| U1105 | A1039 | G974  |      | U846 | U784 |      | G649 |      | A518 | C445 | G379 |      | U236 | U111 |     |
|       | U1040 |       |      | U847 | G785 |      | C650 |      | U519 | G446 | G380 |      | U237 | U12  |     |
| G1106 | G1041 | G978  |      | C848 | C786 |      |      |      | G520 |      | G381 |      | U238 | G115 |     |
| U1107 | U1042 | A979  |      | A849 | U787 |      | A654 |      | U521 | U451 |      |      | U239 | C116 |     |
| U1108 | C1043 | A980  |      | U850 | A788 |      | A655 |      | A522 | G452 | G386 |      | U240 | G117 |     |
| C1109 | A1044 | A981  |      | C851 | U789 |      | G656 |      | C523 | G453 | U387 |      | U241 | A118 |     |
| G1110 | C1045 | C982  |      | U852 | U790 |      | U657 |      | G524 | A454 | U388 |      | U242 | A119 |     |
| A1111 | A1046 | A983  |      | C853 | C791 |      | U658 |      | U525 | C455 | U389 |      | U243 | U120 |     |
| G1112 | G1047 | A984  |      | C854 | G791 |      | G659 |      | A526 | C456 | U390 |      | U244 | G121 |     |
| U1113 | A1048 | C985  |      | G855 | A794 |      | C660 |      | C527 | A457 | A391 |      | U245 | G122 |     |
| C1114 | C1049 | C986  |      | U856 | C795 |      | A661 |      | A528 | G458 | C392 |      | U246 | G123 |     |
| G1115 | A1050 | C987  |      | C857 | C796 |      | G662 |      | U529 | U459 | C393 |      | U247 | G124 |     |
| G1116 | G1051 | A988  |      | U858 | G797 |      | G663 |      | C531 | A460 | C394 |      | U248 | A125 |     |
| C1117 | C1052 | G989  |      | C859 | G798 |      | G664 |      | A532 | C461 | U395 |      | U249 | A126 |     |
|       | G1053 | A990  |      | U860 | C799 |      | U665 |      | G533 |      | G396 |      | U250 | A127 |     |
| U1118 | A1054 | C991  |      | A861 | A800 |      | A666 |      | U534 | U464 | U397 |      | U251 | C128 |     |
| U1119 | G1055 | G992  |      | G862 | G801 |      | A670 |      | A538 | G465 | C398 |      | U252 | C129 |     |
| G1120 | C1056 | G993  |      | U863 | A802 |      | C671 |      | U607 | G469 |      |      | U253 | A190 |     |
| C1121 | U1057 | C994  |      | G864 | U803 |      | C672 |      | G539 | A330 |      |      | U254 | A191 |     |
| G1122 | A1058 | C995  |      | C865 | G804 |      | C673 |      | C540 | G470 |      |      | U255 | A192 |     |
| C1123 | G1059 | A996  |      | A866 | A805 |      | G674 |      | A541 | A472 |      |      | U256 | A193 |     |
| G1124 | U1060 | C997  |      | U870 | C806 |      | G675 |      | U545 | A477 |      |      | U257 | A194 |     |
| A1126 | G1062 | C998  |      | U871 | U807 |      | A676 |      | U546 | A478 |      |      | U258 | A195 |     |
|       | U1063 | U999  |      | U872 | G808 |      | A677 |      | A547 | A479 |      |      | U259 | A196 |     |
| A1129 | G1063 | A1000 |      |      |      |      |      |      |      |      |      |      | U260 | A197 |     |
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|       |       |       |      |      |      |      |      |      |      |      |      |      | U262 | A199 |     |
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| G2067 | C2001 | C1925 | G1863 | G1797 | G1731 | A1665 | U1584 | G1524 | G1455 | A1395 | A1327 | U1258 | G1192 | G1131 |
| G2068 | G2002 | A1926 | G1866 | U1798 | C1732 | G1666 | C1585 | G1524 | U1458 | U1396 | A1328 | G1259 | U1193 | U1132 |
| A2070 | U2007 | A1928 | U1865 | C1800 | G1733 | G1667 | A1586 | A1526 | U1459 | U1397 | U1329 | A1260 | A1194 | A1133 |
| A2071 | C2008 | G1929 | U1866 | C1804 | G1734 | A1668 | G1587 | C1526 | U1460 | C1398 | G1330 | C1261 | C1195 | A1134 |
| C2072 | A2009 | G1930 | G1867 | A1805 | U1736 | C1670 | U1589 | G1527 | U1461 | U1400 | G1332 | G1266 | C1196 | G1135 |
| C2073 | G2010 | U1931 | C1868 | A1806 | G1737 | A1671 | U1590 | G1528 | C1462 | A1401 | G1336 | U1267 | C1197 | G1136 |
| U2074 | G2011 | A1932 | G1869 | C1806 | G1738 | A1672 | A1591 | A1528 | C1463 | U1402 | A1338 | U1268 | U1198 | G1137 |
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| U2079 | A2019 | A1937 | C1874 | G1811 | G1743 | A1677 | A1596 | A1535 | A1470 | U1408 | G1344 | U1273 | A1204 | A1143 |
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| G2083 | U2022 | G1941 | C1879 | A1815 | U1747 | G1681 | C1600 | U1539 | U1474 | U1412 | A1347 | G1277 | C1208 | A1147 |
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| U2086 | C2025 | U1946 | U1882 | U1818 | G1750 | G1684 | C1807 | C1542 | U1476 | C1414 | C1349 | G1283 | G1211 | C1150 |
| G2087 | U2026 | C1947 | U1883 | A1819 | U1751 | C1685 | C1808 | G1543 | A1477 | U1415 | C1350 | A1284 | G1212 | A1151 |
| A2088 | G2027 | G1948 | G1884 | U1820 | C1752 | C1686 | A1608 | A1544 | G1478 | U1416 | C1351 | A1285 | A1213 | C1152 |
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| G2091 | G2029 | U1950 | U1886 | C1822 | G1754 | U1688 | A1610 | G1546 | C1480 | G1418 | A1353 | A1287 | G1215 | G1154 |
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| A2095 | A2033 | A1952 | A1890 | G1826 | U1758 | C1694 | A1616 | C1550 | U1484 | G1422 | C1357 | C1293 | U1222 | C1158 |
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| A2097 | G2035 | U1956 | C1892 | G1828 | C1760 | A1700 | C1622 | A1553 | U1486 | G1424 | G1361 | C1295 | G1227 | G1163 |
| U2098 | C2036 | C1957 | C1893 | A1829 | C1761 | A1701 | G1622 | U1554 | C1488 | A1426 | A1365 | G1296 | G1228 | C1164 |
| U2099 | A2037 | C1958 | C1831 | C1830 | G1762 | C1704 | G1628 | G1555 | A1489 | A1427 | A1366 | C1297 | G1229 | A1165 |
| G2100 | U2038 | G1959 | C1832 | C1832 | C1763 | C1704 | G1628 | G1555 | A1490 | C1428 | A1367 | G1299 | U1231 | G1166 |
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| U2105 | C2043 | C1967 | A1900 | C1836 | C1768 | C1708 | A1635 | C1561 | A1496 | G1432 | C1371 | G1303 | G1236 | C1170 |
| U2106 | G1968 | G1983 | A1901 | C1837 | C1769 | U1709 | U1636 | U1562 | G1499 | A1433 | U1372 | G1304 | A1237 | G1171 |
| G2107 | G2046 | A1969 | A1901 | C1838 | A1773 | C1774 | A1637 | U1563 | C1499 | A1434 | A1373 | C1305 | G1238 | C1172 |
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| U2109 | G2048 | U1971 | G1904 | U1837 | U1775 | U1712 | C1639 | C1565 | G1501 | C1437 | U1375 | A1307 | U1240 | U1174 |
| U2110 | C2050 | G1973 | C1905 | G1842 | G1776 | A1713 | A1640 | A1566 | A1502 | U1438 | C1376 | A1308 | A1241 | A1175 |
| U     | A2051 | C1974 | G1906 | C1843 | U1777 | U1714 | A1641 | G1567 | A1503 | A1439 | G1377 | G1309 | U1242 | U1176 |
| G     | U     | G1983 | C1907 | C1844 | U1778 | G1715 | U1647 | A1568 | A1504 | U1440 | A1378 | G1310 | U1243 | G1177 |
| U     | A2052 | G1984 | C1908 | G1845 | U1779 | A1716 | U1648 | A1570 | A1505 | G1441 | U1379 | G1310 | A1244 | C1178 |
| A     | G2053 | C1984 | C1909 | G1846 | U1780 | A1717 | U1648 | A1571 | U1506 | U1442 | G1380 | U1313 | G1245 | G1179 |
| G     | C2054 | C1985 | A1912 | A1847 | A1785 | G1719 | A1652 | A1572 | C1507 | U1443 | G1381 | C1314 | A1246 | U1180 |
| A     | G2055 | C1985 | A1913 | A1848 | A1786 | U1720 | G1653 | G1573 | A1508 | G1444 | G1382 | C1315 | A1247 | U1181 |
| U     | G2056 | U1991 | C1914 | G1849 | A1788 | G1721 | A1654 | G1574 | A1509 | G1445 | A1383 | C1316 | A1248 | U1182 |
| A     | U2057 | G1992 | A1915 | G1850 | C1788 | A1722 | C1655 | U1575 | G1510 | G1446 | A1384 | C1317 | U1249 | U1183 |
| G     | A2059 | U1993 | A1916 | A1853 | A1789 | G1723 | C1656 | U1576 | C1510 | C1447 | A1385 | U1318 | G1250 | U1184 |
| C     | G2060 | C1994 | U1917 | A1854 | C1790 | G1724 | U1657 | U1577 | U1513 | G1448 | A1386 | C1319 | G1251 | G1185 |
| U     | G2061 | U1995 | A1918 | U1855 | C1791 | U1725 | C1658 | U1578 | G1514 | G1449 | A1387 | C1320 | G1252 | G1186 |
| G     | A2062 | C1996 | A1919 | U1856 | G1792 | C1726 | C1661 | A1579 | A1515 | G1514 | G1388 | A1321 | A1253 | G1187 |
| G     | C2063 | C1997 | C1920 | U1857 | C1793 | C1727 | G1662 | A1580 | G1516 | C1451 | G1389 | A1321 | A1254 | U1188 |
| G     | U2064 | A1998 | C1920 | A1858 | C1794 | C1728 | G1661 | A1581 | G1517 | G1452 | U1390 | G1324 | U1255 | U1189 |
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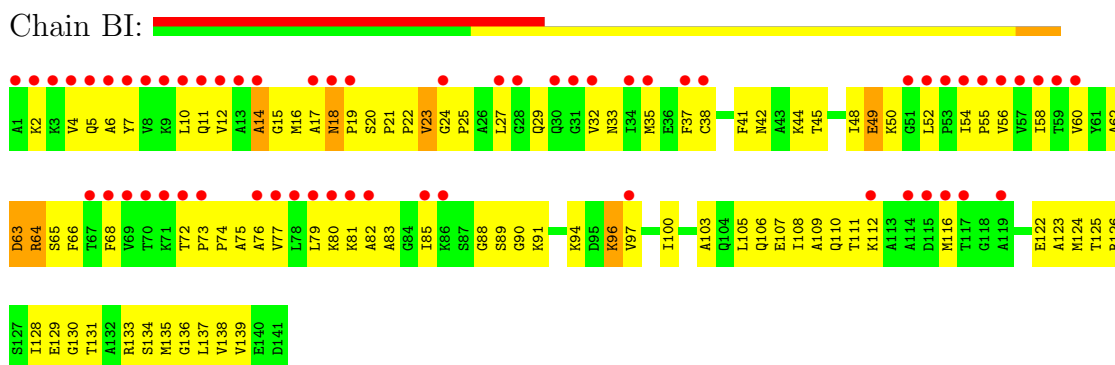




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| A | A | U2109 | G2049 | G1983 | A1848 | A1783 | G1719 | G1653 | U1576 | G1514 | G1449 | A1387 | A1254 | G1185 |
| A | A | G2110 | C2050 | G1984 | G1849 | A1784 | U1720 | A1654 | C1577 | A1515 | G1450 | G1388 | U1255 | G1186 |
| U | A | U     | A2051 | G1985 | G1850 | A1785 | G1721 | A1655 | U1578 | A1516 | C1451 | G1389 | G1256 | G1187 |
| U | G | G     | C1986 | C1986 | U     | A1786 | A1722 | A1656 | A1579 | G1517 | G1452 | U1390 | C1257 | U1188 |
| A | A | U     | G2053 | A1987 | A1853 | A1787 | G1723 | A1657 | U1580 | G1518 | A1453 | U1326 | U1258 | A1189 |
| C | A | U     | A2054 | G1988 | A1854 | C1788 | G1724 | U1657 | G1581 | G1519 | A1454 | A1327 | G1259 | G1190 |
| C | C | G     | C2055 | U     | U1855 | A1789 | U1725 | G1658 | C1582 | U1520 | G1455 | A1328 | A1260 | U1191 |
| A | G | G     | A1916 | A1916 | U1856 | A1790 | C1726 | G1661 | A1583 | G1521 | A1395 | U1329 | C1261 | G1192 |
| C | A | U     | A1917 | A1917 | U1857 | A1791 | C1727 | U1662 | U1584 | A1522 | U1458 | U1397 | U     | G1193 |
| C | A | U     | A1918 | A1918 | G1857 | G1792 | C1728 | U1663 | C1585 | U1523 | G1459 | C1398 | U1267 | A1194 |
| C | A | U     | A1919 | U1983 | U1858 | G1793 | U1729 | A1664 | A1586 | G1524 | U1460 | C1399 | U1268 | G1195 |
| A | A | C     | C1920 | C1920 | U1859 | G1794 | C1730 | A1665 | G1587 | A1525 | C1461 | U1400 | A1269 | C1196 |
| G | G | U     | U1923 | U1923 | G1861 | C1795 | G1731 | U1666 | G1588 | A1526 | C1462 | G1401 | C1270 | U1197 |
| G | C | U     | C1924 | C1924 | G1862 | U1796 | C1732 | U1667 | U1589 | G1527 | C1463 | U1402 | U1198 | U1198 |
| G | G | G     | C1925 | C1925 | U1863 | G1797 | G1733 | U1668 | A1590 | A1528 | G1464 | A1403 | G1271 | U1199 |
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| G | A | G     | A1927 | A1927 | U1865 | G1799 | A1735 | C1670 | C1592 | U1593 | U1405 | U1340 | U1273 | U1201 |
| A | A | G     | C2001 | C2001 | A1866 | C1800 | U1736 | U1671 | A1593 | A1532 | U1406 | A1274 | A1202 | G1202 |
| G | G | U     | G2067 | G2067 | G1867 | U     | G1737 | U1672 | U1594 | C1533 | G1407 | U1275 | U1203 | U1203 |
| C | C | C     | U1930 | U1930 | C1868 | C1804 | G1738 | U1673 | C1595 | U1534 | U1408 | A1276 | A1204 | A1204 |
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| U | U | U     | A1932 | A1932 | C1870 | U     | G1740 | C1675 | A1597 | A1536 | G1471 | G1278 | U     | G1206 |
| U | U | U     | G1933 | G1933 | A1871 | A1809 | C1741 | U1676 | A1598 | G1537 | U1411 | A1347 | U     | G1210 |
| U | U | U     | C2010 | C2010 | A1872 | A1810 | U1742 | U1677 | U1599 | G1538 | U1412 | C1348 | G1283 | G1211 |
| C | C | U     | G1935 | G1935 | A1873 | G1811 | G1743 | A1678 | C1600 | U1539 | U1413 | C1349 | A1285 | G1212 |
| A | A | U     | A1936 | A1936 | C1874 | U1812 | A1744 | A1679 | U     | G1540 | C1414 | C1350 | A1286 | A1213 |
| C | C | U     | A1937 | A1937 | U1875 | G1813 | A1745 | U1680 | A1603 | C1541 | U1415 | U1351 | A1287 | G1215 |
| C | C | U     | U1940 | U1940 | U1876 | U1814 | A1746 | U1681 | U     | U1542 | G1478 | U1352 | A1288 | U1219 |
| C | C | U     | U1941 | U1941 | U1877 | G1815 | U1747 | U1682 | C1607 | G1543 | G1479 | A1353 | U1292 | G1220 |
| C | C | U     | U1942 | U1942 | U1878 | A1816 | C1748 | U1683 | A1608 | U1544 | C1480 | A1354 | G1221 | U1222 |
| C | C | U     | U1943 | U1943 | U1879 | G1817 | A1749 | U1684 | A1609 | A1545 | U1419 | G1355 | U1293 | U1228 |
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| C | C | U     | U1945 | U1945 | U1881 | U1819 | U1751 | U1686 | U1611 | C1547 | G1421 | G1357 | U1298 | U1231 |
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| C | C | U     | C1947 | C1947 | U1883 | U1820 | G1753 | U1688 | U1554 | U1484 | G1423 | A1366 | G1300 | U1235 |
| C | C | U     | G1948 | G1948 | G1884 | A1821 | G1754 | U1689 | A1494 | U1485 | G1424 | A1367 | A1301 | G1236 |
| C | C | U     | G1949 | G1949 | A1885 | G1822 | A1754 | A1614 | G1623 | C1550 | U1486 | G1368 | A1302 | G1237 |
| C | C | U     | U1950 | U1950 | U1886 | G1823 | A1755 | A1690 | U1624 | A1551 | U1487 | G1369 | G1303 | G1238 |
| C | C | U     | G1951 | G1951 | C1887 | G1824 | G1756 | C1691 | U1700 | A1552 | G1426 | C1370 | A1304 | G1239 |
| C | C | U     | U1952 | U1952 | U1888 | U1825 | A1757 | U1692 | G1622 | G1558 | A1427 | G1371 | A1305 | U1240 |
| C | C | U     | A1953 | A1953 | U1889 | G1826 | U1758 | U1693 | G1623 | G1559 | C1428 | A1431 | C1306 | G1241 |
| C | C | U     | G1954 | G1954 | A1890 | U1827 | A1759 | C1694 | G1624 | U1560 | G1429 | G1372 | A1307 | U1242 |
| C | C | U     | U1955 | U1955 | G1891 | G1828 | C1760 | U1700 | U1624 | A1495 | A1431 | G1373 | A1308 | A1241 |
| C | C | U     | U1956 | U1956 | C1892 | A1829 | C1761 | A1701 | U1624 | A1496 | G1432 | G1374 | G1309 | U1242 |
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| C | C | U     | U1958 | U1958 | C1894 | G1831 | G1763 | U1709 | U1624 | A1503 | A1433 | G1376 | U1313 | A1244 |
| C | C | U     | G1964 | G1964 | U1895 | C1832 | C1764 | G1704 | G1622 | G1567 | U1440 | A1378 | U1313 | G1245 |
| C | C | U     | A1966 | A1966 | G1896 | C1833 | U1765 | A1705 | G1633 | U1561 | U1441 | U1379 | C1314 | A1246 |
| C | C | U     | C1967 | C1967 | G1897 | U1834 | G1766 | C1706 | A1634 | U1562 | U1442 | G1380 | C1315 | A1247 |
| C | C | U     | U1968 | U1968 | U1898 | G1835 | G1767 | U1712 | A1635 | C1564 | G1436 | G1381 | U1316 | G1248 |
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| C | C | U     | A1900 | A1900 | U1899 | C1837 | U1709 | U1714 | U1637 | A1566 | U1438 | A1383 | U1318 | G1250 |
| C | C | U     | U1901 | U1901 | U1900 | G1838 | U1709 | G1715 | A1637 | U1567 | A1439 | A1384 | C1319 | G1251 |
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| C | C | U     | G1903 | G1903 | U1902 | U1839 | C1774 | U1717 | A1640 | U1568 | G1441 | U1379 | A1385 | U1321 |
| C | C | U     | U1904 | U1904 | C1903 | G1842 | U1775 | U1712 | A1641 | A1569 | U1442 | G1380 | A1321 | A1253 |
| C | C | U     | A1905 | A1905 | G1904 | G1843 | U1776 | U1714 | U1641 | A1570 | U1443 | G1381 | U1316 | G1248 |
| C | C | U     | C1906 | C1906 | U1905 | G1844 | U1777 | G1715 | U1647 | A1571 | U1444 | G1382 | U1249 | U1249 |
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| C | C | U     | C1918 | C1918 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1919 | U1919 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1920 | C1920 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1921 | U1921 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1922 | C1922 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1923 | U1923 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1924 | C1924 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1925 | U1925 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1926 | C1926 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1927 | U1927 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1928 | C1928 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1929 | U1929 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1930 | C1930 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1931 | U1931 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1932 | C1932 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1933 | U1933 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1934 | C1934 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1935 | U1935 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1936 | C1936 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1937 | U1937 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1938 | C1938 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1939 | U1939 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | C1940 | C1940 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G1448 | A1386 | A1321 | A1253 |
| C | C | U     | U1941 | U1941 | U1909 | A1847 | U1782 | U1718 | U1652 | C1575 | G     |       |       |       |



• Molecule 24: 50S ribosomal protein L11

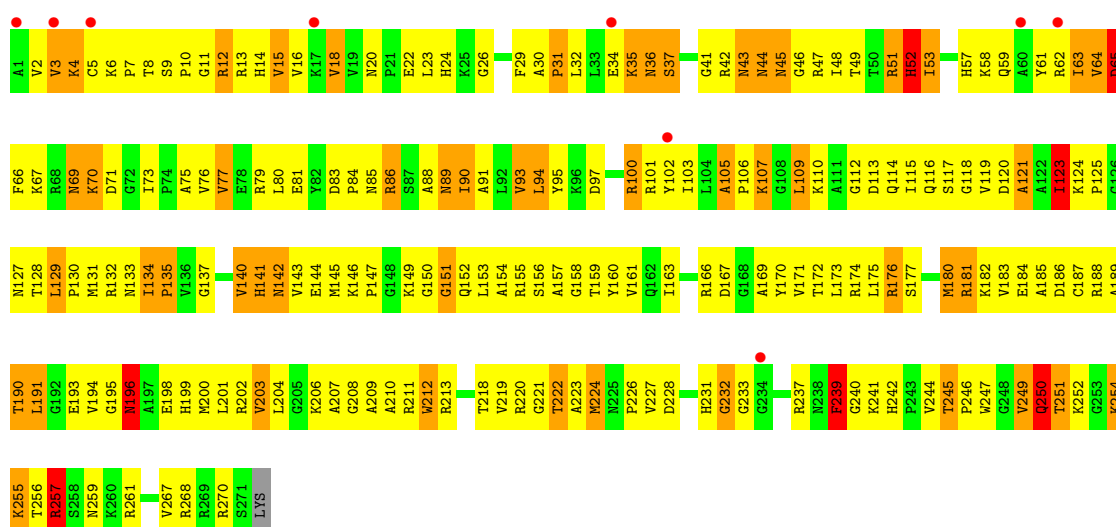


Chain DI:



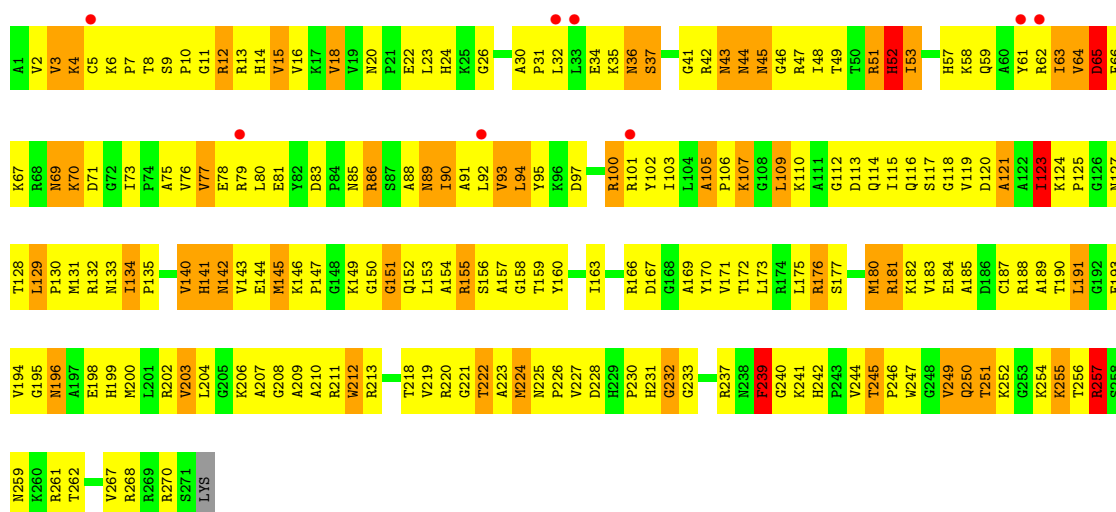
- Molecule 25: 50S ribosomal protein L2

Chain BC:



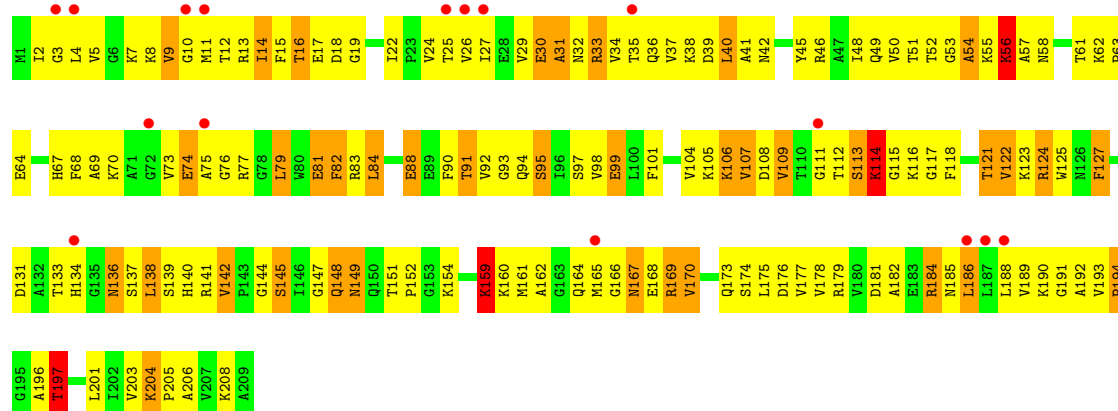
- Molecule 25: 50S ribosomal protein L2

Chain DC:



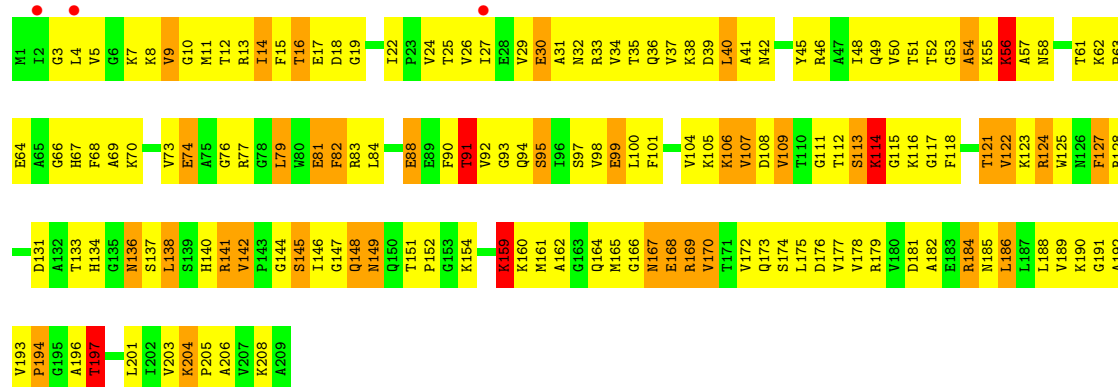
- Molecule 26: 50S ribosomal protein L3

Chain BD: 



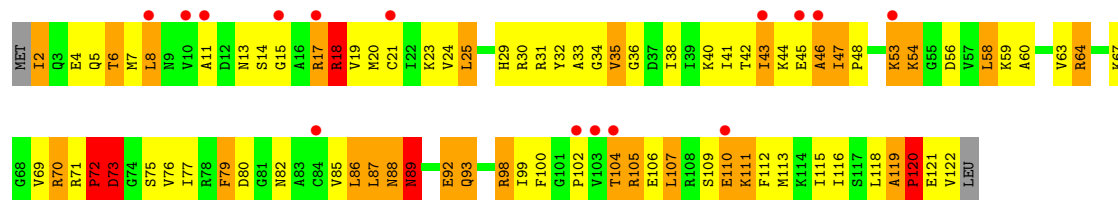
- Molecule 26: 50S ribosomal protein L3

Chain DD: 



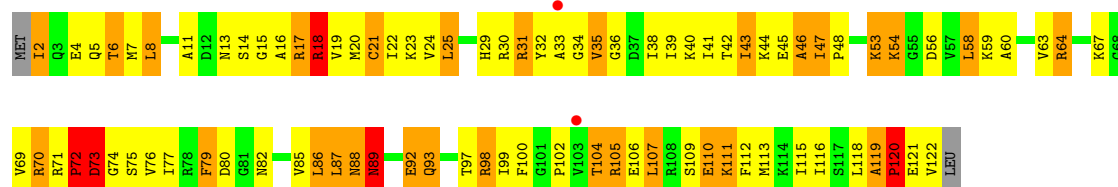
- Molecule 27: 50S ribosomal protein L14

Chain BK: 



- Molecule 27: 50S ribosomal protein L14

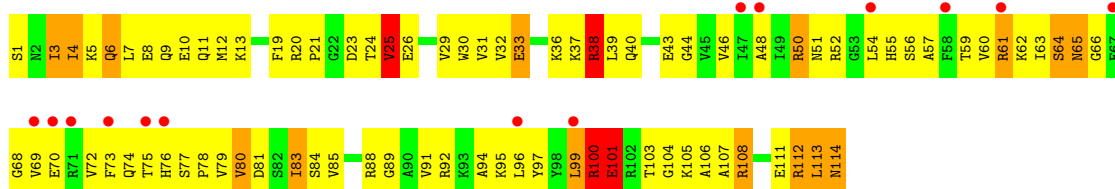
Chain DK: 



- Molecule 28: 50S ribosomal protein L19

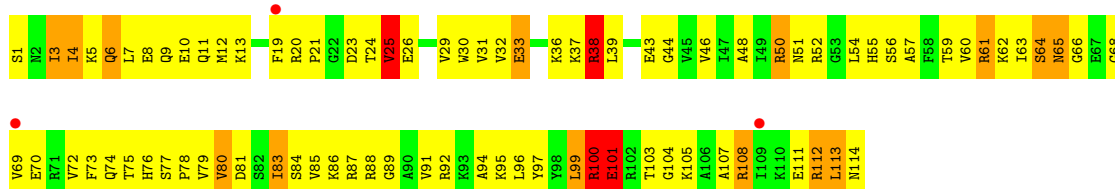


Chain BP:



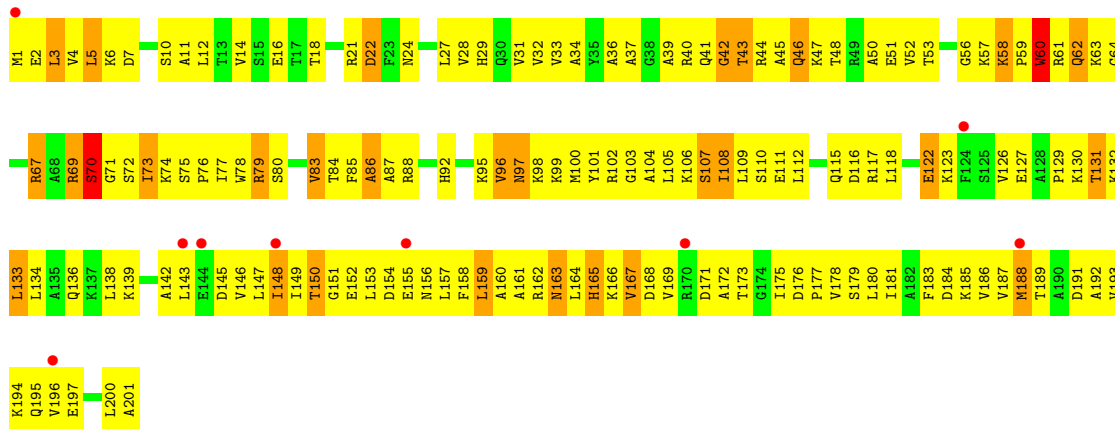
- Molecule 28: 50S ribosomal protein L19

Chain DP:



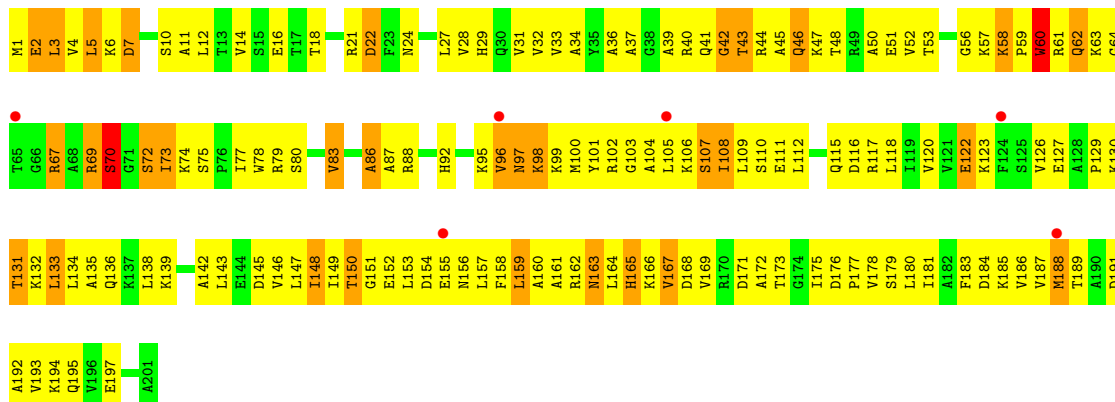
- Molecule 29: 50S ribosomal protein L4

Chain BE:



- Molecule 29: 50S ribosomal protein L4

Chain DE:



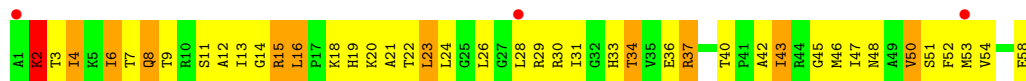
- Molecule 30: 50S ribosomal protein L30

Chain BY: 



- Molecule 30: 50S ribosomal protein L30

Chain DY: 



- Molecule 31: 50S ribosomal protein L32

Chain B0: 



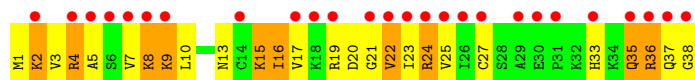
- Molecule 31: 50S ribosomal protein L32

Chain D0: 



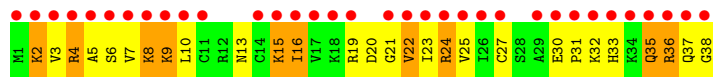
- Molecule 32: 50S ribosomal protein L36

Chain B4: 



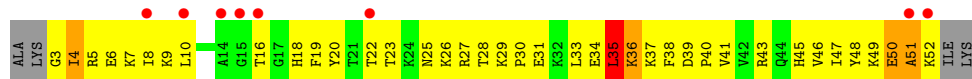
- Molecule 32: 50S ribosomal protein L36

Chain D4: 



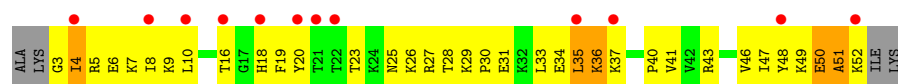
- Molecule 33: 50S ribosomal protein L33

Chain B1: 



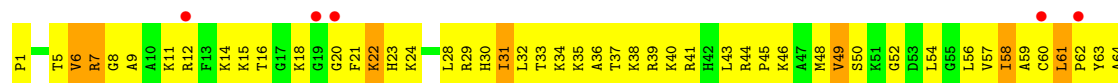
- Molecule 33: 50S ribosomal protein L33

Chain D1: 



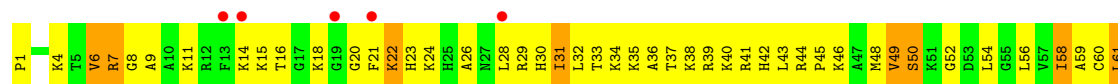
- Molecule 34: 50S ribosomal protein L35

Chain B3:



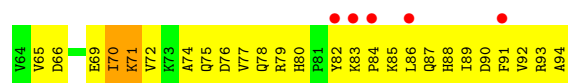
- Molecule 34: 50S ribosomal protein L35

Chain D3:



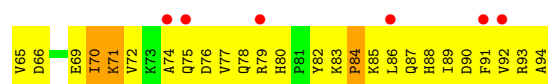
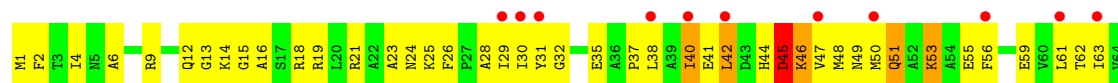
- Molecule 35: 50S ribosomal protein L25

Chain BV:



- Molecule 35: 50S ribosomal protein L25

Chain DV:



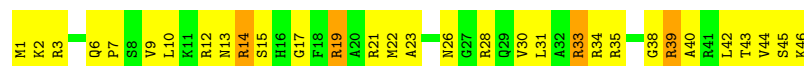
- Molecule 36: 50S ribosomal protein L34

Chain B2:



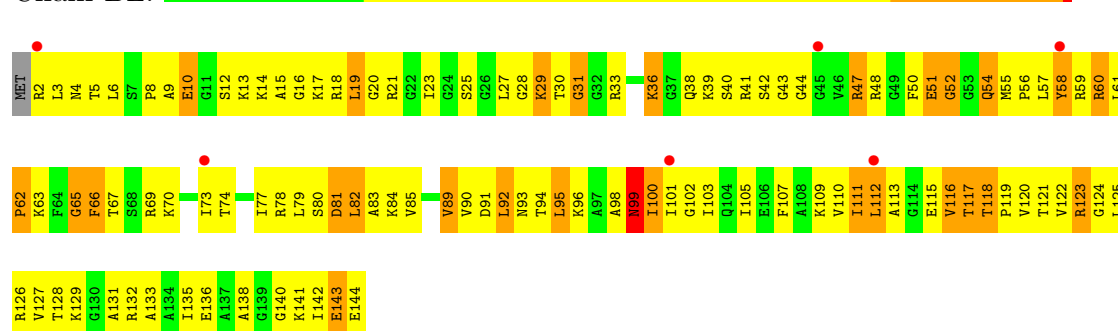
- Molecule 36: 50S ribosomal protein L34

Chain D2:



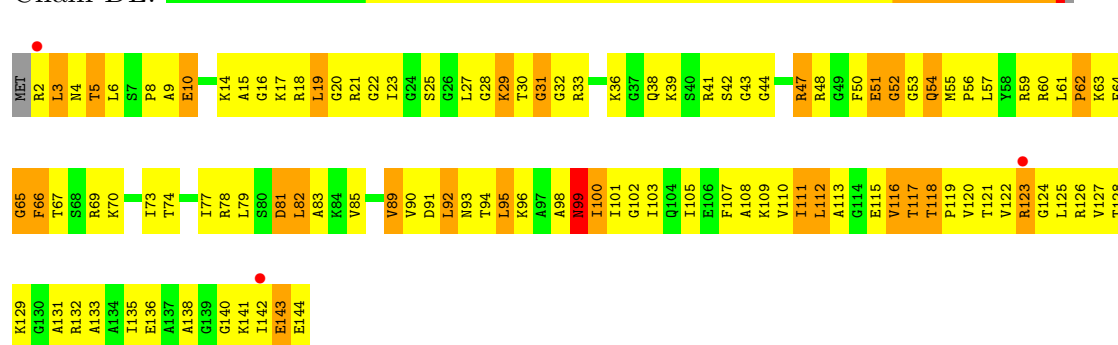
- Molecule 37: 50S ribosomal protein L15

Chain BL:



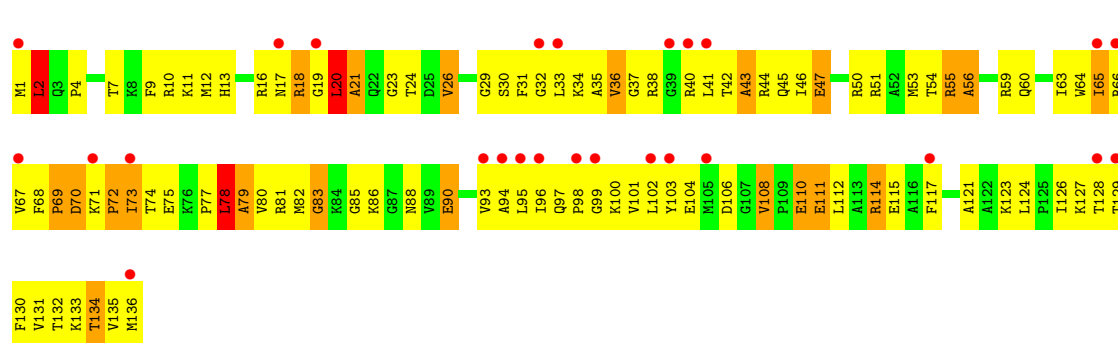
- Molecule 37: 50S ribosomal protein L15

Chain DL:



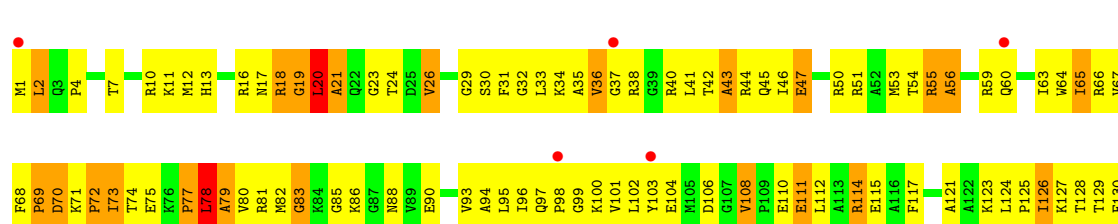
- Molecule 38: 50S ribosomal protein L16

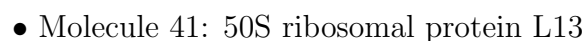
Chain BM:



- Molecule 38: 50S ribosomal protein L16

Chain DM:

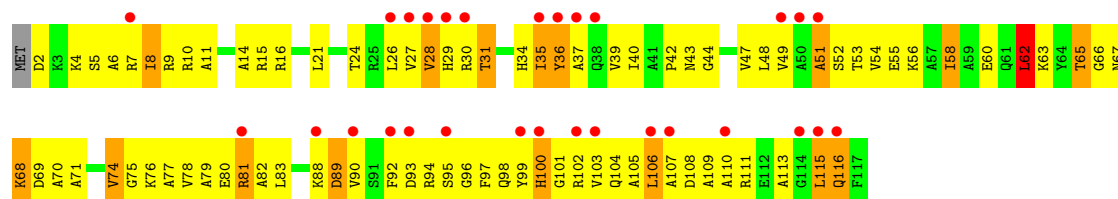




Chain BJ:

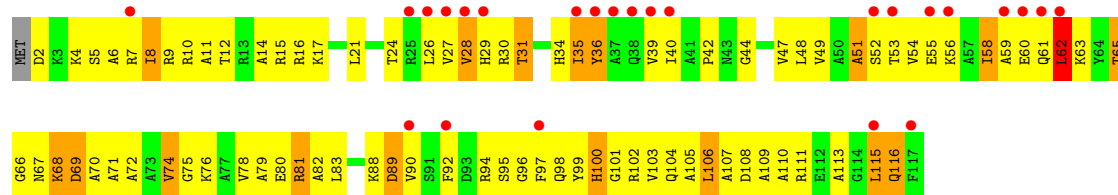


Chain BO: 



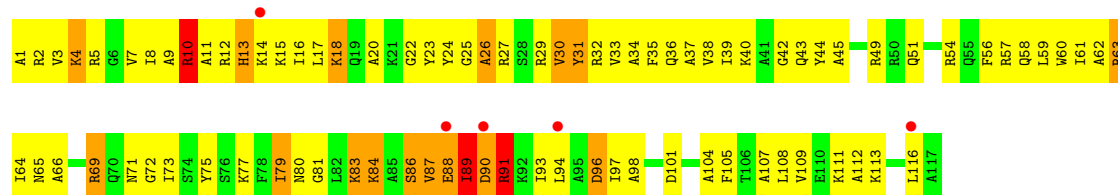
- Molecule 43: 50S ribosomal protein L18

Chain DO: 



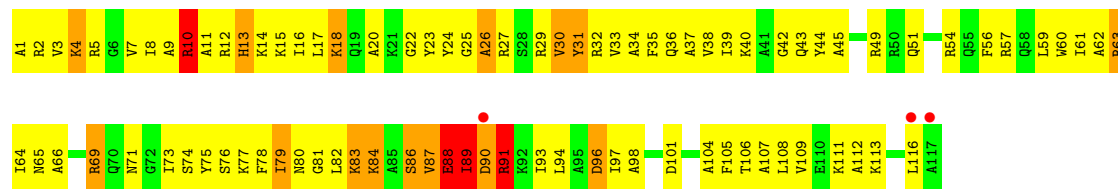
- Molecule 44: 50S ribosomal protein L20

Chain BQ: 



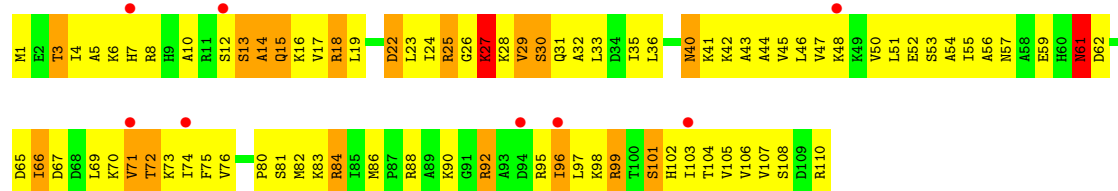
- Molecule 44: 50S ribosomal protein L20

Chain DQ: 



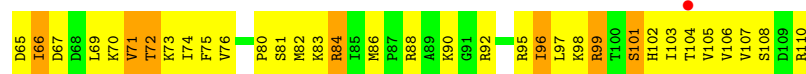
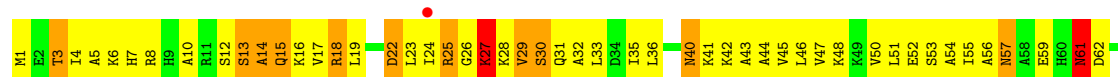
- Molecule 45: 50S ribosomal protein L22

Chain BS: 



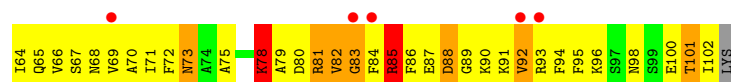
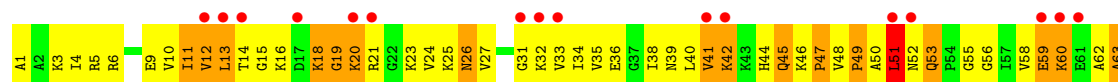
- Molecule 45: 50S ribosomal protein L22

Chain DS: 



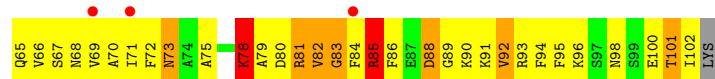
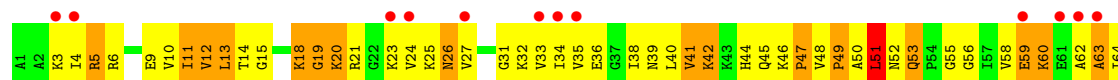
• Molecule 46: 50S ribosomal protein L24

Chain BU:



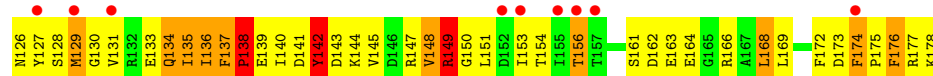
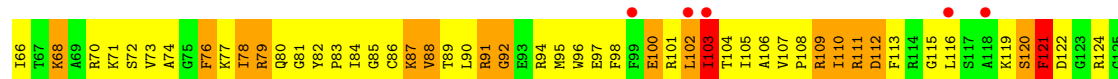
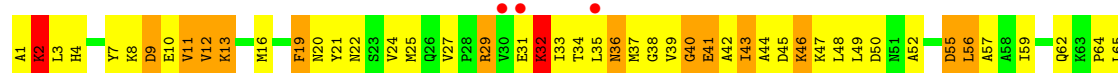
• Molecule 46: 50S ribosomal protein L24

Chain DU:



• Molecule 47: 50S ribosomal protein L5

Chain BF:

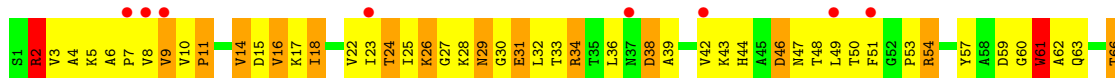






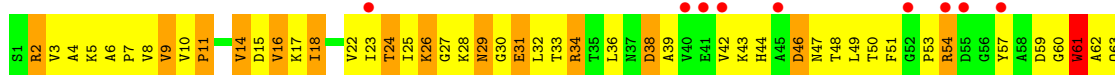
• Molecule 48: 50S ribosomal protein L6

Chain BG:



• Molecule 48: 50S ribosomal protein L6

Chain DG:



• Molecule 49: 50S ribosomal protein L21

Chain BR:



• Molecule 49: 50S ribosomal protein L21

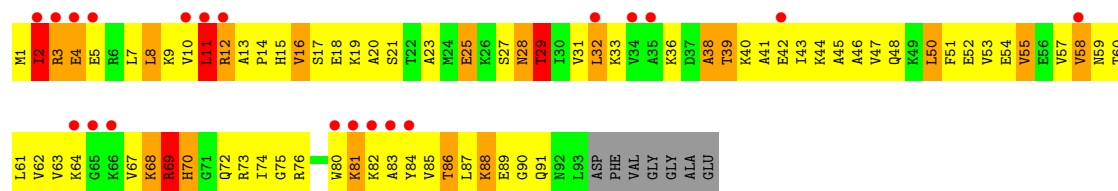
Chain DR:



• Molecule 50: 50S ribosomal protein L23

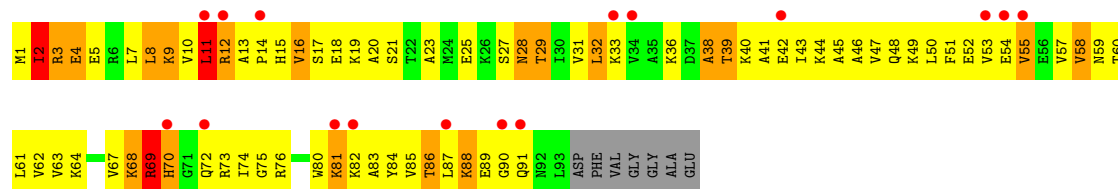


Chain BT:



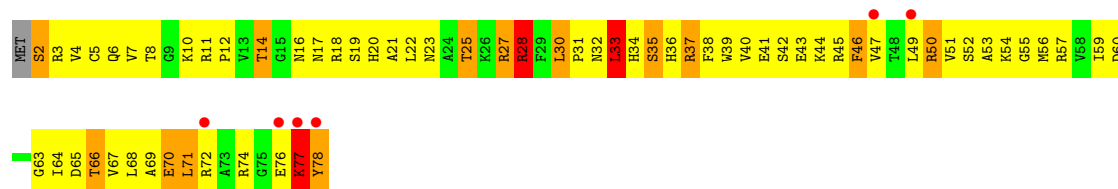
- Molecule 50: 50S ribosomal protein L23

Chain DT:



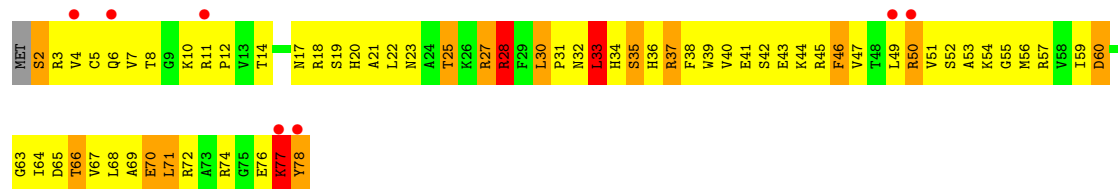
- Molecule 51: 50S ribosomal protein L28

Chain BZ:



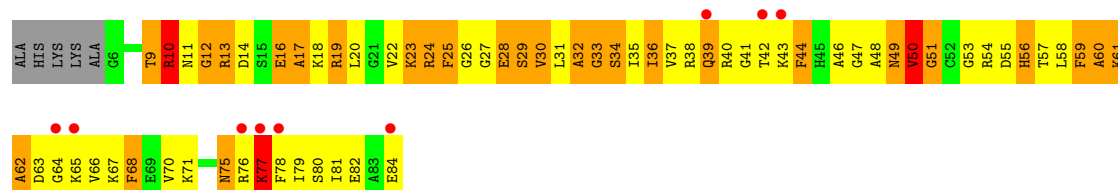
- Molecule 51: 50S ribosomal protein L28

Chain DZ:



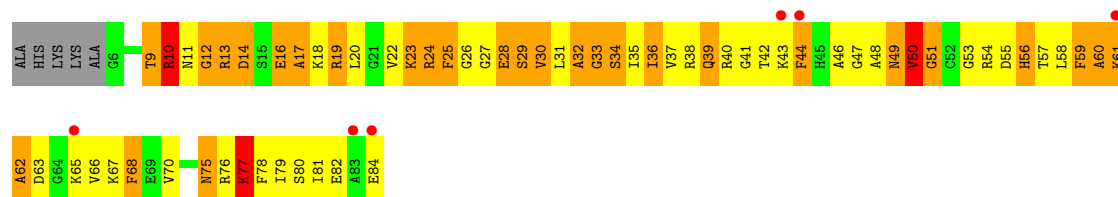
- Molecule 52: 50S ribosomal protein L27

Chain BW:



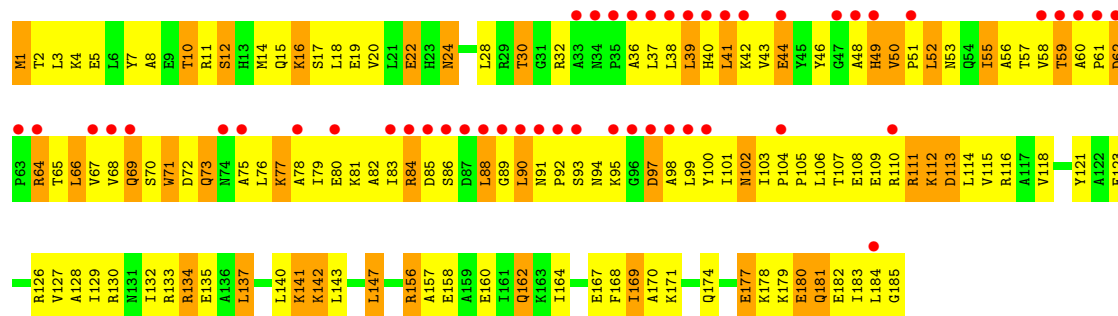
- Molecule 52: 50S ribosomal protein L27

Chain DW:



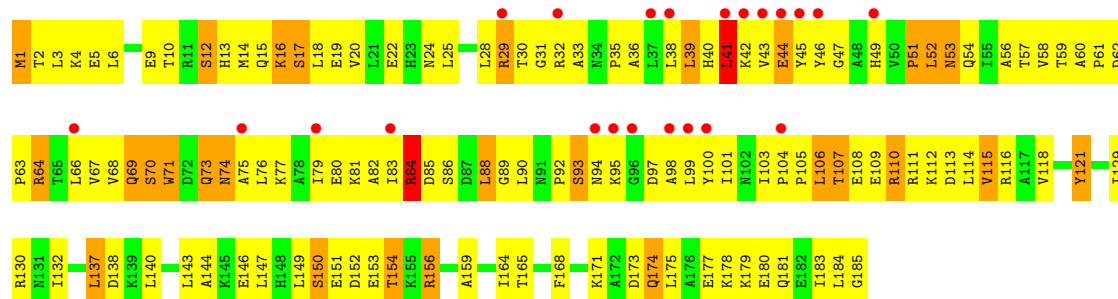
• Molecule 53: 50S ribosomal protein RRF

Chain B6:



• Molecule 53: 50S ribosomal protein RRF

Chain D6:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 208.87Å 378.75Å 738.26Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 40.00 – 4.45<br>69.15 – 4.45                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.7 (40.00-4.45)<br>95.6 (69.15-4.45)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.39 (at 4.46Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.263 , 0.309<br>0.246 , 0.280                              | Depositor<br>DCC |
| $R_{free}$ test set   | 16978 reflections (5.23%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 150.5   | Xtriage          |
| Anisotropy  | 0.297   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.20 , 18.8   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 0 of 341454 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 287128  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 72.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | AA    | 0.28         | 1/36762 (0.0%) | 0.76        | 6/57350 (0.0%)  |
| 1   | CA    | 0.28         | 1/36762 (0.0%) | 0.76        | 10/57350 (0.0%) |
| 2   | AC    | 0.23         | 0/1651         | 0.44        | 0/2225          |
| 2   | CC    | 0.23         | 0/1651         | 0.44        | 0/2225          |
| 3   | AD    | 0.23         | 0/1665         | 0.44        | 0/2227          |
| 3   | CD    | 0.23         | 0/1665         | 0.44        | 0/2227          |
| 4   | AE    | 0.23         | 0/1118         | 0.45        | 0/1504          |
| 4   | CE    | 0.24         | 0/1118         | 0.45        | 0/1504          |
| 5   | AF    | 0.24         | 0/835          | 0.45        | 0/1128          |
| 5   | CF    | 0.24         | 0/835          | 0.45        | 0/1128          |
| 6   | AG    | 0.23         | 0/1187         | 0.45        | 0/1591          |
| 6   | CG    | 0.23         | 0/1211         | 0.45        | 0/1624          |
| 7   | AH    | 0.23         | 0/989          | 0.44        | 0/1326          |
| 7   | CH    | 0.23         | 0/989          | 0.44        | 0/1326          |
| 8   | AI    | 0.24         | 0/1034         | 0.45        | 0/1375          |
| 8   | CI    | 0.24         | 0/1034         | 0.45        | 0/1375          |
| 9   | AJ    | 0.22         | 0/796          | 0.49        | 0/1077          |
| 9   | CJ    | 0.22         | 0/796          | 0.48        | 0/1077          |
| 10  | AK    | 0.24         | 0/893          | 0.46        | 0/1205          |
| 10  | CK    | 0.24         | 0/893          | 0.46        | 0/1205          |
| 11  | AL    | 0.22         | 0/969          | 0.48        | 0/1300          |
| 11  | CL    | 0.22         | 0/969          | 0.48        | 0/1300          |
| 12  | AM    | 0.21         | 0/892          | 0.45        | 0/1193          |
| 12  | CM    | 0.21         | 0/884          | 0.45        | 0/1181          |
| 13  | AN    | 0.24         | 0/785          | 0.46        | 0/1043          |
| 13  | CN    | 0.24         | 0/785          | 0.46        | 0/1043          |
| 14  | AO    | 0.23         | 0/722          | 0.47        | 0/964           |
| 14  | CO    | 0.23         | 0/722          | 0.47        | 0/964           |
| 15  | AP    | 0.25         | 0/659          | 0.46        | 0/884           |
| 15  | CP    | 0.25         | 0/648          | 0.46        | 0/870           |
| 16  | AQ    | 0.23         | 0/657          | 0.47        | 0/881           |
| 16  | CQ    | 0.24         | 0/666          | 0.47        | 0/892           |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 17  | AR    | 0.23         | 0/462          | 0.45        | 0/621            |
| 17  | CR    | 0.23         | 0/462          | 0.45        | 0/621            |
| 18  | AS    | 0.25         | 0/652          | 0.46        | 0/877            |
| 18  | CS    | 0.25         | 0/660          | 0.47        | 0/888            |
| 19  | AT    | 0.24         | 0/671          | 0.40        | 0/888            |
| 19  | CT    | 0.24         | 0/671          | 0.40        | 0/888            |
| 20  | AB    | 0.25         | 0/1735         | 0.45        | 0/2338           |
| 20  | CB    | 0.25         | 0/1735         | 0.45        | 0/2338           |
| 21  | AU    | 0.26         | 0/430          | 0.48        | 0/570            |
| 21  | CU    | 0.26         | 0/430          | 0.47        | 0/570            |
| 22  | BA    | 0.55         | 6/2803 (0.2%)  | 0.83        | 7/4371 (0.2%)    |
| 22  | DA    | 0.56         | 6/2803 (0.2%)  | 0.83        | 7/4371 (0.2%)    |
| 23  | BB    | 0.31         | 8/68314 (0.0%) | 0.79        | 41/106569 (0.0%) |
| 23  | DB    | 0.31         | 7/68314 (0.0%) | 0.79        | 38/106569 (0.0%) |
| 24  | BI    | 0.24         | 0/1046         | 0.47        | 0/1410           |
| 24  | DI    | 0.25         | 0/1046         | 0.48        | 0/1410           |
| 25  | BC    | 0.22         | 0/2121         | 0.48        | 0/2852           |
| 25  | DC    | 0.22         | 0/2121         | 0.48        | 0/2852           |
| 26  | BD    | 0.24         | 0/1586         | 0.48        | 0/2134           |
| 26  | DD    | 0.24         | 0/1586         | 0.48        | 0/2134           |
| 27  | BK    | 0.24         | 0/939          | 0.55        | 0/1258           |
| 27  | DK    | 0.24         | 0/939          | 0.55        | 0/1258           |
| 28  | BP    | 0.24         | 0/929          | 0.51        | 0/1242           |
| 28  | DP    | 0.24         | 0/929          | 0.51        | 0/1242           |
| 29  | BE    | 0.24         | 0/1571         | 0.50        | 0/2113           |
| 29  | DE    | 0.24         | 0/1571         | 0.50        | 0/2113           |
| 30  | BY    | 0.23         | 0/453          | 0.49        | 0/605            |
| 30  | DY    | 0.23         | 0/453          | 0.49        | 0/605            |
| 31  | B0    | 0.22         | 0/450          | 0.55        | 0/599            |
| 31  | D0    | 0.22         | 0/450          | 0.55        | 0/599            |
| 32  | B4    | 0.23         | 0/303          | 0.47        | 0/397            |
| 32  | D4    | 0.23         | 0/303          | 0.47        | 0/397            |
| 33  | B1    | 0.27         | 0/416          | 0.49        | 0/554            |
| 33  | D1    | 0.27         | 0/416          | 0.49        | 0/554            |
| 34  | B3    | 0.24         | 0/513          | 0.48        | 0/676            |
| 34  | D3    | 0.24         | 0/513          | 0.48        | 0/676            |
| 35  | BV    | 0.25         | 0/766          | 0.43        | 0/1025           |
| 35  | DV    | 0.25         | 0/766          | 0.42        | 0/1025           |
| 36  | B2    | 0.26         | 0/380          | 0.46        | 0/498            |
| 36  | D2    | 0.26         | 0/380          | 0.46        | 0/498            |
| 37  | BL    | 0.24         | 0/1054         | 0.48        | 0/1403           |
| 37  | DL    | 0.23         | 0/1054         | 0.48        | 0/1403           |
| 38  | BM    | 0.25         | 0/1093         | 0.48        | 0/1460           |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | DM    | 0.25         | 0/1093           | 0.48        | 0/1460            |
| 39  | BX    | 0.24         | 0/510            | 0.54        | 0/677             |
| 39  | DX    | 0.24         | 0/510            | 0.54        | 0/677             |
| 40  | BH    | 0.25         | 0/1122           | 0.47        | 0/1515            |
| 40  | DH    | 0.25         | 0/1122           | 0.49        | 0/1515            |
| 41  | BJ    | 0.24         | 0/1152           | 0.48        | 0/1551            |
| 41  | DJ    | 0.24         | 0/1152           | 0.48        | 0/1551            |
| 42  | BN    | 0.24         | 0/973            | 0.52        | 0/1301            |
| 42  | DN    | 0.24         | 0/973            | 0.52        | 0/1301            |
| 43  | BO    | 0.23         | 0/902            | 0.48        | 0/1209            |
| 43  | DO    | 0.23         | 0/902            | 0.48        | 0/1209            |
| 44  | BQ    | 0.25         | 0/960            | 0.49        | 0/1278            |
| 44  | DQ    | 0.25         | 0/960            | 0.49        | 0/1278            |
| 45  | BS    | 0.22         | 0/864            | 0.52        | 0/1156            |
| 45  | DS    | 0.22         | 0/864            | 0.52        | 0/1156            |
| 46  | BU    | 0.25         | 0/787            | 0.47        | 0/1051            |
| 46  | DU    | 0.25         | 0/787            | 0.47        | 0/1051            |
| 47  | BF    | 0.26         | 0/1444           | 0.51        | 0/1937            |
| 47  | DF    | 0.26         | 0/1444           | 0.52        | 0/1937            |
| 48  | BG    | 0.23         | 0/1343           | 0.46        | 0/1816            |
| 48  | DG    | 0.23         | 0/1343           | 0.46        | 0/1816            |
| 49  | BR    | 0.25         | 0/829            | 0.48        | 0/1107            |
| 49  | DR    | 0.25         | 0/829            | 0.48        | 0/1107            |
| 50  | BT    | 0.23         | 0/744            | 0.55        | 0/994             |
| 50  | DT    | 0.23         | 0/744            | 0.55        | 0/994             |
| 51  | BZ    | 0.25         | 0/635            | 0.52        | 0/848             |
| 51  | DZ    | 0.25         | 0/635            | 0.52        | 0/848             |
| 52  | BW    | 0.28         | 0/603            | 0.51        | 0/797             |
| 52  | DW    | 0.27         | 0/603            | 0.51        | 0/797             |
| 53  | B6    | 0.23         | 0/1497           | 0.48        | 0/2017            |
| 53  | D6    | 0.24         | 0/1497           | 0.47        | 0/2017            |
| All | All   | 0.29         | 29/309354 (0.0%) | 0.71        | 109/462003 (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                   | 14                  |
| 1   | CA    | 0                   | 12                  |
| 22  | BA    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 22  | DA    | 0                   | 2                   |
| 23  | BB    | 0                   | 50                  |
| 23  | DB    | 0                   | 48                  |
| All | All   | 0                   | 128                 |

All (29) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23  | BB    | 1086 | A    | C5-C6 | -16.24 | 1.26        | 1.41     |
| 23  | DB    | 1086 | A    | C5-C6 | -16.14 | 1.26        | 1.41     |
| 22  | DA    | 28   | C    | C2-O2 | -14.83 | 1.11        | 1.24     |
| 22  | BA    | 28   | C    | C2-O2 | -14.74 | 1.11        | 1.24     |
| 23  | DB    | 2276 | G    | O3'-P | -14.11 | 1.44        | 1.61     |
| 23  | DB    | 1088 | A    | C6-N1 | -10.66 | 1.28        | 1.35     |
| 23  | BB    | 1088 | A    | C6-N1 | -10.60 | 1.28        | 1.35     |
| 23  | BB    | 2276 | G    | O3'-P | -10.35 | 1.48        | 1.61     |
| 22  | DA    | 56   | G    | C2-N2 | 10.01  | 1.44        | 1.34     |
| 22  | BA    | 56   | G    | C2-N2 | 9.96   | 1.44        | 1.34     |
| 22  | BA    | 28   | C    | N3-C4 | -9.82  | 1.27        | 1.33     |
| 22  | DA    | 28   | C    | N3-C4 | -9.78  | 1.27        | 1.33     |
| 23  | BB    | 2318 | G    | O3'-P | 9.68   | 1.72        | 1.61     |
| 22  | DA    | 28   | C    | N1-C6 | -8.22  | 1.32        | 1.37     |
| 22  | BA    | 28   | C    | N1-C6 | -8.15  | 1.32        | 1.37     |
| 23  | DB    | 1060 | U    | C2-N3 | 7.86   | 1.43        | 1.37     |
| 23  | BB    | 1060 | U    | C2-N3 | 7.85   | 1.43        | 1.37     |
| 22  | BA    | 28   | C    | C2-N3 | -7.53  | 1.29        | 1.35     |
| 22  | DA    | 28   | C    | C2-N3 | -7.52  | 1.29        | 1.35     |
| 23  | BB    | 1086 | A    | N3-C4 | -7.06  | 1.30        | 1.34     |
| 23  | DB    | 1086 | A    | N3-C4 | -6.86  | 1.30        | 1.34     |
| 23  | DB    | 2267 | A    | C5-C6 | -6.59  | 1.35        | 1.41     |
| 23  | BB    | 2267 | A    | C5-C6 | -6.42  | 1.35        | 1.41     |
| 23  | DB    | 1086 | A    | N7-C5 | -6.28  | 1.35        | 1.39     |
| 23  | BB    | 1086 | A    | N7-C5 | -6.28  | 1.35        | 1.39     |
| 22  | DA    | 28   | C    | C5-C6 | -6.05  | 1.29        | 1.34     |
| 22  | BA    | 28   | C    | C5-C6 | -5.92  | 1.29        | 1.34     |
| 1   | CA    | 495  | A    | N3-C4 | -5.48  | 1.31        | 1.34     |
| 1   | AA    | 495  | A    | N3-C4 | -5.38  | 1.31        | 1.34     |

All (109) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 23  | DB    | 2204 | G    | O5'-P-OP1 | -29.74 | 75.02       | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 23  | BB    | 2204 | G    | O5'-P-OP2   | -28.61 | 76.37       | 110.70   |
| 23  | BB    | 2791 | G    | O5'-P-OP1   | -27.22 | 78.03       | 110.70   |
| 23  | DB    | 2791 | G    | O5'-P-OP2   | -26.58 | 78.80       | 110.70   |
| 23  | BB    | 2791 | G    | O5'-P-OP2   | 18.87  | 133.34      | 110.70   |
| 23  | DB    | 2791 | G    | O5'-P-OP1   | 18.79  | 133.25      | 110.70   |
| 23  | BB    | 2204 | G    | O5'-P-OP1   | 17.85  | 132.12      | 110.70   |
| 23  | DB    | 2204 | G    | O5'-P-OP2   | 17.59  | 131.81      | 110.70   |
| 23  | BB    | 2790 | U    | OP1-P-O3'   | 14.91  | 138.00      | 105.20   |
| 23  | DB    | 2790 | U    | OP2-P-O3'   | 14.83  | 137.83      | 105.20   |
| 23  | DB    | 2203 | U    | OP1-P-O3'   | 14.37  | 136.81      | 105.20   |
| 23  | BB    | 2203 | U    | OP2-P-O3'   | 14.21  | 136.47      | 105.20   |
| 22  | DA    | 56   | G    | N3-C2-N2    | 8.93   | 126.15      | 119.90   |
| 22  | BA    | 56   | G    | N3-C2-N2    | 8.91   | 126.14      | 119.90   |
| 23  | BB    | 1552 | A    | N9-C1'-C2'  | -8.88  | 102.23      | 112.00   |
| 23  | DB    | 1552 | A    | N9-C1'-C2'  | -8.85  | 102.26      | 112.00   |
| 1   | AA    | 765  | G    | N9-C1'-C2'  | -8.27  | 102.90      | 112.00   |
| 23  | BB    | 1088 | A    | N1-C6-N6    | -8.24  | 113.66      | 118.60   |
| 23  | DB    | 1088 | A    | N1-C6-N6    | -8.23  | 113.66      | 118.60   |
| 1   | CA    | 765  | G    | N9-C1'-C2'  | -8.20  | 102.97      | 112.00   |
| 23  | DB    | 2323 | G    | O3'-P-O5'   | -8.19  | 88.44       | 104.00   |
| 23  | BB    | 1439 | A    | N9-C1'-C2'  | -7.95  | 103.26      | 112.00   |
| 23  | DB    | 1439 | A    | N9-C1'-C2'  | -7.91  | 103.30      | 112.00   |
| 23  | DB    | 1060 | U    | C5-C4-O4    | -7.28  | 121.53      | 125.90   |
| 23  | BB    | 1060 | U    | C5-C4-O4    | -7.26  | 121.54      | 125.90   |
| 23  | BB    | 690  | G    | C5'-C4'-C3' | -7.24  | 104.42      | 116.00   |
| 23  | BB    | 1086 | A    | C4-C5-C6    | 7.17   | 120.58      | 117.00   |
| 23  | BB    | 2283 | C    | O5'-P-OP2   | -7.15  | 99.26       | 105.70   |
| 23  | DB    | 1086 | A    | C4-C5-C6    | 7.10   | 120.55      | 117.00   |
| 1   | CA    | 1049 | U    | O5'-P-OP1   | -6.90  | 99.49       | 105.70   |
| 23  | BB    | 2733 | A    | N9-C1'-C2'  | -6.75  | 104.57      | 112.00   |
| 1   | CA    | 1432 | G    | N9-C1'-C2'  | -6.74  | 104.58      | 112.00   |
| 1   | AA    | 1432 | G    | N9-C1'-C2'  | -6.71  | 104.62      | 112.00   |
| 23  | DB    | 2733 | A    | N9-C1'-C2'  | -6.69  | 104.64      | 112.00   |
| 23  | DB    | 690  | G    | C5'-C4'-C3' | -6.69  | 105.30      | 116.00   |
| 22  | BA    | 28   | C    | C5-C6-N1    | -6.61  | 117.70      | 121.00   |
| 23  | BB    | 2894 | G    | N9-C1'-C2'  | -6.60  | 104.74      | 112.00   |
| 1   | AA    | 1301 | U    | N1-C1'-C2'  | 6.60   | 122.58      | 114.00   |
| 23  | DB    | 2894 | G    | N9-C1'-C2'  | -6.59  | 104.75      | 112.00   |
| 1   | CA    | 1301 | U    | N1-C1'-C2'  | 6.58   | 122.56      | 114.00   |
| 22  | DA    | 28   | C    | C5-C6-N1    | -6.53  | 117.73      | 121.00   |
| 22  | DA    | 27   | C    | C5'-C4'-C3' | -6.51  | 105.59      | 116.00   |
| 23  | DB    | 2619 | C    | C5'-C4'-C3' | -6.48  | 105.63      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | BB    | 2790 | U    | O3'-P-O5'   | -6.45 | 91.74       | 104.00   |
| 23  | BB    | 2759 | G    | C5'-C4'-C3' | -6.42 | 105.72      | 116.00   |
| 23  | BB    | 1088 | A    | C5-C6-N6    | 6.37  | 128.80      | 123.70   |
| 23  | DB    | 1088 | A    | C5-C6-N6    | 6.35  | 128.78      | 123.70   |
| 22  | DA    | 56   | G    | N1-C2-N2    | -6.33 | 110.50      | 116.20   |
| 23  | BB    | 2323 | G    | P-O3'-C3'   | 6.33  | 127.29      | 119.70   |
| 1   | CA    | 1424 | U    | C5'-C4'-C3' | -6.32 | 105.89      | 116.00   |
| 22  | BA    | 56   | G    | N1-C2-N2    | -6.31 | 110.53      | 116.20   |
| 23  | DB    | 2790 | U    | O3'-P-O5'   | -6.26 | 92.10       | 104.00   |
| 23  | BB    | 1086 | A    | C6-C5-N7    | -6.18 | 127.97      | 132.30   |
| 23  | DB    | 1086 | A    | C6-C5-N7    | -6.14 | 128.00      | 132.30   |
| 22  | BA    | 27   | C    | C5'-C4'-C3' | -6.04 | 106.34      | 116.00   |
| 23  | DB    | 2203 | U    | O3'-P-O5'   | -5.95 | 92.69       | 104.00   |
| 23  | DB    | 508  | A    | C4'-C3'-O3' | -5.93 | 96.95       | 109.40   |
| 23  | BB    | 2746 | U    | C4'-C3'-O3' | 5.90  | 124.81      | 113.00   |
| 1   | CA    | 1250 | A    | C5'-C4'-C3' | 5.89  | 125.43      | 116.00   |
| 23  | BB    | 2323 | G    | O3'-P-O5'   | -5.88 | 92.83       | 104.00   |
| 23  | DB    | 131  | A    | C5'-C4'-C3' | 5.87  | 125.39      | 116.00   |
| 23  | BB    | 1043 | C    | C4'-C3'-O3' | 5.87  | 124.74      | 113.00   |
| 23  | BB    | 1126 | A    | C5'-C4'-C3' | -5.87 | 106.61      | 116.00   |
| 23  | DB    | 1047 | G    | C5'-C4'-C3' | -5.85 | 106.64      | 116.00   |
| 23  | BB    | 2480 | C    | C5'-C4'-C3' | 5.83  | 125.33      | 116.00   |
| 23  | DB    | 2267 | A    | C5-C6-N6    | -5.82 | 119.04      | 123.70   |
| 23  | BB    | 2267 | A    | C5-C6-N6    | -5.82 | 119.04      | 123.70   |
| 22  | BA    | 28   | C    | N3-C2-O2    | -5.77 | 117.86      | 121.90   |
| 22  | DA    | 28   | C    | N3-C2-O2    | -5.74 | 117.88      | 121.90   |
| 23  | DB    | 2267 | A    | C4-N9-C1'   | 5.74  | 136.63      | 126.30   |
| 23  | BB    | 2267 | A    | C4-N9-C1'   | 5.73  | 136.61      | 126.30   |
| 23  | DB    | 2480 | C    | C5'-C4'-C3' | 5.72  | 125.16      | 116.00   |
| 23  | DB    | 1397 | U    | C5'-C4'-C3' | -5.69 | 106.89      | 116.00   |
| 23  | BB    | 2108 | A    | C4'-C3'-O3' | 5.67  | 124.33      | 113.00   |
| 23  | BB    | 1060 | U    | N1-C2-O2    | -5.66 | 118.84      | 122.80   |
| 22  | DA    | 28   | C    | C2-N3-C4    | -5.65 | 117.07      | 119.90   |
| 23  | DB    | 1118 | C    | C4'-C3'-O3' | 5.65  | 124.30      | 113.00   |
| 23  | BB    | 1086 | A    | C2-N3-C4    | -5.64 | 107.78      | 110.60   |
| 22  | BA    | 28   | C    | C2-N3-C4    | -5.63 | 117.08      | 119.90   |
| 23  | DB    | 1060 | U    | N1-C2-O2    | -5.62 | 118.86      | 122.80   |
| 23  | BB    | 508  | A    | C4'-C3'-O3' | -5.58 | 97.68       | 109.40   |
| 23  | DB    | 1086 | A    | C2-N3-C4    | -5.58 | 107.81      | 110.60   |
| 23  | DB    | 2324 | U    | P-O5'-C5'   | 5.50  | 129.70      | 120.90   |
| 23  | BB    | 1397 | U    | C5'-C4'-C3' | -5.49 | 107.22      | 116.00   |
| 1   | AA    | 1250 | A    | C5'-C4'-C3' | 5.45  | 124.72      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | BB    | 278  | A    | C5'-C4'-C3' | -5.43 | 107.31      | 116.00   |
| 1   | CA    | 1534 | A    | C2'-C3'-O3' | -5.42 | 97.57       | 109.50   |
| 23  | BB    | 2272 | U    | C5-C4-O4    | -5.41 | 122.66      | 125.90   |
| 23  | BB    | 2203 | U    | O3'-P-O5'   | -5.40 | 93.74       | 104.00   |
| 23  | BB    | 1060 | U    | N3-C2-O2    | 5.35  | 125.95      | 122.20   |
| 1   | CA    | 1049 | U    | C5'-C4'-O4' | 5.31  | 115.47      | 109.10   |
| 23  | DB    | 2267 | A    | C8-N9-C1'   | -5.30 | 118.16      | 127.70   |
| 23  | BB    | 2267 | A    | C8-N9-C1'   | -5.28 | 118.20      | 127.70   |
| 23  | DB    | 2272 | U    | C5-C4-O4    | -5.27 | 122.74      | 125.90   |
| 1   | CA    | 434  | U    | C5'-C4'-C3' | -5.26 | 107.58      | 116.00   |
| 23  | DB    | 1060 | U    | N3-C2-O2    | 5.26  | 125.88      | 122.20   |
| 23  | DB    | 544  | C    | C4'-C3'-O3' | 5.24  | 123.47      | 113.00   |
| 22  | DA    | 28   | C    | O4'-C1'-N1  | 5.23  | 112.38      | 108.20   |
| 22  | BA    | 28   | C    | O4'-C1'-N1  | 5.18  | 112.34      | 108.20   |
| 23  | DB    | 1350 | C    | C5'-C4'-C3' | -5.17 | 107.72      | 116.00   |
| 23  | DB    | 1126 | A    | C5'-C4'-O4' | 5.17  | 115.30      | 109.10   |
| 23  | BB    | 72   | U    | C5'-C4'-C3' | -5.15 | 107.76      | 116.00   |
| 1   | AA    | 1397 | C    | C5'-C4'-C3' | -5.14 | 107.77      | 116.00   |
| 23  | BB    | 479  | A    | C4'-C3'-O3' | -5.11 | 98.67       | 109.40   |
| 1   | AA    | 86   | G    | N9-C1'-C2'  | 5.07  | 120.60      | 114.00   |
| 23  | BB    | 2903 | U    | C4'-C3'-O3' | 5.06  | 123.12      | 113.00   |
| 23  | BB    | 2745 | C    | C5'-C4'-C3' | -5.06 | 107.91      | 116.00   |
| 1   | CA    | 855  | U    | C5'-C4'-C3' | -5.00 | 107.99      | 116.00   |
| 23  | DB    | 2282 | G    | C5'-C4'-C3' | -5.00 | 108.00      | 116.00   |

There are no chirality outliers.

All (128) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1048 | G    | Sidechain |
| 1   | AA    | 1331 | G    | Sidechain |
| 1   | AA    | 1432 | G    | Sidechain |
| 1   | AA    | 1441 | A    | Sidechain |
| 1   | AA    | 187  | G    | Sidechain |
| 1   | AA    | 281  | G    | Sidechain |
| 1   | AA    | 324  | G    | Sidechain |
| 1   | AA    | 437  | U    | Sidechain |
| 1   | AA    | 438  | U    | Sidechain |
| 1   | AA    | 496  | A    | Sidechain |
| 1   | AA    | 575  | G    | Sidechain |
| 1   | AA    | 703  | G    | Sidechain |
| 1   | AA    | 78   | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 86   | G    | Sidechain |
| 22  | BA    | 28   | C    | Sidechain |
| 22  | BA    | 56   | G    | Sidechain |
| 23  | BB    | 1047 | G    | Sidechain |
| 23  | BB    | 1060 | U    | Sidechain |
| 23  | BB    | 1086 | A    | Sidechain |
| 23  | BB    | 1088 | A    | Sidechain |
| 23  | BB    | 1111 | A    | Sidechain |
| 23  | BB    | 1247 | A    | Sidechain |
| 23  | BB    | 1377 | G    | Sidechain |
| 23  | BB    | 1426 | G    | Sidechain |
| 23  | BB    | 1432 | G    | Sidechain |
| 23  | BB    | 1439 | A    | Sidechain |
| 23  | BB    | 1476 | U    | Sidechain |
| 23  | BB    | 1546 | G    | Sidechain |
| 23  | BB    | 1572 | A    | Sidechain |
| 23  | BB    | 1722 | A    | Sidechain |
| 23  | BB    | 1734 | G    | Sidechain |
| 23  | BB    | 1814 | G    | Sidechain |
| 23  | BB    | 1828 | G    | Sidechain |
| 23  | BB    | 2062 | A    | Sidechain |
| 23  | BB    | 2108 | A    | Sidechain |
| 23  | BB    | 221  | A    | Sidechain |
| 23  | BB    | 222  | A    | Sidechain |
| 23  | BB    | 2272 | U    | Sidechain |
| 23  | BB    | 2279 | G    | Sidechain |
| 23  | BB    | 232  | G    | Sidechain |
| 23  | BB    | 2446 | G    | Sidechain |
| 23  | BB    | 2454 | G    | Sidechain |
| 23  | BB    | 2471 | A    | Sidechain |
| 23  | BB    | 2480 | C    | Sidechain |
| 23  | BB    | 2503 | A    | Sidechain |
| 23  | BB    | 2508 | G    | Sidechain |
| 23  | BB    | 2587 | A    | Sidechain |
| 23  | BB    | 2638 | G    | Sidechain |
| 23  | BB    | 2733 | A    | Sidechain |
| 23  | BB    | 2770 | G    | Sidechain |
| 23  | BB    | 2834 | G    | Sidechain |
| 23  | BB    | 2848 | G    | Sidechain |
| 23  | BB    | 2857 | G    | Sidechain |
| 23  | BB    | 2868 | A    | Sidechain |
| 23  | BB    | 2883 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 23  | BB    | 2890 | G    | Sidechain |
| 23  | BB    | 299  | A    | Sidechain |
| 23  | BB    | 361  | G    | Sidechain |
| 23  | BB    | 370  | G    | Sidechain |
| 23  | BB    | 500  | G    | Sidechain |
| 23  | BB    | 51   | G    | Sidechain |
| 23  | BB    | 562  | U    | Sidechain |
| 23  | BB    | 630  | G    | Sidechain |
| 23  | BB    | 727  | A    | Sidechain |
| 23  | BB    | 729  | G    | Sidechain |
| 23  | BB    | 757  | G    | Sidechain |
| 1   | CA    | 1048 | G    | Sidechain |
| 1   | CA    | 1331 | G    | Sidechain |
| 1   | CA    | 1432 | G    | Sidechain |
| 1   | CA    | 1441 | A    | Sidechain |
| 1   | CA    | 187  | G    | Sidechain |
| 1   | CA    | 281  | G    | Sidechain |
| 1   | CA    | 324  | G    | Sidechain |
| 1   | CA    | 437  | U    | Sidechain |
| 1   | CA    | 438  | U    | Sidechain |
| 1   | CA    | 496  | A    | Sidechain |
| 1   | CA    | 575  | G    | Sidechain |
| 1   | CA    | 703  | G    | Sidechain |
| 22  | DA    | 28   | C    | Sidechain |
| 22  | DA    | 56   | G    | Sidechain |
| 23  | DB    | 1047 | G    | Sidechain |
| 23  | DB    | 1060 | U    | Sidechain |
| 23  | DB    | 1086 | A    | Sidechain |
| 23  | DB    | 1088 | A    | Sidechain |
| 23  | DB    | 1247 | A    | Sidechain |
| 23  | DB    | 1377 | G    | Sidechain |
| 23  | DB    | 1426 | G    | Sidechain |
| 23  | DB    | 1432 | G    | Sidechain |
| 23  | DB    | 1439 | A    | Sidechain |
| 23  | DB    | 1476 | U    | Sidechain |
| 23  | DB    | 1546 | G    | Sidechain |
| 23  | DB    | 1572 | A    | Sidechain |
| 23  | DB    | 1722 | A    | Sidechain |
| 23  | DB    | 1734 | G    | Sidechain |
| 23  | DB    | 1814 | G    | Sidechain |
| 23  | DB    | 1828 | G    | Sidechain |
| 23  | DB    | 2062 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 23  | DB    | 2107 | G    | Sidechain |
| 23  | DB    | 221  | A    | Sidechain |
| 23  | DB    | 222  | A    | Sidechain |
| 23  | DB    | 2272 | U    | Sidechain |
| 23  | DB    | 2279 | G    | Sidechain |
| 23  | DB    | 232  | G    | Sidechain |
| 23  | DB    | 2446 | G    | Sidechain |
| 23  | DB    | 2454 | G    | Sidechain |
| 23  | DB    | 2471 | A    | Sidechain |
| 23  | DB    | 2480 | C    | Sidechain |
| 23  | DB    | 2503 | A    | Sidechain |
| 23  | DB    | 2508 | G    | Sidechain |
| 23  | DB    | 2587 | A    | Sidechain |
| 23  | DB    | 2638 | G    | Sidechain |
| 23  | DB    | 2733 | A    | Sidechain |
| 23  | DB    | 2770 | G    | Sidechain |
| 23  | DB    | 2834 | G    | Sidechain |
| 23  | DB    | 2848 | G    | Sidechain |
| 23  | DB    | 2857 | G    | Sidechain |
| 23  | DB    | 2868 | A    | Sidechain |
| 23  | DB    | 2883 | A    | Sidechain |
| 23  | DB    | 2890 | G    | Sidechain |
| 23  | DB    | 299  | A    | Sidechain |
| 23  | DB    | 370  | G    | Sidechain |
| 23  | DB    | 500  | G    | Sidechain |
| 23  | DB    | 51   | G    | Sidechain |
| 23  | DB    | 562  | U    | Sidechain |
| 23  | DB    | 630  | G    | Sidechain |
| 23  | DB    | 727  | A    | Sidechain |
| 23  | DB    | 729  | G    | Sidechain |
| 23  | DB    | 757  | G    | Sidechain |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32831 | 0        | 16521    | 1250    | 0            |
| 1   | CA    | 32831 | 0        | 16521    | 1242    | 0            |
| 2   | AC    | 1624  | 0        | 1699     | 139     | 0            |
| 2   | CC    | 1624  | 0        | 1699     | 141     | 0            |
| 3   | AD    | 1643  | 0        | 1710     | 173     | 0            |
| 3   | CD    | 1643  | 0        | 1710     | 170     | 0            |
| 4   | AE    | 1105  | 0        | 1148     | 99      | 0            |
| 4   | CE    | 1105  | 0        | 1148     | 104     | 0            |
| 5   | AF    | 817   | 0        | 808      | 83      | 0            |
| 5   | CF    | 817   | 0        | 808      | 80      | 0            |
| 6   | AG    | 1174  | 0        | 1230     | 115     | 0            |
| 6   | CG    | 1196  | 0        | 1246     | 98      | 0            |
| 7   | AH    | 979   | 0        | 1034     | 94      | 0            |
| 7   | CH    | 979   | 0        | 1034     | 90      | 0            |
| 8   | AI    | 1022  | 0        | 1070     | 142     | 0            |
| 8   | CI    | 1022  | 0        | 1070     | 134     | 0            |
| 9   | AJ    | 786   | 0        | 828      | 79      | 0            |
| 9   | CJ    | 786   | 0        | 828      | 85      | 0            |
| 10  | AK    | 877   | 0        | 887      | 108     | 0            |
| 10  | CK    | 877   | 0        | 887      | 99      | 0            |
| 11  | AL    | 955   | 0        | 1019     | 82      | 0            |
| 11  | CL    | 955   | 0        | 1019     | 82      | 0            |
| 12  | AM    | 883   | 0        | 944      | 105     | 0            |
| 12  | CM    | 876   | 0        | 937      | 108     | 0            |
| 13  | AN    | 774   | 0        | 827      | 113     | 0            |
| 13  | CN    | 774   | 0        | 827      | 117     | 0            |
| 14  | AO    | 714   | 0        | 734      | 47      | 0            |
| 14  | CO    | 714   | 0        | 734      | 48      | 0            |
| 15  | AP    | 649   | 0        | 666      | 51      | 0            |
| 15  | CP    | 638   | 0        | 656      | 53      | 0            |
| 16  | AQ    | 648   | 0        | 691      | 58      | 0            |
| 16  | CQ    | 657   | 0        | 702      | 61      | 0            |
| 17  | AR    | 455   | 0        | 478      | 45      | 0            |
| 17  | CR    | 455   | 0        | 478      | 49      | 0            |
| 18  | AS    | 637   | 0        | 665      | 89      | 0            |
| 18  | CS    | 644   | 0        | 675      | 88      | 0            |
| 19  | AT    | 665   | 0        | 714      | 58      | 0            |
| 19  | CT    | 665   | 0        | 714      | 55      | 0            |
| 20  | AB    | 1704  | 0        | 1732     | 189     | 0            |
| 20  | CB    | 1704  | 0        | 1732     | 206     | 0            |
| 21  | AU    | 425   | 0        | 449      | 77      | 0            |
| 21  | CU    | 425   | 0        | 449      | 70      | 0            |
| 22  | BA    | 2507  | 0        | 1270     | 119     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | DA    | 2507  | 0        | 1270     | 119     | 1            |
| 23  | BB    | 60995 | 0        | 30679    | 2401    | 0            |
| 23  | DB    | 60995 | 0        | 30677    | 2528    | 1            |
| 24  | BI    | 1032  | 0        | 1088     | 117     | 0            |
| 24  | DI    | 1032  | 0        | 1088     | 185     | 0            |
| 25  | BC    | 2082  | 0        | 2157     | 254     | 0            |
| 25  | DC    | 2082  | 0        | 2157     | 253     | 0            |
| 26  | BD    | 1565  | 0        | 1616     | 196     | 0            |
| 26  | DD    | 1565  | 0        | 1616     | 200     | 0            |
| 27  | BK    | 930   | 0        | 1000     | 107     | 0            |
| 27  | DK    | 930   | 0        | 1000     | 114     | 0            |
| 28  | BP    | 917   | 0        | 965      | 102     | 0            |
| 28  | DP    | 917   | 0        | 965      | 99      | 0            |
| 29  | BE    | 1552  | 0        | 1619     | 211     | 0            |
| 29  | DE    | 1552  | 0        | 1619     | 196     | 0            |
| 30  | BY    | 449   | 0        | 491      | 51      | 0            |
| 30  | DY    | 449   | 0        | 491      | 51      | 0            |
| 31  | B0    | 444   | 0        | 461      | 56      | 0            |
| 31  | D0    | 444   | 0        | 461      | 53      | 0            |
| 32  | B4    | 302   | 0        | 340      | 34      | 0            |
| 32  | D4    | 302   | 0        | 341      | 40      | 0            |
| 33  | B1    | 409   | 0        | 440      | 48      | 0            |
| 33  | D1    | 409   | 0        | 440      | 44      | 0            |
| 34  | B3    | 504   | 0        | 574      | 51      | 0            |
| 34  | D3    | 504   | 0        | 574      | 52      | 0            |
| 35  | BV    | 753   | 0        | 780      | 90      | 0            |
| 35  | DV    | 753   | 0        | 780      | 101     | 0            |
| 36  | B2    | 377   | 0        | 418      | 36      | 0            |
| 36  | D2    | 377   | 0        | 418      | 38      | 0            |
| 37  | BL    | 1045  | 0        | 1117     | 163     | 0            |
| 37  | DL    | 1045  | 0        | 1117     | 163     | 0            |
| 38  | BM    | 1074  | 0        | 1157     | 117     | 0            |
| 38  | DM    | 1074  | 0        | 1157     | 121     | 0            |
| 39  | BX    | 509   | 0        | 543      | 70      | 0            |
| 39  | DX    | 509   | 0        | 543      | 66      | 0            |
| 40  | BH    | 1111  | 0        | 1148     | 207     | 0            |
| 40  | DH    | 1111  | 0        | 1148     | 144     | 0            |
| 41  | BJ    | 1129  | 0        | 1162     | 144     | 0            |
| 41  | DJ    | 1129  | 0        | 1162     | 146     | 0            |
| 42  | BN    | 960   | 0        | 1000     | 123     | 0            |
| 42  | DN    | 960   | 0        | 1000     | 121     | 0            |
| 43  | BO    | 892   | 0        | 923      | 104     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | DO    | 892   | 0        | 923      | 113     | 0            |
| 44  | BQ    | 947   | 0        | 1022     | 156     | 0            |
| 44  | DQ    | 947   | 0        | 1022     | 160     | 0            |
| 45  | BS    | 857   | 0        | 922      | 106     | 0            |
| 45  | DS    | 857   | 0        | 922      | 109     | 0            |
| 46  | BU    | 779   | 0        | 834      | 117     | 0            |
| 46  | DU    | 779   | 0        | 834      | 116     | 0            |
| 47  | BF    | 1420  | 0        | 1460     | 236     | 0            |
| 47  | DF    | 1420  | 0        | 1460     | 248     | 0            |
| 48  | BG    | 1323  | 0        | 1374     | 200     | 0            |
| 48  | DG    | 1323  | 0        | 1374     | 195     | 0            |
| 49  | BR    | 816   | 0        | 839      | 124     | 0            |
| 49  | DR    | 816   | 0        | 839      | 127     | 0            |
| 50  | BT    | 738   | 0        | 807      | 120     | 0            |
| 50  | DT    | 738   | 0        | 807      | 116     | 0            |
| 51  | BZ    | 625   | 0        | 652      | 77      | 0            |
| 51  | DZ    | 625   | 0        | 652      | 71      | 0            |
| 52  | BW    | 596   | 0        | 610      | 124     | 0            |
| 52  | DW    | 596   | 0        | 610      | 130     | 0            |
| 53  | B6    | 1478  | 0        | 1526     | 187     | 0            |
| 53  | D6    | 1478  | 0        | 1526     | 166     | 0            |
| 54  | AA    | 60    | 0        | 0        | 0       | 0            |
| 54  | BB    | 110   | 0        | 0        | 0       | 0            |
| 54  | CA    | 61    | 0        | 0        | 0       | 0            |
| 54  | CE    | 1     | 0        | 0        | 0       | 0            |
| 54  | DB    | 111   | 0        | 0        | 0       | 0            |
| 55  | AA    | 42    | 0        | 45       | 3       | 0            |
| 55  | BB    | 42    | 0        | 45       | 1       | 0            |
| 55  | CA    | 42    | 0        | 45       | 2       | 0            |
| 55  | DB    | 42    | 0        | 45       | 1       | 0            |
| 56  | B4    | 1     | 0        | 0        | 0       | 0            |
| 56  | D4    | 1     | 0        | 0        | 0       | 0            |
| 57  | AA    | 291   | 0        | 0        | 5       | 0            |
| 57  | AL    | 3     | 0        | 0        | 0       | 0            |
| 57  | AN    | 4     | 0        | 0        | 0       | 0            |
| 57  | AT    | 2     | 0        | 0        | 0       | 0            |
| 57  | BB    | 495   | 0        | 0        | 8       | 0            |
| 57  | BC    | 6     | 0        | 0        | 0       | 0            |
| 57  | BD    | 1     | 0        | 0        | 0       | 0            |
| 57  | BE    | 2     | 0        | 0        | 0       | 0            |
| 57  | BL    | 1     | 0        | 0        | 0       | 0            |
| 57  | BT    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57  | CA    | 296    | 0        | 0        | 1       | 0            |
| 57  | CE    | 3      | 0        | 0        | 0       | 0            |
| 57  | CL    | 4      | 0        | 0        | 0       | 0            |
| 57  | CN    | 4      | 0        | 0        | 0       | 0            |
| 57  | CP    | 1      | 0        | 0        | 0       | 0            |
| 57  | CT    | 1      | 0        | 0        | 0       | 0            |
| 57  | DB    | 502    | 0        | 0        | 15      | 0            |
| 57  | DC    | 4      | 0        | 0        | 0       | 0            |
| 57  | DD    | 1      | 0        | 0        | 0       | 0            |
| 57  | DE    | 1      | 0        | 0        | 0       | 0            |
| 57  | DL    | 2      | 0        | 0        | 0       | 0            |
| 57  | DQ    | 1      | 0        | 0        | 0       | 0            |
| 57  | DR    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 287128 | 0        | 193895   | 17520   | 1            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

All (17520) close contacts within the same asymmetric unit are listed below.

| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:DB:1099:G:H8    | 24:DI:3:LYS:N     | 1.37        | 1.19     |
| 49:DR:60:LYS:H     | 49:DR:100:GLY:HA3 | 1.08        | 1.15     |
| 40:BH:31:VAL:HB    | 40:BH:32:PRO:HD2  | 1.28        | 1.15     |
| 2:CC:126:ARG:HH22  | 2:CC:190:THR:HG23 | 1.09        | 1.14     |
| 50:DT:5:GLU:HA     | 50:DT:8:LEU:HB2   | 1.30        | 1.13     |
| 2:AC:126:ARG:HH22  | 2:AC:190:THR:HG23 | 1.08        | 1.13     |
| 50:BT:5:GLU:HA     | 50:BT:8:LEU:HB2   | 1.28        | 1.12     |
| 49:BR:60:LYS:H     | 49:BR:100:GLY:HA3 | 1.09        | 1.10     |
| 10:CK:124:LYS:HA   | 21:CU:34:ARG:HB3  | 1.33        | 1.10     |
| 40:DH:31:VAL:HB    | 40:DH:32:PRO:HD2  | 1.29        | 1.09     |
| 10:AK:124:LYS:HA   | 21:AU:34:ARG:HB3  | 1.34        | 1.09     |
| 23:BB:855:G:H21    | 52:BW:23:LYS:HG2  | 1.14        | 1.08     |
| 25:BC:129:LEU:HD23 | 25:BC:130:PRO:HD2 | 1.33        | 1.08     |
| 23:DB:1099:G:C8    | 24:DI:3:LYS:N     | 2.22        | 1.07     |
| 52:BW:17:ALA:HA    | 52:BW:35:ILE:HG23 | 1.34        | 1.07     |
| 52:DW:39:GLN:HG3   | 52:DW:42:THR:HB   | 1.35        | 1.06     |
| 25:BC:77:VAL:HG23  | 25:BC:112:GLY:H   | 1.21        | 1.05     |
| 48:BG:43:LYS:HB2   | 48:BG:50:THR:HB   | 1.38        | 1.05     |
| 40:DH:133:GLN:HB3  | 40:DH:139:PHE:HB3 | 1.39        | 1.05     |
| 25:DC:129:LEU:HD23 | 25:DC:130:PRO:HD2 | 1.37        | 1.05     |
| 44:BQ:30:VAL:HG13  | 44:BQ:31:TYR:H    | 1.14        | 1.04     |
| 10:AK:33:ILE:HB    | 10:AK:73:VAL:HG11 | 1.38        | 1.04     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DC:77:VAL:HG23  | 25:DC:112:GLY:H    | 1.22        | 1.04     |
| 21:CU:36:PHE:HB3   | 21:CU:40:PRO:HD3   | 1.39        | 1.04     |
| 48:BG:89:VAL:HB    | 48:BG:159:LYS:HA   | 1.36        | 1.04     |
| 44:DQ:30:VAL:HG13  | 44:DQ:31:TYR:H     | 1.15        | 1.04     |
| 52:BW:39:GLN:HG3   | 52:BW:42:THR:HB    | 1.35        | 1.04     |
| 9:CJ:9:ARG:HB2     | 9:CJ:99:GLN:HB3    | 1.40        | 1.04     |
| 23:DB:1098:A:H3'   | 24:DI:3:LYS:HA     | 1.40        | 1.03     |
| 52:DW:17:ALA:HA    | 52:DW:35:ILE:HG23  | 1.35        | 1.03     |
| 47:BF:62:GLN:HE22  | 47:BF:90:LEU:HD13  | 1.22        | 1.03     |
| 34:B3:49:VAL:HG21  | 34:B3:54:LEU:HD13  | 1.39        | 1.03     |
| 6:AG:149:ALA:HB2   | 10:AK:55:ARG:HE    | 1.17        | 1.03     |
| 21:AU:36:PHE:HB3   | 21:AU:40:PRO:HD3   | 1.38        | 1.03     |
| 1:CA:932:C:H5''    | 6:CG:3:ARG:HD2     | 1.40        | 1.02     |
| 10:CK:33:ILE:HB    | 10:CK:73:VAL:HG11  | 1.40        | 1.02     |
| 27:DK:35:VAL:HG23  | 27:DK:36:GLY:H     | 1.22        | 1.02     |
| 23:DB:1099:G:O5'   | 24:DI:4:VAL:N      | 1.91        | 1.02     |
| 48:DG:43:LYS:HB2   | 48:DG:50:THR:HB    | 1.40        | 1.02     |
| 25:BC:144:GLU:HA   | 25:BC:151:GLY:HA2  | 1.42        | 1.01     |
| 1:CA:1533:C:H2'    | 1:CA:1534:A:H3'    | 1.41        | 1.01     |
| 37:DL:123:ARG:HA   | 37:DL:143:GLU:HB3  | 1.42        | 1.01     |
| 37:BL:123:ARG:HA   | 37:BL:143:GLU:HB3  | 1.42        | 1.01     |
| 5:CF:92:THR:HG22   | 5:CF:94:HIS:H      | 1.25        | 1.01     |
| 20:AB:163:ILE:HG23 | 20:AB:164:ASP:H    | 1.26        | 1.00     |
| 16:AQ:6:THR:HG22   | 16:AQ:61:ARG:HB3   | 1.42        | 1.00     |
| 48:DG:89:VAL:HB    | 48:DG:159:LYS:HA   | 1.40        | 1.00     |
| 40:BH:116:ARG:HB2  | 40:BH:133:GLN:HB2  | 1.44        | 1.00     |
| 23:DB:1098:A:H3'   | 24:DI:3:LYS:CA     | 1.90        | 1.00     |
| 25:DC:144:GLU:HA   | 25:DC:151:GLY:HA2  | 1.40        | 1.00     |
| 34:D3:49:VAL:HG21  | 34:D3:54:LEU:HD13  | 1.43        | 1.00     |
| 27:BK:35:VAL:HG23  | 27:BK:36:GLY:H     | 1.24        | 1.00     |
| 26:BD:5:VAL:H      | 26:BD:32:ASN:HD21  | 1.06        | 1.00     |
| 16:CQ:6:THR:HG22   | 16:CQ:61:ARG:HB3   | 1.44        | 0.99     |
| 53:D6:92:PRO:HA    | 53:D6:101:ILE:HG12 | 1.44        | 0.99     |
| 47:DF:62:GLN:HE22  | 47:DF:90:LEU:HD13  | 1.24        | 0.99     |
| 52:DW:51:GLY:HA3   | 52:DW:59:PHE:HB2   | 1.45        | 0.99     |
| 53:B6:32:ARG:HE    | 53:B6:37:LEU:HD23  | 1.24        | 0.99     |
| 23:DB:855:G:H21    | 52:DW:23:LYS:HG2   | 1.27        | 0.99     |
| 23:DB:1420:A:H2'   | 23:DB:2211:A:H62   | 1.28        | 0.99     |
| 23:DB:812:C:H4'    | 44:DQ:12:ARG:HH22  | 1.25        | 0.99     |
| 40:BH:82:SER:H     | 40:BH:146:VAL:HG13 | 1.26        | 0.99     |
| 8:CI:20:ILE:HA     | 8:CI:62:LEU:HD12   | 1.45        | 0.98     |
| 47:DF:115:GLY:HA3  | 47:DF:177:ARG:HD2  | 1.45        | 0.98     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 53:B6:77:LYS:HE2   | 53:B6:94:ASN:HD21 | 1.23        | 0.98     |
| 38:DM:59:ARG:HH11  | 38:DM:60:GLN:HB3  | 1.27        | 0.98     |
| 1:CA:1348:U:H4'    | 8:CI:121:ARG:HG3  | 1.43        | 0.98     |
| 41:BJ:17:VAL:HG23  | 41:BJ:137:PRO:HB2 | 1.44        | 0.98     |
| 25:DC:196:ASN:HD22 | 25:DC:199:HIS:HB2 | 1.29        | 0.98     |
| 44:DQ:63:ARG:HH12  | 44:DQ:96:ASP:HB2  | 1.28        | 0.97     |
| 20:CB:163:ILE:HG23 | 20:CB:164:ASP:H   | 1.28        | 0.97     |
| 27:DK:47:ILE:HG12  | 27:DK:48:PRO:HD2  | 1.46        | 0.97     |
| 8:AI:20:ILE:HA     | 8:AI:62:LEU:HD12  | 1.43        | 0.97     |
| 1:AA:1348:U:H4'    | 8:AI:121:ARG:HG3  | 1.42        | 0.97     |
| 9:AJ:9:ARG:HB2     | 9:AJ:99:GLN:HB3   | 1.43        | 0.97     |
| 5:AF:92:THR:HG22   | 5:AF:94:HIS:H     | 1.26        | 0.97     |
| 28:DP:63:ILE:HA    | 28:DP:68:GLY:HA2  | 1.46        | 0.97     |
| 51:DZ:5:CYS:HB3    | 51:DZ:10:LYS:H    | 1.30        | 0.97     |
| 53:B6:42:LYS:HA    | 53:B6:51:PRO:HA   | 1.43        | 0.96     |
| 35:DV:62:THR:HA    | 35:DV:71:LYS:HA   | 1.48        | 0.96     |
| 38:BM:59:ARG:HH11  | 38:BM:60:GLN:HB3  | 1.31        | 0.95     |
| 47:BF:36:ASN:HA    | 47:BF:87:LYS:HA   | 1.49        | 0.95     |
| 47:DF:71:LYS:HE2   | 47:DF:73:VAL:HB   | 1.47        | 0.95     |
| 30:DY:8:GLN:HG2    | 30:DY:31:ILE:HA   | 1.47        | 0.95     |
| 23:BB:100:U:O2     | 23:BB:100:U:H2'   | 1.65        | 0.95     |
| 27:BK:47:ILE:HG12  | 27:BK:48:PRO:HD2  | 1.49        | 0.95     |
| 1:CA:1493:A:H2'    | 23:DB:1913:A:H61  | 1.31        | 0.95     |
| 53:B6:55:ILE:HG23  | 53:B6:56:ALA:H    | 1.29        | 0.95     |
| 25:BC:128:THR:HA   | 25:BC:190:THR:HA  | 1.48        | 0.95     |
| 23:BB:1420:A:H2'   | 23:BB:2211:A:H62  | 1.28        | 0.95     |
| 23:BB:141:G:H1     | 50:BT:2:ILE:HD12  | 1.32        | 0.95     |
| 26:DD:5:VAL:H      | 26:DD:32:ASN:HD21 | 1.05        | 0.95     |
| 1:AA:981:U:H4'     | 13:AN:60:ARG:HD2  | 1.48        | 0.95     |
| 35:BV:62:THR:HA    | 35:BV:71:LYS:HA   | 1.49        | 0.94     |
| 53:D6:35:PRO:HD3   | 53:D6:60:ALA:HB2  | 1.48        | 0.94     |
| 53:D6:84:ARG:H     | 53:D6:84:ARG:HE   | 1.13        | 0.94     |
| 28:BP:63:ILE:HA    | 28:BP:68:GLY:HA2  | 1.47        | 0.94     |
| 37:DL:79:LEU:HG    | 37:DL:112:LEU:HA  | 1.49        | 0.94     |
| 38:DM:17:ASN:HD21  | 38:DM:95:LEU:HG   | 1.32        | 0.94     |
| 51:DZ:40:VAL:HG21  | 51:DZ:43:GLU:HB3  | 1.46        | 0.94     |
| 47:BF:115:GLY:HA3  | 47:BF:177:ARG:HD2 | 1.49        | 0.94     |
| 41:DJ:17:VAL:HG23  | 41:DJ:137:PRO:HB2 | 1.46        | 0.94     |
| 53:B6:67:VAL:HB    | 53:B6:98:ALA:HB1  | 1.50        | 0.94     |
| 47:DF:45:ASP:HB3   | 47:DF:48:LEU:HD22 | 1.50        | 0.94     |
| 13:CN:68:ARG:HB3   | 13:CN:68:ARG:HH11 | 1.31        | 0.94     |
| 23:DB:142:A:H2'    | 23:DB:143:C:C6    | 2.03        | 0.94     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 45:DS:3:THR:HB     | 45:DS:62:ASP:HB2   | 1.50        | 0.93     |
| 50:DT:53:VAL:HG11  | 50:DT:87:LEU:HD13  | 1.47        | 0.93     |
| 45:BS:3:THR:HB     | 45:BS:62:ASP:HB2   | 1.48        | 0.93     |
| 43:DO:53:THR:HB    | 43:DO:65:THR:HG22  | 1.50        | 0.93     |
| 2:AC:63:ILE:HD12   | 2:AC:98:ALA:HB2    | 1.49        | 0.93     |
| 48:DG:34:ARG:HH11  | 48:DG:34:ARG:H     | 1.17        | 0.93     |
| 52:BW:51:GLY:HA3   | 52:BW:59:PHE:HB2   | 1.50        | 0.93     |
| 1:AA:1296:C:H4'    | 1:AA:1302:C:H41    | 1.30        | 0.93     |
| 23:DB:2393:U:H5''  | 37:DL:62:PRO:HG3   | 1.50        | 0.93     |
| 29:DE:58:LYS:H     | 29:DE:58:LYS:NZ    | 1.67        | 0.93     |
| 1:AA:600:A:H5''    | 7:AH:88:LYS:HD2    | 1.51        | 0.93     |
| 1:CA:600:A:H5''    | 7:CH:88:LYS:HD2    | 1.51        | 0.93     |
| 29:BE:108:ILE:HD11 | 29:BE:181:ILE:HB   | 1.50        | 0.93     |
| 25:DC:128:THR:HA   | 25:DC:190:THR:HA   | 1.51        | 0.93     |
| 30:DY:16:LEU:H     | 30:DY:16:LEU:HD22  | 1.32        | 0.93     |
| 38:BM:17:ASN:HD21  | 38:BM:95:LEU:HG    | 1.34        | 0.93     |
| 42:DN:37:THR:HG22  | 42:DN:39:PRO:HD2   | 1.50        | 0.93     |
| 38:DM:35:ALA:HB3   | 38:DM:99:GLY:H     | 1.33        | 0.93     |
| 52:DW:24:ARG:HA    | 52:DW:66:VAL:H     | 1.33        | 0.92     |
| 53:B6:66:LEU:HD12  | 53:B6:103:ILE:HD11 | 1.48        | 0.92     |
| 23:DB:2548:U:H1'   | 27:DK:23:LYS:NZ    | 1.84        | 0.92     |
| 1:CA:981:U:H4'     | 13:CN:60:ARG:HD2   | 1.47        | 0.92     |
| 50:BT:53:VAL:HG11  | 50:BT:87:LEU:HD13  | 1.50        | 0.92     |
| 47:DF:36:ASN:HA    | 47:DF:87:LYS:HA    | 1.50        | 0.92     |
| 1:CA:1296:C:H4'    | 1:CA:1302:C:H41    | 1.32        | 0.92     |
| 25:DC:76:VAL:HG12  | 25:DC:114:GLN:HG2  | 1.52        | 0.92     |
| 44:BQ:63:ARG:HH12  | 44:BQ:96:ASP:HB2   | 1.33        | 0.92     |
| 48:BG:34:ARG:H     | 48:BG:34:ARG:HH11  | 1.17        | 0.92     |
| 47:DF:147:ARG:HD2  | 47:DF:148:VAL:HG22 | 1.51        | 0.92     |
| 3:CD:25:ARG:HH11   | 3:CD:26:ALA:H      | 1.16        | 0.92     |
| 22:DA:2:G:H2'      | 22:DA:3:C:C6       | 2.05        | 0.92     |
| 1:CA:1328:C:H5''   | 12:CM:27:THR:HG21  | 1.50        | 0.92     |
| 40:BH:100:ALA:HB3  | 40:BH:112:LYS:HA   | 1.50        | 0.92     |
| 7:CH:86:LYS:HD2    | 7:CH:90:GLU:HG2    | 1.50        | 0.92     |
| 51:BZ:5:CYS:HB3    | 51:BZ:10:LYS:H     | 1.35        | 0.92     |
| 13:AN:68:ARG:HB3   | 13:AN:68:ARG:HH11  | 1.33        | 0.92     |
| 25:BC:76:VAL:HG12  | 25:BC:114:GLN:HG2  | 1.52        | 0.91     |
| 46:DU:84:PHE:O     | 46:DU:85:ARG:HB2   | 1.70        | 0.91     |
| 1:AA:1328:C:H5''   | 12:AM:27:THR:HG21  | 1.53        | 0.91     |
| 40:DH:77:THR:HG22  | 40:DH:143:ILE:HB   | 1.49        | 0.91     |
| 46:BU:84:PHE:O     | 46:BU:85:ARG:HB2   | 1.69        | 0.91     |
| 53:B6:129:ILE:HA   | 53:B6:132:ILE:HD12 | 1.52        | 0.91     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 48:BG:15:ASP:HB2   | 48:BG:26:LYS:H    | 1.35        | 0.91     |
| 47:BF:71:LYS:HE2   | 47:BF:73:VAL:HB   | 1.49        | 0.91     |
| 42:BN:37:THR:HG22  | 42:BN:39:PRO:HD2  | 1.53        | 0.91     |
| 12:AM:106:ARG:HH12 | 12:AM:109:LYS:HD2 | 1.36        | 0.91     |
| 34:D3:37:THR:HA    | 34:D3:40:LYS:HE2  | 1.53        | 0.91     |
| 53:D6:38:LEU:HD22  | 53:D6:83:ILE:HD12 | 1.51        | 0.91     |
| 7:AH:86:LYS:HD2    | 7:AH:90:GLU:HG2   | 1.52        | 0.91     |
| 25:BC:64:VAL:O     | 25:BC:65:ASP:HB3  | 1.71        | 0.90     |
| 43:BO:53:THR:HB    | 43:BO:65:THR:HG22 | 1.53        | 0.90     |
| 23:BB:79:C:HO2'    | 23:BB:346:A:H1'   | 1.37        | 0.90     |
| 30:BY:8:GLN:HG2    | 30:BY:31:ILE:HA   | 1.52        | 0.90     |
| 47:DF:42:ALA:HA    | 47:DF:48:LEU:HD21 | 1.52        | 0.90     |
| 3:AD:25:ARG:HH11   | 3:AD:26:ALA:H     | 1.18        | 0.90     |
| 52:BW:24:ARG:HA    | 52:BW:66:VAL:H    | 1.33        | 0.90     |
| 23:BB:1203:U:H1'   | 37:BL:4:ASN:HD21  | 1.33        | 0.90     |
| 1:AA:1206:G:H4'    | 2:AC:192:TYR:HA   | 1.51        | 0.90     |
| 30:BY:16:LEU:H     | 30:BY:16:LEU:HD22 | 1.34        | 0.90     |
| 53:B6:44:GLU:HA    | 53:B6:49:HIS:HA   | 1.52        | 0.90     |
| 51:BZ:40:VAL:HG21  | 51:BZ:43:GLU:HB3  | 1.50        | 0.90     |
| 33:B1:26:LYS:HD3   | 33:B1:52:LYS:HB3  | 1.53        | 0.90     |
| 1:AA:411:A:H62     | 1:AA:413:G:H21    | 1.20        | 0.90     |
| 20:AB:162:VAL:HG13 | 20:AB:184:ALA:HB2 | 1.54        | 0.90     |
| 50:BT:39:THR:HG22  | 50:BT:42:GLU:HG2  | 1.52        | 0.90     |
| 42:BN:83:LEU:HA    | 42:BN:86:ARG:HB2  | 1.52        | 0.90     |
| 23:DB:1060:U:N3    | 23:DB:1088:A:N7   | 2.20        | 0.90     |
| 23:BB:855:G:N2     | 52:BW:23:LYS:HG2  | 1.85        | 0.90     |
| 34:B3:37:THR:HA    | 34:B3:40:LYS:HE2  | 1.51        | 0.90     |
| 23:BB:670:A:H4'    | 23:BB:671:C:H5'   | 1.52        | 0.89     |
| 23:BB:1060:U:N3    | 23:BB:1088:A:N7   | 2.20        | 0.89     |
| 1:CA:1060:U:H4'    | 9:CJ:54:SER:HB2   | 1.54        | 0.89     |
| 47:BF:42:ALA:HA    | 47:BF:48:LEU:HD21 | 1.52        | 0.89     |
| 37:BL:51:GLU:HG3   | 37:BL:56:PRO:HA   | 1.54        | 0.89     |
| 1:CA:1206:G:H4'    | 2:CC:192:TYR:HA   | 1.54        | 0.89     |
| 47:BF:45:ASP:HB3   | 47:BF:48:LEU:HD22 | 1.53        | 0.89     |
| 12:CM:52:ILE:HG23  | 12:CM:56:ARG:HH12 | 1.38        | 0.89     |
| 1:AA:1277:C:HO2'   | 1:AA:1279:G:H8    | 1.19        | 0.89     |
| 5:AF:29:ILE:HG21   | 5:AF:64:VAL:HG11  | 1.54        | 0.89     |
| 46:DU:95:PHE:HE1   | 46:DU:102:ILE:HB  | 1.37        | 0.89     |
| 40:BH:31:VAL:HB    | 40:BH:32:PRO:CD   | 2.02        | 0.89     |
| 47:DF:43:ILE:HG23  | 47:DF:44:ALA:H    | 1.35        | 0.89     |
| 47:BF:43:ILE:HG23  | 47:BF:44:ALA:H    | 1.36        | 0.89     |
| 40:BH:84:ALA:HA    | 40:BH:90:LEU:HA   | 1.54        | 0.89     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 47:BF:11:VAL:HG12  | 47:BF:12:VAL:H     | 1.37        | 0.89     |
| 40:BH:7:ASP:HA     | 40:BH:15:LEU:HD22  | 1.53        | 0.89     |
| 40:DH:31:VAL:HB    | 40:DH:32:PRO:CD    | 2.03        | 0.89     |
| 52:DW:49:ASN:HB3   | 52:DW:81:ILE:HG12  | 1.54        | 0.89     |
| 37:BL:79:LEU:HG    | 37:BL:112:LEU:HA   | 1.53        | 0.89     |
| 23:BB:812:C:H4'    | 44:BQ:12:ARG:HH22  | 1.35        | 0.89     |
| 23:BB:1076:C:H4'   | 24:BI:94:LYS:HE3   | 1.53        | 0.89     |
| 40:BH:116:ARG:HB3  | 40:BH:131:SER:HB2  | 1.54        | 0.89     |
| 25:BC:180:MET:HB3  | 25:BC:267:VAL:HB   | 1.53        | 0.89     |
| 23:DB:1099:G:H8    | 24:DI:3:LYS:H      | 1.00        | 0.89     |
| 2:CC:126:ARG:NH2   | 2:CC:190:THR:HG23  | 1.88        | 0.89     |
| 40:BH:81:ALA:HA    | 40:BH:146:VAL:HA   | 1.55        | 0.89     |
| 23:BB:322:A:H3'    | 29:BE:163:ASN:HD21 | 1.36        | 0.89     |
| 42:DN:83:LEU:HA    | 42:DN:86:ARG:HB2   | 1.52        | 0.89     |
| 23:BB:1458:U:H5''  | 23:BB:1459:G:H5'   | 1.55        | 0.89     |
| 40:DH:84:ALA:HB1   | 40:DH:88:GLY:HA2   | 1.53        | 0.89     |
| 40:DH:5:LEU:HD13   | 40:DH:13:GLY:HA2   | 1.54        | 0.89     |
| 48:DG:15:ASP:HB2   | 48:DG:26:LYS:H     | 1.38        | 0.88     |
| 43:DO:88:LYS:HE2   | 43:DO:116:GLN:HB2  | 1.54        | 0.88     |
| 40:DH:7:ASP:HA     | 40:DH:15:LEU:HD22  | 1.55        | 0.88     |
| 47:BF:147:ARG:HD2  | 47:BF:148:VAL:HG22 | 1.54        | 0.88     |
| 1:AA:1060:U:H4'    | 9:AJ:54:SER:HB2    | 1.55        | 0.88     |
| 1:AA:812:G:HO2'    | 1:AA:813:U:H6      | 0.92        | 0.88     |
| 38:BM:35:ALA:HB3   | 38:BM:99:GLY:H     | 1.37        | 0.88     |
| 2:AC:76:ILE:HA     | 2:AC:83:VAL:HG23   | 1.56        | 0.88     |
| 25:BC:105:ALA:HB1  | 25:BC:109:LEU:HD12 | 1.55        | 0.88     |
| 45:DS:76:VAL:HG12  | 45:DS:103:ILE:HA   | 1.53        | 0.88     |
| 5:CF:29:ILE:HG21   | 5:CF:64:VAL:HG11   | 1.53        | 0.88     |
| 2:CC:63:ILE:HD12   | 2:CC:98:ALA:HB2    | 1.53        | 0.88     |
| 49:DR:7:SER:HB2    | 49:DR:22:LEU:HB3   | 1.55        | 0.88     |
| 42:BN:101:GLY:HA2  | 42:BN:110:MET:H    | 1.38        | 0.88     |
| 4:AE:37:VAL:HG11   | 4:AE:113:VAL:HG12  | 1.56        | 0.88     |
| 29:BE:5:LEU:HD12   | 29:BE:10:SER:HB2   | 1.53        | 0.88     |
| 25:DC:144:GLU:HG3  | 25:DC:151:GLY:H    | 1.38        | 0.88     |
| 29:DE:59:PRO:HB2   | 29:DE:67:ARG:HH22  | 1.35        | 0.88     |
| 23:DB:1168:G:H2'   | 23:DB:1169:A:C8    | 2.08        | 0.88     |
| 23:DB:1141:U:H4'   | 23:DB:1142:A:O4'   | 1.73        | 0.87     |
| 47:DF:11:VAL:HG12  | 47:DF:12:VAL:H     | 1.38        | 0.87     |
| 25:BC:196:ASN:HD22 | 25:BC:199:HIS:HB2  | 1.38        | 0.87     |
| 53:D6:74:ASN:H     | 53:D6:74:ASN:HD22  | 1.19        | 0.87     |
| 1:CA:411:A:H62     | 1:CA:413:G:H21     | 1.21        | 0.87     |
| 35:BV:80:HIS:HD2   | 35:BV:82:TYR:H     | 1.20        | 0.87     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 29:DE:108:ILE:HD11 | 29:DE:181:ILE:HB   | 1.55        | 0.87     |
| 43:BO:88:LYS:HE2   | 43:BO:116:GLN:HB2  | 1.54        | 0.87     |
| 2:AC:126:ARG:NH2   | 2:AC:190:THR:HG23  | 1.88        | 0.87     |
| 7:AH:36:ALA:HA     | 7:AH:39:LEU:HD12   | 1.55        | 0.87     |
| 23:BB:2305:U:H5''  | 47:BF:130:GLY:HA3  | 1.57        | 0.87     |
| 10:AK:111:ASP:HB2  | 21:AU:19:LYS:HE3   | 1.57        | 0.87     |
| 41:DJ:25:LEU:HD22  | 41:DJ:26:GLY:H     | 1.39        | 0.87     |
| 24:BI:27:LEU:HD23  | 24:BI:27:LEU:H     | 1.39        | 0.87     |
| 12:CM:106:ARG:HH12 | 12:CM:109:LYS:HD2  | 1.38        | 0.87     |
| 23:DB:1019:U:H2'   | 23:DB:1020:A:C8    | 2.09        | 0.87     |
| 47:BF:65:LEU:H     | 47:BF:88:VAL:HG22  | 1.40        | 0.86     |
| 20:CB:162:VAL:HG13 | 20:CB:184:ALA:HB2  | 1.55        | 0.86     |
| 4:CE:131:ASN:HD21  | 4:CE:133:ILE:HB    | 1.38        | 0.86     |
| 38:BM:121:ALA:HA   | 38:BM:124:LEU:HD12 | 1.54        | 0.86     |
| 41:BJ:25:LEU:HD22  | 41:BJ:26:GLY:H     | 1.40        | 0.86     |
| 23:BB:2306:C:H3'   | 23:BB:2307:G:C5'   | 2.04        | 0.86     |
| 10:AK:34:THR:HB    | 10:AK:40:ALA:HA    | 1.57        | 0.86     |
| 1:CA:812:G:HO2'    | 1:CA:813:U:H6      | 0.89        | 0.86     |
| 18:CS:48:ILE:HB    | 18:CS:59:VAL:HG23  | 1.57        | 0.86     |
| 37:DL:89:VAL:HG23  | 37:DL:123:ARG:HG3  | 1.57        | 0.86     |
| 4:CE:37:VAL:HG11   | 4:CE:113:VAL:HG12  | 1.56        | 0.86     |
| 45:BS:76:VAL:HG12  | 45:BS:103:ILE:HA   | 1.55        | 0.86     |
| 20:AB:46:VAL:HG13  | 20:AB:47:PRO:HD3   | 1.57        | 0.86     |
| 20:CB:46:VAL:HG13  | 20:CB:47:PRO:HD3   | 1.57        | 0.86     |
| 12:AM:52:ILE:HG23  | 12:AM:56:ARG:HH12  | 1.38        | 0.86     |
| 29:BE:59:PRO:HB2   | 29:BE:67:ARG:HH22  | 1.41        | 0.86     |
| 42:DN:101:GLY:HA2  | 42:DN:110:MET:H    | 1.38        | 0.86     |
| 23:BB:2108:A:H2'   | 23:BB:2109:U:H4'   | 1.57        | 0.86     |
| 23:DB:670:A:H4'    | 23:DB:671:C:H5'    | 1.57        | 0.86     |
| 52:BW:49:ASN:HB3   | 52:BW:81:ILE:HG12  | 1.56        | 0.86     |
| 47:BF:34:THR:HA    | 47:BF:89:THR:HA    | 1.57        | 0.86     |
| 18:AS:48:ILE:HB    | 18:AS:59:VAL:HG23  | 1.57        | 0.86     |
| 23:BB:1019:U:H2'   | 23:BB:1020:A:C8    | 2.10        | 0.86     |
| 41:DJ:81:ILE:HG23  | 41:DJ:82:GLY:H     | 1.40        | 0.86     |
| 10:AK:86:LYS:HB3   | 10:AK:112:VAL:HG23 | 1.56        | 0.86     |
| 33:D1:26:LYS:HD3   | 33:D1:52:LYS:HB3   | 1.57        | 0.86     |
| 25:DC:180:MET:HB3  | 25:DC:267:VAL:HB   | 1.55        | 0.86     |
| 23:BB:1141:U:H4'   | 23:BB:1142:A:O4'   | 1.75        | 0.86     |
| 46:BU:85:ARG:HD3   | 46:BU:86:PHE:H     | 1.38        | 0.86     |
| 4:AE:131:ASN:HD21  | 4:AE:133:ILE:HB    | 1.37        | 0.86     |
| 49:BR:7:SER:HB2    | 49:BR:22:LEU:HB3   | 1.56        | 0.86     |
| 47:DF:34:THR:HA    | 47:DF:89:THR:HA    | 1.57        | 0.86     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 11:AL:49:ARG:HG2   | 11:AL:89:LEU:HD21  | 1.57        | 0.86     |
| 25:DC:105:ALA:HB1  | 25:DC:109:LEU:HD12 | 1.55        | 0.86     |
| 6:AG:149:ALA:H     | 10:AK:55:ARG:HH21  | 1.20        | 0.86     |
| 8:AI:26:LYS:H      | 8:AI:61:ASP:HB3    | 1.41        | 0.86     |
| 46:DU:85:ARG:HD3   | 46:DU:86:PHE:H     | 1.38        | 0.86     |
| 10:AK:91:GLY:HA2   | 10:AK:94:SER:HB3   | 1.57        | 0.86     |
| 10:CK:34:THR:HB    | 10:CK:40:ALA:HA    | 1.57        | 0.86     |
| 23:BB:1024:G:H3'   | 23:BB:1025:G:H5''  | 1.58        | 0.86     |
| 38:DM:126:ILE:H    | 38:DM:126:ILE:HD12 | 1.41        | 0.86     |
| 23:BB:2866:U:H4'   | 23:BB:2867:G:H4'   | 1.57        | 0.86     |
| 52:DW:39:GLN:HG2   | 52:DW:40:ARG:N     | 1.91        | 0.85     |
| 8:AI:94:ARG:HH11   | 8:AI:94:ARG:HB3    | 1.41        | 0.85     |
| 25:DC:64:VAL:O     | 25:DC:65:ASP:HB3   | 1.72        | 0.85     |
| 23:DB:2306:C:H3'   | 23:DB:2307:G:C5'   | 2.05        | 0.85     |
| 43:DO:49:VAL:HG21  | 43:DO:82:ALA:HB2   | 1.58        | 0.85     |
| 29:BE:58:LYS:NZ    | 29:BE:58:LYS:H     | 1.73        | 0.85     |
| 10:CK:86:LYS:HB3   | 10:CK:112:VAL:HG23 | 1.56        | 0.85     |
| 25:DC:144:GLU:HG3  | 25:DC:151:GLY:N    | 1.90        | 0.85     |
| 47:DF:65:LEU:H     | 47:DF:88:VAL:HG22  | 1.41        | 0.85     |
| 23:BB:2472:G:H2'   | 23:BB:2475:C:H42   | 1.38        | 0.85     |
| 51:BZ:54:LYS:HA    | 51:BZ:57:ARG:HD3   | 1.59        | 0.85     |
| 52:BW:39:GLN:HG2   | 52:BW:40:ARG:N     | 1.92        | 0.85     |
| 37:BL:89:VAL:HG23  | 37:BL:123:ARG:HG3  | 1.58        | 0.85     |
| 22:DA:2:G:H2'      | 22:DA:3:C:H6       | 1.41        | 0.85     |
| 13:AN:73:LEU:HD12  | 13:AN:83:VAL:HG21  | 1.58        | 0.85     |
| 23:BB:1060:U:C5    | 24:BI:131:THR:HG22 | 2.11        | 0.85     |
| 23:DB:1244:A:H5''  | 37:DL:8:PRO:HD3    | 1.55        | 0.85     |
| 46:DU:46:LYS:HG2   | 46:DU:47:PRO:HD2   | 1.58        | 0.85     |
| 9:AJ:57:VAL:HG22   | 9:AJ:58:ASN:H      | 1.41        | 0.85     |
| 1:AA:79:G:H2'      | 1:AA:80:A:C8       | 2.12        | 0.85     |
| 2:CC:76:ILE:HA     | 2:CC:83:VAL:HG23   | 1.57        | 0.85     |
| 51:DZ:54:LYS:HA    | 51:DZ:57:ARG:HD3   | 1.57        | 0.85     |
| 50:DT:39:THR:HG22  | 50:DT:42:GLU:HG2   | 1.57        | 0.85     |
| 6:CG:74:VAL:HA     | 6:CG:87:PRO:HA     | 1.59        | 0.85     |
| 29:DE:136:GLN:HE22 | 29:DE:139:LYS:HD3  | 1.42        | 0.85     |
| 25:DC:16:VAL:HB    | 25:DC:203:VAL:HB   | 1.56        | 0.85     |
| 32:B4:2:LYS:HG2    | 32:B4:4:ARG:HE     | 1.42        | 0.85     |
| 22:DA:98:G:H1      | 35:DV:14:LYS:HB2   | 1.41        | 0.85     |
| 26:DD:62:LYS:HD2   | 26:DD:62:LYS:H     | 1.42        | 0.85     |
| 7:CH:36:ALA:HA     | 7:CH:39:LEU:HD12   | 1.56        | 0.85     |
| 3:AD:173:ASP:HB3   | 3:AD:178:GLU:HB2   | 1.57        | 0.85     |
| 9:AJ:55:PRO:HA     | 13:AN:80:ARG:NH2   | 1.91        | 0.85     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 40:BH:80:ILE:HD12  | 40:BH:144:VAL:HG22 | 1.59        | 0.84     |
| 37:DL:116:VAL:HG13 | 37:DL:117:THR:H    | 1.42        | 0.84     |
| 53:D6:174:GLN:NE2  | 53:D6:175:LEU:HD12 | 1.92        | 0.84     |
| 48:DG:96:ALA:HB3   | 48:DG:103:ASN:HB3  | 1.59        | 0.84     |
| 50:BT:57:VAL:HG22  | 50:BT:58:VAL:H     | 1.42        | 0.84     |
| 16:AQ:60:ILE:HG22  | 16:AQ:74:LEU:HA    | 1.59        | 0.84     |
| 23:BB:2389:G:H5''  | 23:BB:2390:U:H5'   | 1.59        | 0.84     |
| 23:DB:2472:G:H2'   | 23:DB:2475:C:H42   | 1.42        | 0.84     |
| 33:B1:49:LYS:HG3   | 33:B1:50:GLU:H     | 1.41        | 0.84     |
| 37:BL:116:VAL:HG13 | 37:BL:117:THR:H    | 1.41        | 0.84     |
| 23:BB:1244:A:H5''  | 37:BL:8:PRO:HD3    | 1.59        | 0.84     |
| 41:BJ:81:ILE:HG23  | 41:BJ:82:GLY:H     | 1.41        | 0.84     |
| 45:DS:52:GLU:HA    | 45:DS:55:ILE:HG22  | 1.59        | 0.84     |
| 25:BC:144:GLU:HG3  | 25:BC:151:GLY:H    | 1.42        | 0.84     |
| 40:BH:103:VAL:HG23 | 40:BH:110:VAL:HG21 | 1.59        | 0.84     |
| 26:DD:7:LYS:HB2    | 26:DD:77:ARG:HH12  | 1.42        | 0.84     |
| 33:D1:49:LYS:HG3   | 33:D1:50:GLU:H     | 1.40        | 0.84     |
| 38:DM:121:ALA:HA   | 38:DM:124:LEU:HD12 | 1.57        | 0.84     |
| 39:DX:3:ALA:HA     | 39:DX:6:LEU:HD23   | 1.59        | 0.84     |
| 24:DI:27:LEU:HD23  | 24:DI:27:LEU:H     | 1.42        | 0.84     |
| 23:DB:1099:G:H8    | 24:DI:3:LYS:CA     | 1.89        | 0.84     |
| 5:CF:3:HIS:HB2     | 5:CF:92:THR:HA     | 1.57        | 0.84     |
| 24:DI:11:GLN:HG2   | 24:DI:55:PRO:HB3   | 1.60        | 0.84     |
| 6:AG:112:ASP:HB2   | 6:AG:118:ARG:HG2   | 1.57        | 0.84     |
| 23:BB:2751:G:H5'   | 48:BG:2:ARG:HD2    | 1.59        | 0.84     |
| 23:BB:2787:C:H1'   | 26:BD:63:PRO:HG3   | 1.59        | 0.84     |
| 2:CC:106:ARG:HD2   | 2:CC:106:ARG:H     | 1.42        | 0.84     |
| 37:DL:51:GLU:HG3   | 37:DL:56:PRO:HA    | 1.60        | 0.84     |
| 47:DF:62:GLN:HG3   | 47:DF:91:ARG:HH11  | 1.40        | 0.84     |
| 47:DF:137:PHE:HB2  | 47:DF:138:PRO:HD2  | 1.60        | 0.84     |
| 23:DB:972:A:H3'    | 23:DB:973:A:H5''   | 1.60        | 0.84     |
| 6:CG:2:ARG:HH11    | 6:CG:2:ARG:HB3     | 1.42        | 0.84     |
| 52:BW:43:LYS:HD2   | 52:BW:79:ILE:HD11  | 1.58        | 0.84     |
| 6:AG:74:VAL:HA     | 6:AG:87:PRO:HA     | 1.58        | 0.84     |
| 37:DL:124:GLY:N    | 37:DL:143:GLU:HG3  | 1.93        | 0.84     |
| 40:BH:5:LEU:HD13   | 40:BH:13:GLY:HA2   | 1.60        | 0.84     |
| 53:B6:109:GLU:HA   | 53:B6:112:LYS:HE3  | 1.58        | 0.84     |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:C8     | 2.12        | 0.84     |
| 1:AA:1412:C:H2'    | 1:AA:1413:A:H8     | 1.42        | 0.84     |
| 23:DB:1024:G:H3'   | 23:DB:1025:G:H5''  | 1.57        | 0.84     |
| 23:BB:1173:U:H2'   | 23:BB:1174:U:H4'   | 1.59        | 0.84     |
| 23:BB:532:A:H4'    | 23:BB:533:G:C8     | 2.13        | 0.84     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:865:A:H5'     | 1:AA:1078:U:O4     | 1.77        | 0.84     |
| 46:DU:27:VAL:HG23  | 46:DU:33:VAL:HG12  | 1.59        | 0.84     |
| 12:AM:85:TYR:HA    | 12:AM:88:LEU:HD12  | 1.59        | 0.84     |
| 40:BH:108:VAL:HG12 | 40:BH:109:GLU:H    | 1.43        | 0.84     |
| 1:AA:72:A:H61      | 1:AA:98:A:H2       | 1.26        | 0.84     |
| 23:DB:161:A:H3'    | 23:DB:162:U:H5''   | 1.59        | 0.84     |
| 46:BU:46:LYS:HG2   | 46:BU:47:PRO:HD2   | 1.58        | 0.84     |
| 3:CD:173:ASP:HB3   | 3:CD:178:GLU:HB2   | 1.57        | 0.84     |
| 11:CL:49:ARG:HG2   | 11:CL:89:LEU:HD21  | 1.59        | 0.84     |
| 25:BC:143:VAL:HB   | 25:BC:153:LEU:HB2  | 1.60        | 0.83     |
| 40:DH:129:GLU:HA   | 40:DH:143:ILE:HA   | 1.60        | 0.83     |
| 46:BU:27:VAL:HG23  | 46:BU:33:VAL:HG12  | 1.58        | 0.83     |
| 52:BW:9:THR:HG23   | 52:BW:10:ARG:HD3   | 1.58        | 0.83     |
| 23:BB:1032:A:H1'   | 32:B4:23:ILE:HD13  | 1.59        | 0.83     |
| 33:D1:7:LYS:HD3    | 34:D3:33:THR:HG21  | 1.59        | 0.83     |
| 16:CQ:60:ILE:HG22  | 16:CQ:74:LEU:HA    | 1.58        | 0.83     |
| 23:BB:161:A:H3'    | 23:BB:162:U:H5''   | 1.60        | 0.83     |
| 23:DB:27:G:H22     | 23:DB:512:G:H2'    | 1.43        | 0.83     |
| 52:DW:39:GLN:HG3   | 52:DW:42:THR:CB    | 2.07        | 0.83     |
| 53:B6:32:ARG:HH12  | 53:B6:88:LEU:HD23  | 1.43        | 0.83     |
| 50:DT:57:VAL:HG22  | 50:DT:58:VAL:H     | 1.43        | 0.83     |
| 38:DM:50:ARG:HA    | 38:DM:53:MET:HE3   | 1.60        | 0.83     |
| 6:CG:112:ASP:HB2   | 6:CG:118:ARG:HG2   | 1.60        | 0.83     |
| 37:DL:6:LEU:H      | 37:DL:6:LEU:HD23   | 1.43        | 0.83     |
| 46:BU:95:PHE:HE1   | 46:BU:102:ILE:HB   | 1.43        | 0.83     |
| 10:CK:91:GLY:HA2   | 10:CK:94:SER:HB3   | 1.60        | 0.83     |
| 23:DB:2267:A:C8    | 23:DB:2267:A:H3'   | 2.13        | 0.83     |
| 29:DE:5:LEU:HD12   | 29:DE:10:SER:HB2   | 1.60        | 0.83     |
| 20:AB:221:ARG:HB3  | 20:AB:221:ARG:HH11 | 1.43        | 0.83     |
| 23:DB:532:A:H4'    | 23:DB:533:G:C8     | 2.13        | 0.83     |
| 37:BL:124:GLY:N    | 37:BL:143:GLU:HG3  | 1.92        | 0.83     |
| 20:CB:202:ASN:ND2  | 20:CB:204:ASP:H    | 1.77        | 0.83     |
| 32:B4:7:VAL:HG23   | 32:B4:35:GLN:HB2   | 1.59        | 0.83     |
| 13:AN:51:PRO:HB2   | 13:AN:54:SER:HB3   | 1.60        | 0.83     |
| 44:DQ:81:GLY:HA3   | 44:DQ:112:ALA:HB1  | 1.59        | 0.83     |
| 20:CB:221:ARG:HH11 | 20:CB:221:ARG:HB3  | 1.44        | 0.83     |
| 47:DF:87:LYS:HG3   | 47:DF:88:VAL:H     | 1.43        | 0.83     |
| 17:AR:62:ARG:HD3   | 17:AR:69:TYR:HA    | 1.59        | 0.83     |
| 13:CN:73:LEU:HD12  | 13:CN:83:VAL:HG21  | 1.61        | 0.83     |
| 37:DL:29:LYS:HG3   | 37:DL:30:THR:HG23  | 1.60        | 0.83     |
| 46:BU:12:VAL:HG22  | 46:BU:69:VAL:HG12  | 1.58        | 0.83     |
| 23:BB:2039:U:H2'   | 23:BB:2040:G:H8    | 1.44        | 0.83     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 9:CJ:57:VAL:HG22   | 9:CJ:58:ASN:H      | 1.43        | 0.83     |
| 23:DB:1287:A:OP1   | 42:DN:104:ALA:HB3  | 1.79        | 0.83     |
| 19:AT:4:LYS:HE3    | 19:AT:6:ALA:H      | 1.44        | 0.83     |
| 52:BW:39:GLN:HG3   | 52:BW:42:THR:CB    | 2.08        | 0.83     |
| 44:BQ:30:VAL:HG13  | 44:BQ:31:TYR:N     | 1.93        | 0.83     |
| 48:BG:96:ALA:HB3   | 48:BG:103:ASN:HB3  | 1.60        | 0.83     |
| 40:DH:90:LEU:HD12  | 40:DH:90:LEU:H     | 1.41        | 0.83     |
| 23:BB:2267:A:C8    | 23:BB:2267:A:H3'   | 2.13        | 0.83     |
| 8:CI:33:SER:HB3    | 8:CI:36:GLN:HB2    | 1.61        | 0.83     |
| 10:CK:111:ASP:HB2  | 21:CU:19:LYS:HE3   | 1.61        | 0.83     |
| 23:BB:2886:A:H62   | 31:B0:39:ARG:NE    | 1.75        | 0.83     |
| 52:DW:43:LYS:HD2   | 52:DW:79:ILE:HD11  | 1.59        | 0.83     |
| 48:BG:16:VAL:HG13  | 48:BG:49:LEU:HD11  | 1.60        | 0.83     |
| 23:BB:2267:A:H8    | 23:BB:2267:A:H3'   | 1.43        | 0.83     |
| 15:AP:6:LEU:HB3    | 15:AP:17:TYR:HB3   | 1.60        | 0.83     |
| 1:CA:699:C:H2'     | 1:CA:700:G:H5''    | 1.59        | 0.83     |
| 9:CJ:55:PRO:HA     | 13:CN:80:ARG:NH2   | 1.94        | 0.83     |
| 21:AU:48:LYS:HA    | 21:AU:51:ALA:HB3   | 1.58        | 0.83     |
| 2:AC:5:HIS:HB3     | 13:AN:88:MET:SD    | 2.18        | 0.83     |
| 23:DB:2866:U:H4'   | 23:DB:2867:G:H4'   | 1.59        | 0.83     |
| 2:AC:106:ARG:HD2   | 2:AC:106:ARG:H     | 1.44        | 0.83     |
| 44:DQ:57:ARG:HH12  | 44:DQ:61:ILE:HD11  | 1.43        | 0.82     |
| 23:BB:1060:U:C2    | 23:BB:1088:A:N7    | 2.47        | 0.82     |
| 23:DB:2267:A:H3'   | 23:DB:2267:A:H8    | 1.43        | 0.82     |
| 53:B6:162:GLN:HA   | 53:B6:162:GLN:HE21 | 1.41        | 0.82     |
| 23:DB:2389:G:H5''  | 23:DB:2390:U:H5'   | 1.61        | 0.82     |
| 8:AI:33:SER:HB3    | 8:AI:36:GLN:HB2    | 1.59        | 0.82     |
| 23:DB:850:U:H5''   | 30:DY:18:LYS:HD3   | 1.60        | 0.82     |
| 53:D6:31:GLY:HA2   | 53:D6:106:LEU:HD13 | 1.61        | 0.82     |
| 40:BH:128:HIS:HB3  | 40:BH:144:VAL:HB   | 1.61        | 0.82     |
| 24:DI:121:ILE:HD13 | 24:DI:121:ILE:H    | 1.44        | 0.82     |
| 1:CA:1323:G:H2'    | 1:CA:1324:A:H8     | 1.43        | 0.82     |
| 26:DD:107:VAL:HG13 | 26:DD:203:VAL:HG23 | 1.59        | 0.82     |
| 23:DB:45:G:H5'     | 23:DB:46:G:H5'     | 1.60        | 0.82     |
| 2:AC:149:LYS:HB3   | 2:AC:200:TRP:HB2   | 1.61        | 0.82     |
| 32:D4:7:VAL:HG23   | 32:D4:35:GLN:HB2   | 1.62        | 0.82     |
| 48:DG:148:ARG:HA   | 48:DG:161:VAL:HB   | 1.61        | 0.82     |
| 29:BE:149:ILE:HD11 | 29:BE:172:ALA:HA   | 1.61        | 0.82     |
| 52:BW:65:LYS:HG3   | 52:BW:84:GLU:HB3   | 1.61        | 0.82     |
| 44:DQ:30:VAL:HG13  | 44:DQ:31:TYR:N     | 1.93        | 0.82     |
| 53:B6:41:LEU:HD11  | 53:B6:88:LEU:HD11  | 1.60        | 0.82     |
| 40:DH:90:LEU:HD23  | 40:DH:94:ILE:HD13  | 1.58        | 0.82     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:243:A:H4'     | 1:CA:244:U:H5'     | 1.62        | 0.82     |
| 3:CD:138:PRO:HA    | 3:CD:181:PHE:HD2   | 1.44        | 0.82     |
| 52:DW:9:THR:HG23   | 52:DW:10:ARG:HD3   | 1.61        | 0.82     |
| 44:BQ:81:GLY:HA3   | 44:BQ:112:ALA:HB1  | 1.62        | 0.82     |
| 29:BE:136:GLN:HE22 | 29:BE:139:LYS:HD3  | 1.43        | 0.82     |
| 23:BB:1082:U:C4    | 23:BB:1086:A:C2    | 2.67        | 0.82     |
| 37:BL:143:GLU:HG2  | 37:BL:144:GLU:H    | 1.45        | 0.82     |
| 5:AF:3:HIS:HB2     | 5:AF:92:THR:HA     | 1.61        | 0.82     |
| 28:DP:91:VAL:HG11  | 28:DP:96:LEU:HD11  | 1.60        | 0.82     |
| 23:DB:2502:G:H5'   | 23:DB:2503:A:H5''  | 1.59        | 0.82     |
| 23:DB:1099:G:P     | 24:DI:4:VAL:H      | 2.02        | 0.82     |
| 51:DZ:7:VAL:HG13   | 51:DZ:8:THR:HG23   | 1.62        | 0.82     |
| 47:DF:49:LEU:HD11  | 47:DF:66:ILE:HD12  | 1.61        | 0.82     |
| 23:DB:328:U:H4'    | 46:DU:65:GLN:HE22  | 1.45        | 0.82     |
| 41:DJ:1:MET:HG2    | 41:DJ:2:LYS:HG2    | 1.62        | 0.82     |
| 23:DB:2039:U:H2'   | 23:DB:2040:G:H8    | 1.44        | 0.82     |
| 23:BB:141:G:N1     | 50:BT:2:ILE:HD12   | 1.93        | 0.82     |
| 28:BP:91:VAL:HG11  | 28:BP:96:LEU:HD11  | 1.62        | 0.82     |
| 12:CM:85:TYR:HA    | 12:CM:88:LEU:HD12  | 1.61        | 0.82     |
| 2:AC:48:LYS:H      | 2:AC:48:LYS:HD3    | 1.45        | 0.82     |
| 44:BQ:57:ARG:HH12  | 44:BQ:61:ILE:HD11  | 1.43        | 0.82     |
| 13:CN:51:PRO:HB2   | 13:CN:54:SER:HB3   | 1.60        | 0.82     |
| 23:DB:1082:U:C4    | 23:DB:1086:A:C2    | 2.67        | 0.82     |
| 23:BB:2331:G:H21   | 23:BB:2336:A:H8    | 1.27        | 0.81     |
| 23:DB:1060:U:C2    | 23:DB:1088:A:N7    | 2.48        | 0.81     |
| 23:BB:547:A:H3'    | 23:BB:548:G:H8     | 1.45        | 0.81     |
| 23:BB:972:A:H3'    | 23:BB:973:A:H5''   | 1.61        | 0.81     |
| 51:BZ:64:ILE:H     | 51:BZ:64:ILE:HD12  | 1.44        | 0.81     |
| 20:AB:202:ASN:ND2  | 20:AB:204:ASP:H    | 1.77        | 0.81     |
| 10:AK:22:ILE:HG12  | 10:AK:31:VAL:HG12  | 1.62        | 0.81     |
| 43:DO:67:ASN:HB3   | 43:DO:70:ALA:HB2   | 1.63        | 0.81     |
| 2:AC:120:THR:HB    | 2:AC:188:ALA:HB2   | 1.62        | 0.81     |
| 1:AA:1288:A:N1     | 1:AA:1371:G:H1'    | 1.96        | 0.81     |
| 43:BO:49:VAL:HG21  | 43:BO:82:ALA:HB2   | 1.60        | 0.81     |
| 23:DB:2379:G:H5'   | 43:DO:21:LEU:HD11  | 1.62        | 0.81     |
| 35:DV:80:HIS:HD2   | 35:DV:82:TYR:H     | 1.23        | 0.81     |
| 26:DD:29:VAL:HB    | 26:DD:98:VAL:HG22  | 1.62        | 0.81     |
| 23:DB:1458:U:H5''  | 23:DB:1459:G:H5'   | 1.61        | 0.81     |
| 1:AA:1238:A:H5'    | 1:AA:1336:C:N4     | 1.94        | 0.81     |
| 26:BD:7:LYS:HB2    | 26:BD:77:ARG:HH12  | 1.44        | 0.81     |
| 23:DB:636:G:H3'    | 37:DL:128:THR:HG21 | 1.62        | 0.81     |
| 31:B0:27:LEU:H     | 31:B0:27:LEU:HD12  | 1.45        | 0.81     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:45:G:H5'     | 23:BB:46:G:H5'     | 1.60        | 0.81     |
| 39:DX:28:LEU:HD13  | 39:DX:37:LEU:HD11  | 1.61        | 0.81     |
| 22:DA:104:A:H2'    | 22:DA:105:G:O4'    | 1.81        | 0.81     |
| 30:DY:4:ILE:HD12   | 30:DY:58:GLU:HG3   | 1.63        | 0.81     |
| 23:BB:2502:G:H5'   | 23:BB:2503:A:H5''  | 1.61        | 0.81     |
| 48:DG:16:VAL:HG13  | 48:DG:49:LEU:HD11  | 1.62        | 0.81     |
| 1:CA:1323:G:H2'    | 1:CA:1324:A:C8     | 2.14        | 0.81     |
| 23:BB:2769:U:H2'   | 23:BB:2770:G:H8    | 1.46        | 0.81     |
| 3:AD:138:PRO:HA    | 3:AD:181:PHE:HD2   | 1.45        | 0.81     |
| 48:BG:148:ARG:HA   | 48:BG:161:VAL:HB   | 1.62        | 0.81     |
| 23:DB:2484:G:OP1   | 38:DM:44:ARG:HD3   | 1.79        | 0.81     |
| 47:BF:128:SER:HB3  | 47:BF:154:THR:HG23 | 1.62        | 0.81     |
| 24:BI:129:GLU:HB3  | 24:BI:133:ARG:HH12 | 1.42        | 0.81     |
| 23:DB:2108:A:H5''  | 23:DB:2150:C:H4'   | 1.63        | 0.81     |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:H8     | 1.45        | 0.81     |
| 51:DZ:64:ILE:HD12  | 51:DZ:64:ILE:H     | 1.44        | 0.81     |
| 39:BX:3:ALA:HA     | 39:BX:6:LEU:HD23   | 1.61        | 0.81     |
| 25:BC:144:GLU:HG3  | 25:BC:151:GLY:N    | 1.94        | 0.81     |
| 9:CJ:36:VAL:HG22   | 9:CJ:76:ILE:HG22   | 1.63        | 0.81     |
| 15:CP:6:LEU:HB3    | 15:CP:17:TYR:HB3   | 1.62        | 0.81     |
| 45:BS:66:ILE:H     | 45:BS:66:ILE:HD13  | 1.45        | 0.81     |
| 52:DW:65:LYS:HG3   | 52:DW:84:GLU:HB3   | 1.62        | 0.81     |
| 23:BB:79:C:O2'     | 23:BB:346:A:H1'    | 1.80        | 0.81     |
| 47:BF:137:PHE:HB2  | 47:BF:138:PRO:HD2  | 1.60        | 0.81     |
| 18:CS:30:LEU:HB2   | 18:CS:48:ILE:HG23  | 1.63        | 0.81     |
| 42:BN:72:ASP:HB3   | 42:BN:75:ILE:HG12  | 1.62        | 0.81     |
| 1:AA:1432:G:H5'    | 28:BP:105:LYS:HG2  | 1.61        | 0.81     |
| 23:DB:1412:U:H2'   | 23:DB:1413:A:H8    | 1.46        | 0.81     |
| 25:BC:16:VAL:HB    | 25:BC:203:VAL:HB   | 1.62        | 0.81     |
| 29:DE:161:ALA:HA   | 29:DE:164:LEU:HB2  | 1.62        | 0.81     |
| 26:BD:62:LYS:HD2   | 26:BD:62:LYS:H     | 1.44        | 0.81     |
| 1:CA:120:A:H2'     | 1:CA:121:U:H5''    | 1.60        | 0.81     |
| 27:BK:54:LYS:H     | 27:BK:54:LYS:HD2   | 1.45        | 0.81     |
| 27:DK:41:ILE:HG13  | 27:DK:42:THR:H     | 1.46        | 0.81     |
| 20:AB:198:VAL:HG12 | 20:AB:200:PRO:HD3  | 1.63        | 0.81     |
| 41:BJ:57:LEU:HG    | 41:BJ:128:ASN:H    | 1.44        | 0.80     |
| 24:BI:55:PRO:HD3   | 24:BI:74:PRO:HD3   | 1.63        | 0.80     |
| 32:D4:2:LYS:HG2    | 32:D4:4:ARG:HE     | 1.46        | 0.80     |
| 17:CR:62:ARG:HD3   | 17:CR:69:TYR:HA    | 1.61        | 0.80     |
| 31:D0:27:LEU:H     | 31:D0:27:LEU:HD12  | 1.46        | 0.80     |
| 53:D6:1:MET:HB3    | 53:D6:143:LEU:HD21 | 1.64        | 0.80     |
| 37:DL:143:GLU:HG2  | 37:DL:144:GLU:H    | 1.43        | 0.80     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 40:BH:82:SER:N     | 40:BH:146:VAL:HG13 | 1.96        | 0.80     |
| 8:AI:21:LYS:O      | 8:AI:60:LEU:HB2    | 1.81        | 0.80     |
| 42:BN:101:GLY:HA2  | 42:BN:110:MET:N    | 1.95        | 0.80     |
| 18:AS:30:LEU:HB2   | 18:AS:48:ILE:HG23  | 1.62        | 0.80     |
| 10:CK:22:ILE:HG12  | 10:CK:31:VAL:HG12  | 1.62        | 0.80     |
| 37:BL:6:LEU:H      | 37:BL:6:LEU:HD23   | 1.44        | 0.80     |
| 53:B6:20:VAL:O     | 53:B6:24:ASN:HB2   | 1.81        | 0.80     |
| 48:DG:8:VAL:HG11   | 48:DG:49:LEU:HB2   | 1.62        | 0.80     |
| 1:AA:203:G:H1'     | 1:AA:465:A:N6      | 1.97        | 0.80     |
| 23:DB:2722:G:H4'   | 42:DN:4:ARG:HB2    | 1.62        | 0.80     |
| 45:DS:66:ILE:H     | 45:DS:66:ILE:HD13  | 1.46        | 0.80     |
| 27:DK:71:ARG:HG3   | 27:DK:105:ARG:NH2  | 1.96        | 0.80     |
| 23:DB:2141:G:H2'   | 23:DB:2142:A:C8    | 2.15        | 0.80     |
| 48:DG:120:ILE:HD11 | 48:DG:132:LEU:HB2  | 1.62        | 0.80     |
| 23:BB:1060:U:H5    | 24:BI:131:THR:HG22 | 1.46        | 0.80     |
| 23:DB:1168:G:H2'   | 23:DB:1169:A:H8    | 1.45        | 0.80     |
| 1:AA:978:A:H5'     | 1:AA:1362:A:N6     | 1.96        | 0.80     |
| 23:DB:1283:G:H22   | 23:DB:1286:A:H5'   | 1.46        | 0.80     |
| 8:CI:94:ARG:HH11   | 8:CI:94:ARG:HB3    | 1.45        | 0.80     |
| 29:DE:149:ILE:HD11 | 29:DE:172:ALA:HA   | 1.61        | 0.80     |
| 52:DW:37:VAL:HG12  | 52:DW:38:ARG:H     | 1.46        | 0.80     |
| 48:BG:120:ILE:HD11 | 48:BG:132:LEU:HB2  | 1.63        | 0.80     |
| 1:AA:411:A:N6      | 1:AA:413:G:H21     | 1.79        | 0.80     |
| 22:BA:104:A:H2'    | 22:BA:105:G:O4'    | 1.81        | 0.80     |
| 1:AA:699:C:H2'     | 1:AA:700:G:H5''    | 1.62        | 0.80     |
| 23:BB:968:C:H2'    | 23:BB:969:G:H8     | 1.46        | 0.80     |
| 42:BN:114:GLU:HG2  | 42:BN:115:LEU:N    | 1.95        | 0.80     |
| 8:CI:21:LYS:O      | 8:CI:60:LEU:HB2    | 1.81        | 0.80     |
| 44:BQ:77:LYS:HE2   | 44:BQ:116:LEU:HD23 | 1.63        | 0.80     |
| 23:DB:2787:C:H1'   | 26:DD:63:PRO:HG3   | 1.64        | 0.80     |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:C8     | 2.15        | 0.80     |
| 45:BS:52:GLU:HA    | 45:BS:55:ILE:HG22  | 1.62        | 0.80     |
| 29:DE:189:THR:HG23 | 29:DE:192:ALA:H    | 1.45        | 0.80     |
| 30:BY:4:ILE:HD12   | 30:BY:58:GLU:HG3   | 1.64        | 0.80     |
| 23:BB:590:A:H2'    | 23:BB:591:U:C6     | 2.17        | 0.80     |
| 23:BB:27:G:H22     | 23:BB:512:G:H2'    | 1.45        | 0.80     |
| 1:CA:1236:A:H4'    | 1:CA:1304:G:H4'    | 1.64        | 0.80     |
| 23:DB:845:A:H2'    | 23:DB:846:U:H5''   | 1.64        | 0.80     |
| 26:BD:91:THR:HG23  | 26:BD:92:VAL:H     | 1.46        | 0.80     |
| 47:BF:111:ARG:NH2  | 47:BF:113:PHE:HB2  | 1.96        | 0.80     |
| 24:DI:21:PRO:HB2   | 24:DI:22:PRO:HD3   | 1.64        | 0.80     |
| 46:DU:12:VAL:HG22  | 46:DU:69:VAL:HG12  | 1.63        | 0.80     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 20:AB:53:LEU:HD11  | 20:AB:216:VAL:HG12 | 1.64        | 0.80     |
| 26:BD:107:VAL:HG13 | 26:BD:203:VAL:HG23 | 1.63        | 0.80     |
| 51:BZ:7:VAL:HG13   | 51:BZ:8:THR:HG23   | 1.64        | 0.80     |
| 42:DN:101:GLY:HA2  | 42:DN:110:MET:N    | 1.96        | 0.80     |
| 27:DK:54:LYS:H     | 27:DK:54:LYS:HD2   | 1.46        | 0.80     |
| 19:CT:4:LYS:HE3    | 19:CT:6:ALA:H      | 1.45        | 0.80     |
| 23:BB:571:U:H3'    | 49:BR:80:ARG:NH1   | 1.96        | 0.80     |
| 23:BB:2444:G:OP2   | 29:BE:63:LYS:HD2   | 1.82        | 0.80     |
| 40:BH:83:LYS:HB3   | 40:BH:91:PHE:HB2   | 1.64        | 0.80     |
| 44:DQ:77:LYS:HE2   | 44:DQ:116:LEU:HD23 | 1.63        | 0.80     |
| 23:DB:2769:U:H2'   | 23:DB:2770:G:H8    | 1.45        | 0.80     |
| 25:DC:75:ALA:HB2   | 25:DC:95:TYR:HA    | 1.63        | 0.80     |
| 37:BL:29:LYS:HG3   | 37:BL:30:THR:HG23  | 1.62        | 0.80     |
| 1:AA:1238:A:H5'    | 1:AA:1336:C:H41    | 1.47        | 0.80     |
| 26:BD:29:VAL:HB    | 26:BD:98:VAL:HG22  | 1.64        | 0.80     |
| 40:BH:14:SER:HB2   | 40:BH:17:ASP:HB2   | 1.63        | 0.80     |
| 5:CF:38:ARG:HH21   | 5:CF:63:ASN:ND2    | 1.78        | 0.80     |
| 52:BW:37:VAL:HG12  | 52:BW:38:ARG:H     | 1.46        | 0.80     |
| 8:CI:26:LYS:H      | 8:CI:61:ASP:HB3    | 1.47        | 0.80     |
| 23:BB:345:A:H1'    | 23:BB:346:A:H2     | 1.45        | 0.80     |
| 29:BE:189:THR:HG23 | 29:BE:192:ALA:H    | 1.45        | 0.80     |
| 2:CC:120:THR:HB    | 2:CC:188:ALA:HB2   | 1.62        | 0.80     |
| 20:CB:198:VAL:HG12 | 20:CB:200:PRO:HD3  | 1.63        | 0.80     |
| 23:BB:845:A:H2'    | 23:BB:846:U:H5''   | 1.64        | 0.80     |
| 38:DM:43:ALA:O     | 38:DM:46:ILE:HG12  | 1.82        | 0.80     |
| 46:BU:80:ASP:HB2   | 46:BU:95:PHE:HB3   | 1.63        | 0.79     |
| 1:CA:1238:A:H5'    | 1:CA:1336:C:N4     | 1.97        | 0.79     |
| 48:BG:79:THR:HG22  | 48:BG:80:GLU:HG2   | 1.64        | 0.79     |
| 38:BM:50:ARG:HA    | 38:BM:53:MET:HE2   | 1.64        | 0.79     |
| 2:CC:48:LYS:HD3    | 2:CC:48:LYS:H      | 1.46        | 0.79     |
| 47:DF:111:ARG:NH2  | 47:DF:113:PHE:HB2  | 1.96        | 0.79     |
| 45:BS:24:ILE:HD11  | 45:BS:36:LEU:HD11  | 1.64        | 0.79     |
| 29:DE:145:ASP:HA   | 29:DE:166:LYS:HB3  | 1.62        | 0.79     |
| 27:BK:41:ILE:HG13  | 27:BK:42:THR:H     | 1.46        | 0.79     |
| 43:BO:67:ASN:HB3   | 43:BO:70:ALA:HB2   | 1.62        | 0.79     |
| 1:CA:437:U:H2'     | 1:CA:438:U:O4'     | 1.82        | 0.79     |
| 22:BA:52:A:OP1     | 22:BA:52:A:H4'     | 1.82        | 0.79     |
| 22:DA:52:A:H4'     | 22:DA:52:A:OP1     | 1.82        | 0.79     |
| 41:BJ:1:MET:HG2    | 41:BJ:2:LYS:HG2    | 1.63        | 0.79     |
| 29:BE:145:ASP:HA   | 29:BE:166:LYS:HB3  | 1.63        | 0.79     |
| 23:DB:1019:U:H2'   | 23:DB:1020:A:H8    | 1.46        | 0.79     |
| 1:AA:116:A:H61     | 1:AA:313:A:H1'     | 1.45        | 0.79     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:AD:187:ARG:HH12  | 3:AD:191:SER:HA    | 1.45        | 0.79     |
| 23:DB:1722:A:H2'   | 23:DB:1723:G:H8    | 1.47        | 0.79     |
| 23:DB:2886:A:H62   | 31:D0:39:ARG:NE    | 1.80        | 0.79     |
| 29:BE:147:LEU:HB3  | 29:BE:186:VAL:HG23 | 1.64        | 0.79     |
| 23:DB:2849:U:H4'   | 23:DB:2850:A:H5'   | 1.65        | 0.79     |
| 27:BK:71:ARG:HG3   | 27:BK:105:ARG:NH2  | 1.98        | 0.79     |
| 23:DB:590:A:H2'    | 23:DB:591:U:C6     | 2.16        | 0.79     |
| 40:DH:14:SER:HB2   | 40:DH:17:ASP:HB2   | 1.63        | 0.79     |
| 1:CA:1288:A:N1     | 1:CA:1371:G:H1'    | 1.97        | 0.79     |
| 11:CL:56:LEU:HD21  | 11:CL:81:ILE:HG13  | 1.64        | 0.79     |
| 42:DN:72:ASP:HB3   | 42:DN:75:ILE:HG12  | 1.63        | 0.79     |
| 42:DN:33:ILE:HG22  | 42:DN:114:GLU:HB2  | 1.63        | 0.79     |
| 21:CU:33:ARG:CZ    | 21:CU:34:ARG:HG2   | 2.12        | 0.79     |
| 41:DJ:57:LEU:HG    | 41:DJ:128:ASN:H    | 1.46        | 0.79     |
| 1:CA:21:G:H2'      | 1:CA:22:G:C8       | 2.18        | 0.79     |
| 1:CA:1412:C:H2'    | 1:CA:1413:A:H8     | 1.46        | 0.79     |
| 38:BM:126:ILE:HD12 | 38:BM:126:ILE:H    | 1.46        | 0.79     |
| 8:CI:38:PHE:HZ     | 8:CI:74:GLN:HB3    | 1.48        | 0.79     |
| 2:CC:149:LYS:HB3   | 2:CC:200:TRP:HB2   | 1.63        | 0.79     |
| 47:BF:87:LYS:HG3   | 47:BF:88:VAL:H     | 1.46        | 0.79     |
| 49:DR:6:GLN:HE22   | 49:DR:10:LYS:N     | 1.81        | 0.79     |
| 49:BR:6:GLN:HE22   | 49:BR:10:LYS:N     | 1.80        | 0.79     |
| 1:CA:978:A:H5'     | 1:CA:1362:A:N6     | 1.98        | 0.79     |
| 12:AM:3:ILE:HA     | 12:AM:56:ARG:HG2   | 1.64        | 0.79     |
| 43:DO:58:ILE:HG22  | 43:DO:62:LEU:HD23  | 1.64        | 0.79     |
| 23:DB:1654:A:O2'   | 26:DD:118:PHE:HB2  | 1.82        | 0.79     |
| 42:DN:70:THR:HB    | 42:DN:75:ILE:HD11  | 1.64        | 0.79     |
| 49:BR:49:ILE:HD13  | 49:BR:53:PHE:N     | 1.98        | 0.79     |
| 15:CP:26:ASN:HD21  | 15:CP:31:ARG:HD3   | 1.48        | 0.79     |
| 23:BB:855:G:H21    | 52:BW:23:LYS:CG    | 1.95        | 0.79     |
| 8:AI:56:MET:HA     | 8:AI:59:LYS:HB2    | 1.65        | 0.79     |
| 4:AE:35:LEU:HD21   | 4:AE:136:VAL:HG11  | 1.65        | 0.79     |
| 38:BM:19:GLY:HA2   | 38:BM:98:PRO:HD2   | 1.64        | 0.79     |
| 27:DK:99:ILE:HB    | 27:DK:118:LEU:HD22 | 1.66        | 0.79     |
| 40:BH:73:ASN:HB3   | 40:BH:141:LYS:HZ3  | 1.48        | 0.79     |
| 23:DB:1099:G:OP2   | 24:DI:3:LYS:HA     | 1.82        | 0.78     |
| 23:DB:855:G:N2     | 52:DW:23:LYS:HG2   | 1.97        | 0.78     |
| 47:BF:49:LEU:HD11  | 47:BF:66:ILE:HD12  | 1.64        | 0.78     |
| 1:CA:920:U:H2'     | 1:CA:921:U:C6      | 2.18        | 0.78     |
| 9:AJ:52:LEU:HA     | 9:AJ:62:ARG:HA     | 1.65        | 0.78     |
| 42:DN:114:GLU:HG2  | 42:DN:115:LEU:N    | 1.95        | 0.78     |
| 49:DR:49:ILE:HD13  | 49:DR:53:PHE:N     | 1.98        | 0.78     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 46:DU:80:ASP:HB2   | 46:DU:95:PHE:HB3   | 1.66        | 0.78     |
| 1:CA:411:A:N6      | 1:CA:413:G:H21     | 1.81        | 0.78     |
| 43:BO:58:ILE:HG22  | 43:BO:62:LEU:HD23  | 1.65        | 0.78     |
| 2:CC:149:LYS:HA    | 2:CC:168:ARG:HB2   | 1.65        | 0.78     |
| 44:BQ:109:VAL:HG12 | 44:BQ:113:LYS:HE3  | 1.66        | 0.78     |
| 24:BI:21:PRO:HB2   | 24:BI:22:PRO:HD3   | 1.63        | 0.78     |
| 29:DE:69:ARG:O     | 29:DE:70:SER:HB3   | 1.81        | 0.78     |
| 2:AC:69:THR:HG21   | 2:AC:75:VAL:HG21   | 1.64        | 0.78     |
| 27:BK:99:ILE:HB    | 27:BK:118:LEU:HD22 | 1.65        | 0.78     |
| 1:AA:21:G:H2'      | 1:AA:22:G:C8       | 2.18        | 0.78     |
| 47:BF:62:GLN:HG3   | 47:BF:91:ARG:HH11  | 1.48        | 0.78     |
| 40:DH:78:VAL:HB    | 40:DH:144:VAL:HG13 | 1.65        | 0.78     |
| 13:AN:30:ILE:H     | 13:AN:30:ILE:HD12  | 1.49        | 0.78     |
| 23:DB:2346:A:H3'   | 23:DB:2347:C:H5''  | 1.65        | 0.78     |
| 26:DD:178:VAL:HB   | 26:DD:188:LEU:HB2  | 1.66        | 0.78     |
| 37:DL:103:ILE:H    | 37:DL:103:ILE:HD12 | 1.48        | 0.78     |
| 23:DB:1338:G:H4'   | 50:DT:18:GLU:HG3   | 1.64        | 0.78     |
| 23:BB:2143:C:H2'   | 23:BB:2144:G:O4'   | 1.83        | 0.78     |
| 38:BM:55:ARG:HH21  | 38:BM:55:ARG:HA    | 1.47        | 0.78     |
| 53:D6:56:ALA:HB2   | 53:D6:79:ILE:HD13  | 1.65        | 0.78     |
| 39:BX:28:LEU:HD13  | 39:BX:37:LEU:HD11  | 1.63        | 0.78     |
| 39:BX:31:GLN:HG2   | 39:BX:37:LEU:HB2   | 1.66        | 0.78     |
| 47:DF:109:ARG:HB3  | 47:DF:135:ILE:HD12 | 1.66        | 0.78     |
| 21:CU:48:LYS:HA    | 21:CU:51:ALA:HB3   | 1.63        | 0.78     |
| 10:CK:24:ALA:HA    | 10:CK:29:THR:HG23  | 1.65        | 0.78     |
| 10:CK:83:VAL:HB    | 10:CK:109:ILE:HG23 | 1.65        | 0.78     |
| 23:BB:1412:U:H2'   | 23:BB:1413:A:H8    | 1.48        | 0.78     |
| 23:DB:9:G:H21      | 23:DB:10:A:H62     | 1.29        | 0.78     |
| 1:AA:437:U:H2'     | 1:AA:438:U:O4'     | 1.83        | 0.78     |
| 23:DB:1099:G:P     | 24:DI:3:LYS:HA     | 2.23        | 0.78     |
| 23:BB:918:A:H2'    | 23:BB:919:U:H5'    | 1.65        | 0.78     |
| 25:DC:77:VAL:HG23  | 25:DC:112:GLY:N    | 1.99        | 0.78     |
| 1:AA:920:U:H2'     | 1:AA:921:U:C6      | 2.19        | 0.78     |
| 23:DB:140:C:H4'    | 23:DB:141:G:C6     | 2.18        | 0.78     |
| 23:DB:1796:U:H2'   | 23:DB:1797:G:H8    | 1.48        | 0.78     |
| 48:DG:30:GLY:HA3   | 48:DG:78:VAL:HA    | 1.66        | 0.78     |
| 38:DM:19:GLY:HA2   | 38:DM:98:PRO:HD2   | 1.64        | 0.78     |
| 8:CI:56:MET:HA     | 8:CI:59:LYS:HB2    | 1.66        | 0.78     |
| 23:DB:968:C:H2'    | 23:DB:969:G:H8     | 1.47        | 0.78     |
| 47:BF:163:GLU:HA   | 47:BF:166:ARG:HH11 | 1.49        | 0.78     |
| 44:BQ:10:ARG:HH21  | 44:BQ:14:LYS:HD3   | 1.49        | 0.78     |
| 23:BB:2867:G:H2'   | 23:BB:2867:G:N3    | 1.98        | 0.78     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 2:AC:149:LYS:HA   | 2:AC:168:ARG:HB2   | 1.65        | 0.78     |
| 23:DB:1412:U:H2'  | 23:DB:1413:A:C8    | 2.19        | 0.78     |
| 24:DI:45:THR:HA   | 24:DI:48:ILE:HG22  | 1.66        | 0.78     |
| 35:BV:40:ILE:HD13 | 35:BV:40:ILE:H     | 1.48        | 0.78     |
| 1:CA:116:A:H61    | 1:CA:313:A:H1'     | 1.48        | 0.78     |
| 34:B3:22:LYS:HA   | 34:B3:48:MET:HA    | 1.66        | 0.78     |
| 21:CU:36:PHE:CB   | 21:CU:40:PRO:HD3   | 2.14        | 0.78     |
| 8:AI:24:ASN:ND2   | 8:AI:25:GLY:H      | 1.82        | 0.78     |
| 12:CM:3:ILE:HA    | 12:CM:56:ARG:HG2   | 1.65        | 0.78     |
| 1:AA:1347:G:N2    | 1:AA:1373:G:H2'    | 1.99        | 0.78     |
| 3:CD:187:ARG:HH12 | 3:CD:191:SER:HA    | 1.48        | 0.78     |
| 1:CA:1347:G:N2    | 1:CA:1373:G:H2'    | 1.99        | 0.78     |
| 48:DG:79:THR:HG22 | 48:DG:80:GLU:HG2   | 1.66        | 0.78     |
| 38:DM:55:ARG:HH21 | 38:DM:55:ARG:HA    | 1.47        | 0.78     |
| 40:BH:68:ARG:NH1  | 40:BH:134:VAL:HG21 | 1.99        | 0.78     |
| 51:DZ:5:CYS:HB3   | 51:DZ:10:LYS:N     | 1.99        | 0.78     |
| 35:BV:4:ILE:HB    | 35:BV:63:ILE:HA    | 1.66        | 0.78     |
| 35:DV:40:ILE:HD13 | 35:DV:40:ILE:H     | 1.49        | 0.78     |
| 44:DQ:10:ARG:HH21 | 44:DQ:14:LYS:HD3   | 1.49        | 0.78     |
| 23:BB:460:A:H4'   | 50:BT:72:GLN:HB2   | 1.64        | 0.78     |
| 26:BD:178:VAL:HB  | 26:BD:188:LEU:HB2  | 1.66        | 0.78     |
| 23:DB:918:A:H2'   | 23:DB:919:U:H5'    | 1.64        | 0.77     |
| 8:AI:25:GLY:HA2   | 8:AI:60:LEU:O      | 1.83        | 0.77     |
| 26:DD:51:THR:CG2  | 26:DD:76:GLY:HA3   | 2.14        | 0.77     |
| 47:DF:149:ARG:HA  | 47:DF:149:ARG:HH11 | 1.48        | 0.77     |
| 1:CA:1238:A:H5'   | 1:CA:1336:C:H41    | 1.49        | 0.77     |
| 26:BD:10:GLY:HA3  | 26:BD:26:VAL:H     | 1.49        | 0.77     |
| 47:DF:35:LEU:HD23 | 47:DF:153:ILE:HG12 | 1.66        | 0.77     |
| 27:BK:58:LEU:HD11 | 27:BK:86:LEU:HB3   | 1.66        | 0.77     |
| 11:CL:78:VAL:HG12 | 11:CL:101:LEU:HD13 | 1.65        | 0.77     |
| 49:DR:60:LYS:N    | 49:DR:100:GLY:HA3  | 1.94        | 0.77     |
| 47:DF:126:ASN:HB3 | 47:DF:156:THR:HA   | 1.67        | 0.77     |
| 9:CJ:52:LEU:HA    | 9:CJ:62:ARG:HA     | 1.65        | 0.77     |
| 23:BB:1287:A:OP1  | 42:BN:104:ALA:HB3  | 1.84        | 0.77     |
| 1:CA:279:A:H5''   | 1:CA:280:C:H3'     | 1.66        | 0.77     |
| 29:BE:176:ASP:HB3 | 29:BE:179:SER:HB2  | 1.67        | 0.77     |
| 9:CJ:8:ILE:HG13   | 9:CJ:100:ILE:HG22  | 1.65        | 0.77     |
| 46:BU:58:VAL:HG12 | 46:BU:59:GLU:H     | 1.48        | 0.77     |
| 51:DZ:31:PRO:HB2  | 51:DZ:33:LEU:HD11  | 1.64        | 0.77     |
| 25:BC:75:ALA:HB2  | 25:BC:95:TYR:HA    | 1.65        | 0.77     |
| 40:DH:127:GLU:HA  | 40:DH:145:ASN:HA   | 1.65        | 0.77     |
| 29:BE:161:ALA:HA  | 29:BE:164:LEU:HB2  | 1.65        | 0.77     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:18:C:H4'     | 1:CA:1078:U:O2     | 1.84        | 0.77     |
| 23:BB:172:A:H2'   | 23:BB:173:A:C8     | 2.20        | 0.77     |
| 1:AA:1299:A:H2'   | 1:AA:1301:U:H1'    | 1.66        | 0.77     |
| 23:BB:9:G:H21     | 23:BB:10:A:H62     | 1.30        | 0.77     |
| 38:DM:40:ARG:HD3  | 38:DM:93:VAL:HG21  | 1.65        | 0.77     |
| 23:DB:1098:A:H2'  | 24:DI:4:VAL:N      | 1.99        | 0.77     |
| 47:DF:40:GLY:HA2  | 47:DF:84:ILE:HG23  | 1.66        | 0.77     |
| 10:AK:22:ILE:HG21 | 10:AK:95:THR:HG21  | 1.67        | 0.77     |
| 10:CK:22:ILE:HG21 | 10:CK:95:THR:HG21  | 1.66        | 0.77     |
| 23:DB:2867:G:N3   | 23:DB:2867:G:H2'   | 1.99        | 0.77     |
| 23:BB:2148:G:H3'  | 23:BB:2149:U:O4'   | 1.84        | 0.77     |
| 4:CE:52:ALA:HB2   | 4:CE:61:LYS:HE2    | 1.66        | 0.77     |
| 1:AA:843:U:H5'    | 1:AA:844:G:N7      | 1.99        | 0.77     |
| 23:BB:364:C:H2'   | 23:BB:365:U:C6     | 2.19        | 0.77     |
| 6:CG:145:GLU:HA   | 6:CG:148:LYS:HB2   | 1.66        | 0.77     |
| 35:BV:79:ARG:HA   | 35:BV:86:LEU:HA    | 1.67        | 0.77     |
| 33:D1:33:LEU:H    | 33:D1:51:ALA:HB3   | 1.50        | 0.77     |
| 47:DF:128:SER:HB3 | 47:DF:154:THR:HG23 | 1.66        | 0.77     |
| 22:BA:28:C:C5     | 22:BA:56:G:N2      | 2.53        | 0.77     |
| 4:CE:23:THR:HA    | 4:CE:28:ARG:HA     | 1.66        | 0.77     |
| 45:DS:24:ILE:HG22 | 45:DS:71:VAL:HG11  | 1.67        | 0.77     |
| 43:BO:11:ALA:HB2  | 43:BO:96:GLY:N     | 1.99        | 0.77     |
| 23:BB:1283:G:H22  | 23:BB:1286:A:H5'   | 1.49        | 0.77     |
| 1:AA:715:A:H2'    | 1:AA:716:A:H8      | 1.49        | 0.77     |
| 23:BB:1416:G:HO2' | 23:BB:1417:C:H6    | 1.33        | 0.77     |
| 49:BR:60:LYS:N    | 49:BR:100:GLY:HA3  | 1.94        | 0.77     |
| 53:B6:43:VAL:HB   | 53:B6:55:ILE:HG21  | 1.65        | 0.77     |
| 45:DS:24:ILE:HD11 | 45:DS:36:LEU:HD11  | 1.66        | 0.77     |
| 45:BS:24:ILE:HG22 | 45:BS:71:VAL:HG11  | 1.66        | 0.77     |
| 29:DE:147:LEU:HB3 | 29:DE:186:VAL:HG23 | 1.64        | 0.77     |
| 23:DB:1778:U:H2'  | 23:DB:1784:A:N6    | 2.00        | 0.77     |
| 1:AA:1391:U:H2'   | 1:AA:1392:G:C8     | 2.18        | 0.77     |
| 1:CA:203:G:H1'    | 1:CA:465:A:N6      | 1.99        | 0.77     |
| 1:AA:243:A:H4'    | 1:AA:244:U:H5'     | 1.64        | 0.77     |
| 52:DW:67:LYS:O    | 52:DW:68:PHE:HB2   | 1.85        | 0.77     |
| 2:CC:137:VAL:HA   | 2:CC:148:ILE:HD13  | 1.65        | 0.77     |
| 43:DO:11:ALA:HB2  | 43:DO:96:GLY:N     | 1.99        | 0.77     |
| 52:BW:67:LYS:O    | 52:BW:68:PHE:HB2   | 1.83        | 0.77     |
| 1:AA:120:A:H2'    | 1:AA:121:U:H5''    | 1.66        | 0.77     |
| 26:DD:151:THR:HB  | 26:DD:152:PRO:HD3  | 1.66        | 0.77     |
| 2:CC:69:THR:HG21  | 2:CC:75:VAL:HG21   | 1.66        | 0.77     |
| 24:DI:72:THR:HG21 | 24:DI:112:LYS:HA   | 1.67        | 0.77     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 7:AH:49:LYS:HB3    | 7:AH:59:GLU:HB2    | 1.65        | 0.77     |
| 23:BB:287:G:H2'    | 23:BB:288:U:C6     | 2.19        | 0.77     |
| 24:BI:106:GLN:O    | 24:BI:110:GLN:HG3  | 1.85        | 0.77     |
| 26:BD:105:LYS:H    | 26:BD:106:LYS:HZ3  | 1.33        | 0.76     |
| 47:BF:66:ILE:HD11  | 47:BF:83:PRO:HB3   | 1.67        | 0.76     |
| 23:BB:321:U:OP2    | 29:BE:130:LYS:HA   | 1.84        | 0.76     |
| 23:BB:2849:U:H4'   | 23:BB:2850:A:H5'   | 1.66        | 0.76     |
| 13:CN:30:ILE:H     | 13:CN:30:ILE:HD12  | 1.50        | 0.76     |
| 26:DD:68:PHE:HB3   | 26:DD:73:VAL:HG23  | 1.67        | 0.76     |
| 1:AA:1221:G:O3'    | 18:AS:76:THR:HG21  | 1.85        | 0.76     |
| 11:AL:78:VAL:HG12  | 11:AL:101:LEU:HD13 | 1.66        | 0.76     |
| 23:DB:571:U:H3'    | 49:DR:80:ARG:NH1   | 1.99        | 0.76     |
| 21:AU:33:ARG:CZ    | 21:AU:34:ARG:HG2   | 2.14        | 0.76     |
| 53:D6:73:GLN:HA    | 53:D6:76:LEU:HD12  | 1.67        | 0.76     |
| 23:DB:328:U:H4'    | 46:DU:65:GLN:NE2   | 2.00        | 0.76     |
| 23:BB:2548:U:H1'   | 27:BK:23:LYS:NZ    | 2.01        | 0.76     |
| 42:BN:70:THR:HB    | 42:BN:75:ILE:HD11  | 1.66        | 0.76     |
| 23:BB:850:U:H5''   | 30:BY:18:LYS:HD3   | 1.66        | 0.76     |
| 1:CA:1391:U:H2'    | 1:CA:1392:G:C8     | 2.20        | 0.76     |
| 24:DI:105:LEU:HD13 | 24:DI:129:GLU:HG2  | 1.66        | 0.76     |
| 26:DD:91:THR:HG23  | 26:DD:92:VAL:H     | 1.49        | 0.76     |
| 48:BG:8:VAL:HG11   | 48:BG:49:LEU:HB2   | 1.67        | 0.76     |
| 47:BF:40:GLY:HA2   | 47:BF:84:ILE:HG23  | 1.66        | 0.76     |
| 24:BI:27:LEU:HD12  | 24:BI:32:VAL:HG11  | 1.66        | 0.76     |
| 1:CA:1221:G:O3'    | 18:CS:76:THR:HG21  | 1.85        | 0.76     |
| 23:DB:2141:G:H2'   | 23:DB:2142:A:H8    | 1.50        | 0.76     |
| 47:BF:35:LEU:HD23  | 47:BF:153:ILE:HG12 | 1.67        | 0.76     |
| 23:DB:1551:A:H3'   | 23:DB:1552:A:H5''  | 1.68        | 0.76     |
| 25:DC:196:ASN:ND2  | 25:DC:199:HIS:HB2  | 1.99        | 0.76     |
| 22:DA:28:C:C5      | 22:DA:56:G:N2      | 2.54        | 0.76     |
| 33:B1:33:LEU:H     | 33:B1:51:ALA:HB3   | 1.50        | 0.76     |
| 23:DB:571:U:H3'    | 49:DR:80:ARG:HH12  | 1.51        | 0.76     |
| 26:DD:186:LEU:HD21 | 28:DP:3:ILE:HD11   | 1.68        | 0.76     |
| 53:B6:118:VAL:HG11 | 53:B6:180:GLU:HB2  | 1.67        | 0.76     |
| 21:AU:36:PHE:CB    | 21:AU:40:PRO:HD3   | 2.14        | 0.76     |
| 13:CN:5:MET:HB3    | 13:CN:62:ARG:HH12  | 1.51        | 0.76     |
| 29:BE:155:GLU:HA   | 29:BE:158:PHE:HB3  | 1.67        | 0.76     |
| 29:BE:69:ARG:O     | 29:BE:70:SER:HB3   | 1.85        | 0.76     |
| 23:BB:1558:C:H4'   | 23:BB:1559:U:H5'   | 1.65        | 0.76     |
| 23:BB:1722:A:H2'   | 23:BB:1723:G:H8    | 1.49        | 0.76     |
| 36:B2:34:ARG:HB3   | 36:B2:39:ARG:HB2   | 1.64        | 0.76     |
| 23:DB:455:C:N3     | 23:DB:472:A:H2'    | 2.00        | 0.76     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1236:A:H4'    | 1:AA:1304:G:H4'    | 1.66        | 0.76     |
| 26:BD:51:THR:CG2   | 26:BD:76:GLY:HA3   | 2.16        | 0.76     |
| 44:DQ:86:SER:HB2   | 49:DR:51:VAL:HA    | 1.68        | 0.76     |
| 44:DQ:4:LYS:HZ1    | 44:DQ:7:VAL:HG22   | 1.51        | 0.76     |
| 1:AA:82:G:H2'      | 1:AA:84:U:H5       | 1.50        | 0.76     |
| 9:AJ:17:LEU:HD22   | 9:AJ:96:VAL:HG13   | 1.68        | 0.76     |
| 40:DH:72:ILE:HD11  | 40:DH:140:ALA:HB3  | 1.66        | 0.76     |
| 47:BF:126:ASN:HB3  | 47:BF:156:THR:HA   | 1.68        | 0.76     |
| 47:BF:109:ARG:HB3  | 47:BF:135:ILE:HD12 | 1.68        | 0.76     |
| 23:BB:1019:U:H2'   | 23:BB:1020:A:H8    | 1.49        | 0.76     |
| 32:B4:23:ILE:HB    | 32:B4:38:GLY:HA3   | 1.66        | 0.76     |
| 1:AA:279:A:H5''    | 1:AA:280:C:H3'     | 1.67        | 0.76     |
| 23:DB:1700:A:H2'   | 23:DB:1701:A:H5'   | 1.67        | 0.76     |
| 23:DB:1080:A:H2'   | 23:DB:1081:U:H6    | 1.50        | 0.76     |
| 44:BQ:26:ALA:O     | 44:BQ:30:VAL:HG12  | 1.86        | 0.76     |
| 51:BZ:31:PRO:HB2   | 51:BZ:33:LEU:HD11  | 1.68        | 0.76     |
| 3:AD:24:VAL:HG23   | 3:AD:25:ARG:H      | 1.50        | 0.76     |
| 4:AE:23:THR:HA     | 4:AE:28:ARG:HA     | 1.68        | 0.76     |
| 46:DU:47:PRO:HD3   | 46:DU:55:GLY:HA3   | 1.67        | 0.76     |
| 46:DU:12:VAL:HA    | 46:DU:69:VAL:HA    | 1.68        | 0.76     |
| 44:DQ:109:VAL:HG12 | 44:DQ:113:LYS:HE3  | 1.66        | 0.76     |
| 26:BD:151:THR:HB   | 26:BD:152:PRO:HD3  | 1.67        | 0.76     |
| 24:BI:33:ASN:HD21  | 24:BI:64:ARG:HH11  | 1.34        | 0.76     |
| 29:DE:176:ASP:HB3  | 29:DE:179:SER:HB2  | 1.67        | 0.76     |
| 48:BG:9:VAL:HG12   | 48:BG:11:PRO:HD3   | 1.68        | 0.76     |
| 43:DO:89:ASP:HA    | 43:DO:116:GLN:O    | 1.86        | 0.76     |
| 38:DM:36:VAL:HB    | 38:DM:127:LYS:O    | 1.86        | 0.76     |
| 48:BG:166:GLU:HG2  | 48:BG:168:VAL:HG23 | 1.67        | 0.76     |
| 20:CB:53:LEU:HD11  | 20:CB:216:VAL:HG12 | 1.66        | 0.76     |
| 23:BB:1338:G:H4'   | 50:BT:18:GLU:HG3   | 1.65        | 0.76     |
| 11:AL:51:VAL:HG12  | 11:AL:52:CYS:H     | 1.50        | 0.76     |
| 1:CA:843:U:H5'     | 1:CA:844:G:N7      | 2.00        | 0.76     |
| 36:D2:21:ARG:HG2   | 36:D2:31:LEU:HG    | 1.68        | 0.76     |
| 25:BC:77:VAL:HG23  | 25:BC:112:GLY:N    | 1.99        | 0.76     |
| 25:DC:144:GLU:HB3  | 25:DC:187:CYS:HB3  | 1.68        | 0.76     |
| 23:BB:1178:C:H2'   | 23:BB:1179:G:C8    | 2.21        | 0.76     |
| 46:BU:47:PRO:HD3   | 46:BU:55:GLY:HA3   | 1.68        | 0.76     |
| 21:CU:3:ILE:HD13   | 21:CU:19:LYS:HA    | 1.68        | 0.76     |
| 23:BB:125:A:H3'    | 23:BB:126:A:C5'    | 2.15        | 0.76     |
| 23:BB:1437:C:H2'   | 23:BB:1438:U:C6    | 2.21        | 0.76     |
| 23:BB:1551:A:H3'   | 23:BB:1552:A:H5''  | 1.67        | 0.76     |
| 25:DC:156:SER:O    | 25:DC:194:VAL:HG11 | 1.85        | 0.76     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 14:CO:89:ARG:HA    | 14:CO:89:ARG:HH11  | 1.51        | 0.76     |
| 23:DB:1099:G:H5'   | 24:DI:3:LYS:N      | 2.01        | 0.75     |
| 7:AH:77:VAL:HG23   | 7:AH:126:CYS:HA    | 1.68        | 0.75     |
| 49:DR:4:VAL:O      | 49:DR:38:VAL:HA    | 1.86        | 0.75     |
| 23:DB:1548:A:H2'   | 23:DB:1549:A:C8    | 2.21        | 0.75     |
| 25:BC:156:SER:O    | 25:BC:194:VAL:HG11 | 1.85        | 0.75     |
| 9:CJ:17:LEU:HD22   | 9:CJ:96:VAL:HG13   | 1.68        | 0.75     |
| 48:BG:30:GLY:HA3   | 48:BG:78:VAL:HA    | 1.66        | 0.75     |
| 25:BC:43:ASN:ND2   | 25:BC:44:ASN:H     | 1.84        | 0.75     |
| 47:BF:149:ARG:HA   | 47:BF:149:ARG:HH11 | 1.52        | 0.75     |
| 20:CB:31:PHE:HB2   | 20:CB:41:ASN:HA    | 1.68        | 0.75     |
| 53:D6:174:GLN:HE21 | 53:D6:175:LEU:N    | 1.85        | 0.75     |
| 35:DV:79:ARG:HA    | 35:DV:86:LEU:HA    | 1.67        | 0.75     |
| 42:BN:33:ILE:HG22  | 42:BN:114:GLU:HB2  | 1.67        | 0.75     |
| 23:BB:2185:U:H2'   | 23:BB:2186:G:C8    | 2.21        | 0.75     |
| 20:CB:143:LEU:HD22 | 20:CB:147:LEU:HD12 | 1.68        | 0.75     |
| 9:AJ:8:ILE:HG13    | 9:AJ:100:ILE:HG22  | 1.67        | 0.75     |
| 20:AB:143:LEU:HD22 | 20:AB:147:LEU:HD12 | 1.68        | 0.75     |
| 23:BB:1104:C:H2'   | 23:BB:1105:U:H6    | 1.50        | 0.75     |
| 48:DG:115:GLN:H    | 48:DG:115:GLN:CD   | 1.90        | 0.75     |
| 7:CH:11:THR:HG22   | 7:CH:14:ARG:HH12   | 1.49        | 0.75     |
| 12:CM:49:GLU:O     | 12:CM:52:ILE:HG22  | 1.86        | 0.75     |
| 47:DF:102:LEU:HA   | 47:DF:106:ALA:CB   | 2.17        | 0.75     |
| 2:AC:137:VAL:HA    | 2:AC:148:ILE:HD13  | 1.68        | 0.75     |
| 3:CD:137:SER:HB2   | 3:CD:138:PRO:HD2   | 1.66        | 0.75     |
| 23:DB:2243:U:H2'   | 23:DB:2244:U:C6    | 2.21        | 0.75     |
| 2:CC:5:HIS:HB3     | 13:CN:88:MET:SD    | 2.26        | 0.75     |
| 40:DH:46:PHE:HA    | 40:DH:50:ARG:HH21  | 1.52        | 0.75     |
| 23:DB:2102:G:H2'   | 23:DB:2103:C:O4'   | 1.86        | 0.75     |
| 23:DB:2331:G:H21   | 23:DB:2336:A:H8    | 1.30        | 0.75     |
| 40:BH:6:LEU:HD13   | 40:BH:36:ALA:HA    | 1.66        | 0.75     |
| 23:BB:1447:C:H2'   | 23:BB:1448:G:H8    | 1.51        | 0.75     |
| 23:DB:2425:A:H5'   | 23:DB:2427:C:O4'   | 1.87        | 0.75     |
| 26:BD:186:LEU:HD21 | 28:BP:3:ILE:HD11   | 1.67        | 0.75     |
| 23:DB:2615:U:H1'   | 31:D0:3:GLN:HB3    | 1.68        | 0.75     |
| 34:D3:22:LYS:HA    | 34:D3:48:MET:HA    | 1.66        | 0.75     |
| 38:BM:43:ALA:O     | 38:BM:46:ILE:HG12  | 1.86        | 0.75     |
| 23:DB:2769:U:H2'   | 23:DB:2770:G:C8    | 2.22        | 0.75     |
| 23:BB:845:A:C2     | 23:BB:847:U:H1'    | 2.22        | 0.75     |
| 1:CA:1338:G:H2'    | 1:CA:1339:A:C8     | 2.21        | 0.75     |
| 23:BB:2743:U:H2'   | 23:BB:2744:G:O4'   | 1.86        | 0.75     |
| 23:BB:2653:U:O2'   | 48:BG:109:SER:HB2  | 1.85        | 0.75     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 11:AL:56:LEU:HD21  | 11:AL:81:ILE:HG13  | 1.68        | 0.75     |
| 4:AE:81:GLN:H      | 4:AE:146:MET:HE3   | 1.51        | 0.75     |
| 47:DF:31:GLU:HB3   | 47:DF:156:THR:O    | 1.87        | 0.75     |
| 18:AS:18:VAL:HG21  | 18:AS:43:MET:HB3   | 1.69        | 0.75     |
| 23:BB:1092:C:OP1   | 23:BB:2475:C:H4'   | 1.86        | 0.75     |
| 50:DT:21:SER:O     | 50:DT:25:GLU:HB2   | 1.86        | 0.75     |
| 20:AB:96:LEU:HD21  | 20:AB:146:SER:HB2  | 1.69        | 0.75     |
| 26:BD:37:VAL:HG23  | 26:BD:91:THR:HA    | 1.68        | 0.75     |
| 35:DV:4:ILE:HB     | 35:DV:63:ILE:HA    | 1.68        | 0.75     |
| 12:CM:38:ILE:HG13  | 12:CM:55:LEU:HD21  | 1.69        | 0.75     |
| 3:AD:137:SER:HB2   | 3:AD:138:PRO:HD2   | 1.67        | 0.75     |
| 51:DZ:17:ASN:HB2   | 51:DZ:25:THR:OG1   | 1.86        | 0.75     |
| 1:CA:1299:A:H2'    | 1:CA:1301:U:H1'    | 1.67        | 0.75     |
| 20:AB:120:SER:HA   | 20:AB:125:PHE:HB3  | 1.69        | 0.75     |
| 47:DF:163:GLU:HA   | 47:DF:166:ARG:HH11 | 1.51        | 0.75     |
| 8:CI:24:ASN:ND2    | 8:CI:25:GLY:H      | 1.85        | 0.75     |
| 12:CM:70:ARG:HH21  | 47:DF:136:ILE:HB   | 1.51        | 0.75     |
| 37:DL:56:PRO:HD2   | 37:DL:59:ARG:HG3   | 1.68        | 0.75     |
| 32:D4:23:ILE:HB    | 32:D4:38:GLY:HA3   | 1.69        | 0.75     |
| 48:BG:84:LYS:HG2   | 48:BG:85:LYS:H     | 1.52        | 0.75     |
| 53:D6:43:VAL:HG21  | 53:D6:52:LEU:HD12  | 1.69        | 0.75     |
| 50:BT:29:THR:HA    | 50:BT:86:THR:HA    | 1.69        | 0.75     |
| 53:D6:174:GLN:HE22 | 53:D6:175:LEU:HD12 | 1.49        | 0.75     |
| 8:CI:87:MET:HG2    | 8:CI:91:GLU:HG2    | 1.68        | 0.75     |
| 26:DD:10:GLY:HA3   | 26:DD:26:VAL:H     | 1.50        | 0.75     |
| 38:DM:114:ARG:HB2  | 38:DM:114:ARG:HH21 | 1.51        | 0.75     |
| 16:CQ:57:VAL:HB    | 16:CQ:79:GLU:HB3   | 1.69        | 0.75     |
| 45:BS:81:SER:HA    | 45:BS:99:ARG:HA    | 1.69        | 0.75     |
| 26:BD:106:LYS:HB3  | 26:BD:206:ALA:H    | 1.51        | 0.74     |
| 24:DI:55:PRO:HD3   | 24:DI:74:PRO:HD3   | 1.68        | 0.74     |
| 48:DG:166:GLU:HG2  | 48:DG:168:VAL:HG23 | 1.68        | 0.74     |
| 27:DK:102:PRO:HA   | 27:DK:120:PRO:HB3  | 1.69        | 0.74     |
| 28:BP:4:ILE:HG22   | 28:BP:5:LYS:H      | 1.51        | 0.74     |
| 45:DS:81:SER:HA    | 45:DS:99:ARG:HA    | 1.68        | 0.74     |
| 16:AQ:57:VAL:HB    | 16:AQ:79:GLU:HB3   | 1.67        | 0.74     |
| 44:DQ:26:ALA:O     | 44:DQ:30:VAL:HG12  | 1.86        | 0.74     |
| 53:D6:53:ASN:HD22  | 53:D6:53:ASN:H     | 1.35        | 0.74     |
| 53:D6:53:ASN:ND2   | 53:D6:53:ASN:H     | 1.83        | 0.74     |
| 23:DB:137:U:H2'    | 23:DB:138:U:O4'    | 1.87        | 0.74     |
| 50:DT:29:THR:HA    | 50:DT:86:THR:HA    | 1.69        | 0.74     |
| 23:BB:1082:U:N3    | 23:BB:1086:A:C2    | 2.55        | 0.74     |
| 1:AA:1338:G:H2'    | 1:AA:1339:A:C8     | 2.22        | 0.74     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 39:DX:31:GLN:HG2  | 39:DX:37:LEU:HB2   | 1.67        | 0.74     |
| 27:DK:41:ILE:HG13 | 27:DK:42:THR:N     | 2.02        | 0.74     |
| 23:BB:172:A:H2'   | 23:BB:173:A:H8     | 1.51        | 0.74     |
| 23:DB:1324:G:H1'  | 23:DB:1616:A:N6    | 2.01        | 0.74     |
| 43:DO:5:SER:HA    | 43:DO:8:ILE:HD12   | 1.69        | 0.74     |
| 1:CA:1004:A:H2'   | 1:CA:1005:A:O4'    | 1.87        | 0.74     |
| 25:DC:43:ASN:ND2  | 25:DC:44:ASN:H     | 1.85        | 0.74     |
| 25:DC:91:ALA:HB2  | 25:DC:105:ALA:HB2  | 1.68        | 0.74     |
| 48:DG:9:VAL:HG12  | 48:DG:11:PRO:HD3   | 1.67        | 0.74     |
| 26:DD:30:GLU:HG3  | 26:DD:52:THR:HG22  | 1.68        | 0.74     |
| 21:AU:3:ILE:HD13  | 21:AU:19:LYS:HA    | 1.69        | 0.74     |
| 23:BB:1081:U:H5'  | 24:BI:126:ARG:HD2  | 1.69        | 0.74     |
| 26:DD:114:LYS:HB2 | 26:DD:116:LYS:HE3  | 1.69        | 0.74     |
| 23:DB:1447:C:H2'  | 23:DB:1448:G:H8    | 1.52        | 0.74     |
| 1:CA:270:A:H2'    | 1:CA:271:C:C6      | 2.22        | 0.74     |
| 49:DR:31:GLU:H    | 49:DR:63:VAL:HG22  | 1.53        | 0.74     |
| 37:BL:103:ILE:H   | 37:BL:103:ILE:HD12 | 1.50        | 0.74     |
| 8:AI:117:LEU:HD22 | 8:AI:123:ARG:HG2   | 1.70        | 0.74     |
| 20:CB:122:ASP:OD2 | 20:CB:124:THR:HG22 | 1.87        | 0.74     |
| 23:DB:2331:G:O2'  | 52:DW:40:ARG:HB2   | 1.87        | 0.74     |
| 43:DO:51:ALA:HB3  | 43:DO:78:VAL:HG22  | 1.70        | 0.74     |
| 8:AI:87:MET:HG2   | 8:AI:91:GLU:HG2    | 1.69        | 0.74     |
| 23:BB:873:C:H4'   | 38:BM:64:TRP:HE1   | 1.51        | 0.74     |
| 23:BB:1412:U:H2'  | 23:BB:1413:A:C8    | 2.21        | 0.74     |
| 38:DM:19:GLY:H    | 38:DM:38:ARG:HH12  | 1.35        | 0.74     |
| 45:DS:43:ALA:HA   | 45:DS:46:LEU:HD12  | 1.69        | 0.74     |
| 53:D6:110:ARG:HB3 | 53:D6:110:ARG:HH11 | 1.51        | 0.74     |
| 1:AA:108:G:H5'    | 1:AA:109:A:H5''    | 1.68        | 0.74     |
| 23:DB:172:A:H2'   | 23:DB:173:A:C8     | 2.22        | 0.74     |
| 28:DP:89:GLY:HA2  | 28:DP:112:ARG:N    | 2.03        | 0.74     |
| 1:CA:673:A:H2'    | 1:CA:674:G:C8      | 2.21        | 0.74     |
| 23:DB:580:U:H2'   | 23:DB:581:C:C6     | 2.22        | 0.74     |
| 8:AI:23:GLY:H     | 8:AI:60:LEU:HA     | 1.52        | 0.74     |
| 40:BH:105:ALA:HB3 | 40:BH:108:VAL:HG21 | 1.68        | 0.74     |
| 44:BQ:86:SER:HB2  | 49:BR:51:VAL:HA    | 1.70        | 0.74     |
| 1:AA:269:C:H2'    | 1:AA:270:A:C8      | 2.23        | 0.74     |
| 1:CA:108:G:H5'    | 1:CA:109:A:H5''    | 1.70        | 0.74     |
| 23:DB:1911:U:H2'  | 23:DB:1918:A:N1    | 2.02        | 0.74     |
| 23:BB:2425:A:H5'  | 23:BB:2427:C:O4'   | 1.88        | 0.74     |
| 48:BG:15:ASP:HB3  | 48:BG:25:ILE:HA    | 1.68        | 0.74     |
| 23:BB:287:G:H2'   | 23:BB:288:U:H6     | 1.52        | 0.74     |
| 23:DB:1437:C:H2'  | 23:DB:1438:U:C6    | 2.21        | 0.74     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 5:CF:98:GLU:HG2   | 5:CF:99:ALA:N      | 2.03        | 0.74     |
| 2:AC:154:GLY:HA3  | 2:AC:162:ALA:HB1   | 1.69        | 0.74     |
| 23:DB:775:G:H4'   | 23:DB:776:G:H5'    | 1.69        | 0.74     |
| 10:AK:24:ALA:HA   | 10:AK:29:THR:HG23  | 1.69        | 0.74     |
| 1:AA:1011:C:H2'   | 1:AA:1012:A:C8     | 2.21        | 0.74     |
| 23:DB:1804:C:OP1  | 25:DC:256:THR:HB   | 1.88        | 0.74     |
| 29:DE:155:GLU:HA  | 29:DE:158:PHE:HB3  | 1.67        | 0.74     |
| 23:BB:923:G:H1'   | 52:BW:23:LYS:HZ2   | 1.51        | 0.74     |
| 7:CH:77:VAL:HG23  | 7:CH:126:CYS:HA    | 1.69        | 0.74     |
| 42:DN:38:LEU:HB3  | 42:DN:39:PRO:HD3   | 1.69        | 0.74     |
| 36:B2:21:ARG:HG2  | 36:B2:31:LEU:HG    | 1.67        | 0.74     |
| 36:D2:34:ARG:HB3  | 36:D2:39:ARG:HB2   | 1.67        | 0.74     |
| 1:CA:33:A:H2'     | 1:CA:34:C:H6       | 1.52        | 0.74     |
| 23:BB:62:U:H3'    | 23:BB:63:A:C8      | 2.23        | 0.74     |
| 53:B6:102:ASN:N   | 53:B6:102:ASN:HD22 | 1.86        | 0.74     |
| 47:BF:31:GLU:HB3  | 47:BF:156:THR:O    | 1.87        | 0.74     |
| 8:CI:23:GLY:H     | 8:CI:60:LEU:HA     | 1.53        | 0.74     |
| 53:B6:84:ARG:HA   | 53:B6:89:GLY:HA2   | 1.70        | 0.74     |
| 35:BV:72:VAL:HG12 | 35:BV:94:ALA:H     | 1.53        | 0.74     |
| 29:BE:29:HIS:NE2  | 37:BL:8:PRO:HG3    | 2.02        | 0.74     |
| 19:CT:2:ASN:ND2   | 19:CT:3:ILE:H      | 1.86        | 0.74     |
| 23:DB:172:A:H2'   | 23:DB:173:A:H8     | 1.53        | 0.74     |
| 27:DK:53:LYS:H    | 27:DK:53:LYS:HD3   | 1.53        | 0.74     |
| 51:BZ:14:THR:HA   | 51:BZ:28:ARG:HA    | 1.70        | 0.74     |
| 51:DZ:76:GLU:HG3  | 51:DZ:77:LYS:H     | 1.52        | 0.74     |
| 41:DJ:24:THR:HA   | 41:DJ:63:ALA:HB3   | 1.70        | 0.74     |
| 47:BF:102:LEU:HA  | 47:BF:106:ALA:CB   | 2.17        | 0.74     |
| 21:CU:24:LYS:HD2  | 21:CU:25:ALA:H     | 1.50        | 0.74     |
| 44:BQ:4:LYS:NZ    | 44:BQ:7:VAL:HG22   | 2.03        | 0.74     |
| 1:AA:270:A:H2'    | 1:AA:271:C:C6      | 2.22        | 0.74     |
| 23:BB:775:G:H4'   | 23:BB:776:G:H5'    | 1.69        | 0.74     |
| 31:B0:31:LYS:HD2  | 31:B0:31:LYS:H     | 1.52        | 0.74     |
| 23:BB:181:A:H2'   | 23:BB:182:A:C8     | 2.23        | 0.74     |
| 33:B1:7:LYS:HD3   | 34:B3:33:THR:HG21  | 1.68        | 0.74     |
| 6:CG:78:ARG:HG2   | 6:CG:83:THR:HG22   | 1.67        | 0.74     |
| 2:CC:129:PHE:HE2  | 2:CC:165:GLU:HG2   | 1.53        | 0.74     |
| 3:AD:103:ARG:HH21 | 3:AD:110:ARG:HH22  | 1.35        | 0.74     |
| 1:AA:93:U:H5''    | 1:AA:94:G:OP2      | 1.88        | 0.74     |
| 53:D6:109:GLU:HA  | 53:D6:112:LYS:HE3  | 1.69        | 0.74     |
| 23:DB:191:A:H2'   | 23:DB:192:C:C6     | 2.22        | 0.74     |
| 23:DB:1579:A:H2'  | 23:DB:1580:A:C8    | 2.23        | 0.74     |
| 20:AB:187:ASP:OD1 | 20:AB:203:ASP:HB3  | 1.87        | 0.74     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 8:AI:38:PHE:HZ    | 8:AI:74:GLN:HB3    | 1.51        | 0.74     |
| 26:DD:5:VAL:H     | 26:DD:32:ASN:ND2   | 1.84        | 0.74     |
| 3:CD:25:ARG:HD3   | 3:CD:26:ALA:N      | 2.03        | 0.74     |
| 23:BB:2393:U:H5'  | 37:BL:62:PRO:HG3   | 1.67        | 0.74     |
| 19:AT:2:ASN:ND2   | 19:AT:3:ILE:H      | 1.86        | 0.74     |
| 23:DB:1082:U:N3   | 23:DB:1086:A:C2    | 2.55        | 0.74     |
| 38:BM:36:VAL:HB   | 38:BM:127:LYS:O    | 1.88        | 0.74     |
| 23:BB:38:A:O2'    | 29:BE:43:THR:HA    | 1.87        | 0.74     |
| 1:AA:41:G:H2'     | 1:AA:42:G:C8       | 2.23        | 0.74     |
| 2:AC:26:LYS:HG3   | 2:AC:27:GLU:H      | 1.53        | 0.74     |
| 23:DB:276:U:H3    | 23:DB:362:A:H61    | 1.36        | 0.74     |
| 1:AA:320:A:H2'    | 1:AA:321:A:C8      | 2.23        | 0.74     |
| 12:CM:9:PRO:HB2   | 12:CM:17:ALA:HB1   | 1.70        | 0.73     |
| 20:CB:96:LEU:H    | 20:CB:99:MET:HE3   | 1.53        | 0.73     |
| 20:AB:27:LYS:HA   | 20:AB:30:ILE:HD12  | 1.68        | 0.73     |
| 48:BG:155:PRO:HA  | 48:BG:170:THR:HG22 | 1.70        | 0.73     |
| 5:AF:38:ARG:HH21  | 5:AF:63:ASN:ND2    | 1.85        | 0.73     |
| 40:BH:90:LEU:HD11 | 40:BH:146:VAL:HG12 | 1.69        | 0.73     |
| 40:DH:6:LEU:HD13  | 40:DH:36:ALA:HA    | 1.69        | 0.73     |
| 44:DQ:4:LYS:NZ    | 44:DQ:7:VAL:HG22   | 2.03        | 0.73     |
| 23:DB:62:U:H3'    | 23:DB:63:A:C8      | 2.22        | 0.73     |
| 23:BB:1790:C:O2'  | 25:BC:207:ALA:HB2  | 1.89        | 0.73     |
| 52:DW:35:ILE:HA   | 52:DW:57:THR:HG23  | 1.69        | 0.73     |
| 48:DG:84:LYS:HG2  | 48:DG:85:LYS:H     | 1.51        | 0.73     |
| 37:BL:79:LEU:HB2  | 37:BL:113:ALA:H    | 1.52        | 0.73     |
| 1:CA:812:G:O2'    | 1:CA:813:U:H6      | 1.69        | 0.73     |
| 23:BB:2267:A:C8   | 23:BB:2267:A:C3'   | 2.71        | 0.73     |
| 27:DK:71:ARG:HG3  | 27:DK:105:ARG:HH21 | 1.53        | 0.73     |
| 23:DB:2078:C:H2'  | 23:DB:2079:U:C6    | 2.24        | 0.73     |
| 23:DB:1098:A:H2'  | 24:DI:4:VAL:CA     | 2.18        | 0.73     |
| 6:AG:145:GLU:HA   | 6:AG:148:LYS:HB2   | 1.69        | 0.73     |
| 40:BH:78:VAL:HG21 | 40:BH:142:VAL:HG12 | 1.67        | 0.73     |
| 8:AI:34:LEU:HD11  | 8:AI:47:VAL:HG21   | 1.69        | 0.73     |
| 42:BN:38:LEU:HB3  | 42:BN:39:PRO:HD3   | 1.69        | 0.73     |
| 47:BF:110:ILE:HA  | 47:BF:111:ARG:CZ   | 2.19        | 0.73     |
| 10:AK:83:VAL:HB   | 10:AK:109:ILE:HG23 | 1.68        | 0.73     |
| 18:AS:4:LEU:HD11  | 18:AS:9:PHE:HB3    | 1.68        | 0.73     |
| 46:BU:12:VAL:HA   | 46:BU:69:VAL:HA    | 1.69        | 0.73     |
| 49:BR:4:VAL:O     | 49:BR:38:VAL:HA    | 1.88        | 0.73     |
| 46:DU:35:VAL:HB   | 46:DU:38:ILE:HG21  | 1.71        | 0.73     |
| 1:CA:715:A:H2'    | 1:CA:716:A:H8      | 1.54        | 0.73     |
| 1:AA:1057:G:H4'   | 2:AC:196:GLY:H     | 1.52        | 0.73     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 43:BO:5:SER:HA    | 43:BO:8:ILE:HD12  | 1.70        | 0.73     |
| 25:DC:91:ALA:CB   | 25:DC:105:ALA:HB2 | 2.18        | 0.73     |
| 53:D6:80:GLU:HA   | 53:D6:83:ILE:HG12 | 1.69        | 0.73     |
| 8:CI:25:GLY:HA2   | 8:CI:60:LEU:O     | 1.89        | 0.73     |
| 38:DM:35:ALA:HB3  | 38:DM:99:GLY:N    | 2.04        | 0.73     |
| 4:CE:35:LEU:HD21  | 4:CE:136:VAL:HG11 | 1.70        | 0.73     |
| 24:DI:20:SER:HB3  | 24:DI:21:PRO:HD3  | 1.68        | 0.73     |
| 23:BB:2443:C:H2'  | 23:BB:2444:G:H8   | 1.53        | 0.73     |
| 28:DP:4:ILE:HG22  | 28:DP:5:LYS:H     | 1.54        | 0.73     |
| 40:BH:125:THR:HA  | 40:BH:146:VAL:HB  | 1.70        | 0.73     |
| 1:CA:1412:C:H2'   | 1:CA:1413:A:C8    | 2.23        | 0.73     |
| 23:DB:62:U:C2'    | 23:DB:63:A:H5'    | 2.19        | 0.73     |
| 23:BB:773:U:H5'   | 23:BB:774:G:OP2   | 1.87        | 0.73     |
| 14:CO:24:SER:HB3  | 14:CO:27:VAL:HG23 | 1.70        | 0.73     |
| 37:DL:79:LEU:HB2  | 37:DL:113:ALA:H   | 1.50        | 0.73     |
| 13:CN:68:ARG:HH12 | 13:CN:70:HIS:HB2  | 1.54        | 0.73     |
| 53:B6:108:GLU:HA  | 53:B6:111:ARG:HB2 | 1.70        | 0.73     |
| 23:BB:2769:U:H2'  | 23:BB:2770:G:C8   | 2.23        | 0.73     |
| 1:AA:85:U:O3'     | 1:AA:86:G:H4'     | 1.89        | 0.73     |
| 46:DU:26:ASN:N    | 46:DU:26:ASN:HD22 | 1.85        | 0.73     |
| 31:D0:31:LYS:H    | 31:D0:31:LYS:HD2  | 1.54        | 0.73     |
| 26:BD:68:PHE:HB3  | 26:BD:73:VAL:HG23 | 1.71        | 0.73     |
| 23:DB:558:U:OP1   | 41:DJ:113:PRO:HG2 | 1.89        | 0.73     |
| 46:DU:58:VAL:HG12 | 46:DU:59:GLU:H    | 1.52        | 0.73     |
| 27:DK:35:VAL:HG23 | 27:DK:36:GLY:N    | 2.02        | 0.73     |
| 47:DF:110:ILE:HA  | 47:DF:111:ARG:CZ  | 2.18        | 0.73     |
| 23:BB:1548:A:H2'  | 23:BB:1549:A:C8   | 2.24        | 0.73     |
| 46:BU:34:ILE:HG12 | 46:BU:63:ALA:HB2  | 1.71        | 0.73     |
| 23:DB:181:A:H2'   | 23:DB:182:A:C8    | 2.24        | 0.73     |
| 21:AU:10:PRO:HB2  | 2:CC:71:ARG:HD3   | 1.71        | 0.73     |
| 25:DC:143:VAL:HB  | 25:DC:153:LEU:HB2 | 1.69        | 0.73     |
| 47:DF:62:GLN:HG3  | 47:DF:91:ARG:NH1  | 2.02        | 0.73     |
| 8:CI:20:ILE:HD13  | 8:CI:85:ALA:HB3   | 1.69        | 0.73     |
| 29:BE:58:LYS:HZ3  | 29:BE:58:LYS:H    | 1.37        | 0.73     |
| 26:DD:37:VAL:HG23 | 26:DD:91:THR:HA   | 1.70        | 0.73     |
| 23:BB:1104:C:H2'  | 23:BB:1105:U:C6   | 2.24        | 0.73     |
| 23:BB:1324:G:H1'  | 23:BB:1616:A:N6   | 2.04        | 0.73     |
| 7:CH:49:LYS:HB3   | 7:CH:59:GLU:HB2   | 1.69        | 0.73     |
| 40:DH:115:VAL:HB  | 40:DH:132:PHE:CD1 | 2.23        | 0.73     |
| 52:BW:35:ILE:HA   | 52:BW:57:THR:HG23 | 1.71        | 0.73     |
| 40:BH:97:ARG:HA   | 40:BH:112:LYS:HB2 | 1.70        | 0.73     |
| 25:BC:91:ALA:HB2  | 25:BC:105:ALA:HB2 | 1.69        | 0.73     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 37:BL:56:PRO:HD2   | 37:BL:59:ARG:HG3   | 1.68        | 0.73     |
| 13:AN:30:ILE:HG22  | 13:AN:41:TRP:HB2   | 1.71        | 0.73     |
| 13:CN:30:ILE:HG22  | 13:CN:41:TRP:HB2   | 1.71        | 0.73     |
| 26:BD:24:VAL:HG21  | 26:BD:188:LEU:HB3  | 1.71        | 0.73     |
| 23:DB:1681:G:N3    | 23:DB:1762:A:H2'   | 2.03        | 0.73     |
| 23:DB:1131:G:N2    | 23:DB:2024:G:H21   | 1.87        | 0.73     |
| 11:CL:51:VAL:HG12  | 11:CL:52:CYS:H     | 1.52        | 0.73     |
| 1:AA:973:G:H3'     | 1:AA:974:A:H5''    | 1.69        | 0.73     |
| 48:BG:115:GLN:CD   | 48:BG:115:GLN:H    | 1.91        | 0.73     |
| 23:DB:2144:G:O2'   | 23:DB:2145:C:H5'   | 1.89        | 0.73     |
| 29:DE:148:ILE:HD13 | 29:DE:187:VAL:HG21 | 1.69        | 0.73     |
| 25:BC:144:GLU:HB3  | 25:BC:187:CYS:HB3  | 1.71        | 0.72     |
| 1:AA:1216:A:H5''   | 13:AN:4:SER:HB3    | 1.69        | 0.72     |
| 47:DF:66:ILE:HD11  | 47:DF:83:PRO:HB3   | 1.71        | 0.72     |
| 42:BN:102:PHE:H    | 42:BN:109:PRO:HA   | 1.52        | 0.72     |
| 24:BI:20:SER:HB3   | 24:BI:21:PRO:HD3   | 1.69        | 0.72     |
| 23:BB:280:U:H2'    | 23:BB:281:C:C6     | 2.24        | 0.72     |
| 1:AA:1004:A:H2'    | 1:AA:1005:A:O4'    | 1.89        | 0.72     |
| 5:AF:98:GLU:HG2    | 5:AF:99:ALA:N      | 2.03        | 0.72     |
| 23:BB:1681:G:N3    | 23:BB:1762:A:H2'   | 2.03        | 0.72     |
| 51:BZ:17:ASN:HB2   | 51:BZ:25:THR:OG1   | 1.89        | 0.72     |
| 23:DB:1099:G:O4'   | 24:DI:3:LYS:C      | 2.27        | 0.72     |
| 8:AI:26:LYS:N      | 8:AI:61:ASP:HB3    | 2.03        | 0.72     |
| 50:BT:11:LEU:HD22  | 50:BT:11:LEU:H     | 1.54        | 0.72     |
| 12:AM:49:GLU:O     | 12:AM:52:ILE:HG22  | 1.87        | 0.72     |
| 10:CK:28:ASN:HD21  | 10:CK:47:GLY:H     | 1.37        | 0.72     |
| 1:CA:973:G:H3'     | 1:CA:974:A:H5''    | 1.70        | 0.72     |
| 8:CI:34:LEU:HD11   | 8:CI:47:VAL:HG21   | 1.71        | 0.72     |
| 26:DD:51:THR:HG21  | 26:DD:76:GLY:HA3   | 1.71        | 0.72     |
| 25:BC:91:ALA:CB    | 25:BC:105:ALA:HB2  | 2.19        | 0.72     |
| 43:BO:89:ASP:HA    | 43:BO:116:GLN:O    | 1.89        | 0.72     |
| 23:BB:2734:A:H2'   | 23:BB:2735:G:H5'   | 1.71        | 0.72     |
| 1:CA:269:C:H2'     | 1:CA:270:A:C8      | 2.25        | 0.72     |
| 3:AD:103:ARG:HH21  | 3:AD:110:ARG:NH2   | 1.87        | 0.72     |
| 14:AO:89:ARG:HA    | 14:AO:89:ARG:HH11  | 1.54        | 0.72     |
| 12:AM:9:PRO:HB2    | 12:AM:17:ALA:HB1   | 1.70        | 0.72     |
| 23:DB:90:U:H3'     | 23:DB:91:A:H5''    | 1.69        | 0.72     |
| 10:AK:45:THR:HG23  | 10:AK:48:GLY:HA3   | 1.71        | 0.72     |
| 28:BP:26:GLU:HB3   | 28:BP:84:SER:HB3   | 1.70        | 0.72     |
| 1:CA:41:G:H2'      | 1:CA:42:G:C8       | 2.23        | 0.72     |
| 10:CK:45:THR:HG23  | 10:CK:48:GLY:HA3   | 1.71        | 0.72     |
| 35:BV:42:LEU:HD23  | 35:BV:42:LEU:H     | 1.55        | 0.72     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:90:U:H3'     | 23:BB:91:A:H5''    | 1.70        | 0.72     |
| 53:D6:84:ARG:H     | 53:D6:84:ARG:NE    | 1.88        | 0.72     |
| 52:DW:49:ASN:HB2   | 52:DW:61:LYS:H     | 1.54        | 0.72     |
| 24:BI:77:VAL:HA    | 24:BI:80:LYS:HE2   | 1.72        | 0.72     |
| 1:CA:946:A:H2'     | 1:CA:947:G:C8      | 2.23        | 0.72     |
| 18:CS:48:ILE:HG22  | 18:CS:49:ALA:H     | 1.54        | 0.72     |
| 24:BI:122:GLU:O    | 24:BI:126:ARG:HG3  | 1.89        | 0.72     |
| 22:BA:75:G:H1      | 22:BA:102:G:N2     | 1.88        | 0.72     |
| 23:BB:616:A:H3'    | 23:BB:617:G:H8     | 1.54        | 0.72     |
| 23:DB:2548:U:H1'   | 27:DK:23:LYS:HZ1   | 1.53        | 0.72     |
| 23:DB:1778:U:H2'   | 23:DB:1784:A:H62   | 1.54        | 0.72     |
| 9:AJ:44:THR:HG23   | 9:AJ:69:THR:O      | 1.90        | 0.72     |
| 2:AC:59:PRO:HG2    | 2:AC:62:SER:OG     | 1.89        | 0.72     |
| 21:AU:40:PRO:HA    | 21:AU:44:ARG:HD3   | 1.72        | 0.72     |
| 48:BG:17:LYS:HB3   | 48:BG:24:THR:H     | 1.54        | 0.72     |
| 51:BZ:76:GLU:HG3   | 51:BZ:77:LYS:H     | 1.53        | 0.72     |
| 23:BB:322:A:C3'    | 29:BE:163:ASN:HD21 | 2.03        | 0.72     |
| 23:DB:2267:A:C8    | 23:DB:2267:A:C3'   | 2.71        | 0.72     |
| 26:DD:186:LEU:HD11 | 28:DP:3:ILE:HG13   | 1.72        | 0.72     |
| 23:BB:62:U:C2'     | 23:BB:63:A:H5'     | 2.19        | 0.72     |
| 20:CB:96:LEU:HD21  | 20:CB:146:SER:HB2  | 1.72        | 0.72     |
| 10:AK:105:ARG:NH2  | 21:AU:10:PRO:HB3   | 2.05        | 0.72     |
| 49:BR:24:LYS:HA    | 49:BR:94:THR:HG23  | 1.71        | 0.72     |
| 23:DB:215:G:H4'    | 23:DB:216:A:H4'    | 1.71        | 0.72     |
| 43:BO:76:LYS:O     | 43:BO:80:GLU:HG2   | 1.90        | 0.72     |
| 51:DZ:14:THR:HA    | 51:DZ:28:ARG:HA    | 1.72        | 0.72     |
| 23:BB:191:A:H2'    | 23:BB:192:C:C6     | 2.24        | 0.72     |
| 9:AJ:36:VAL:HG22   | 9:AJ:76:ILE:HG22   | 1.70        | 0.72     |
| 23:BB:2155:U:H2'   | 23:BB:2156:G:O4'   | 1.90        | 0.72     |
| 27:DK:58:LEU:HD11  | 27:DK:86:LEU:HB3   | 1.70        | 0.72     |
| 48:DG:9:VAL:HA     | 48:DG:48:THR:HG22  | 1.69        | 0.72     |
| 47:DF:34:THR:HG22  | 47:DF:89:THR:HG22  | 1.72        | 0.72     |
| 50:BT:21:SER:O     | 50:BT:25:GLU:HB2   | 1.88        | 0.72     |
| 1:CA:17:U:H2'      | 1:CA:18:C:C6       | 2.24        | 0.72     |
| 22:BA:32:U:H1'     | 22:BA:52:A:N7      | 2.05        | 0.72     |
| 44:BQ:104:ALA:HA   | 49:BR:46:GLU:CD    | 2.10        | 0.72     |
| 1:CA:706:A:H4'     | 10:CK:30:ILE:HD11  | 1.72        | 0.72     |
| 20:CB:60:ALA:HA    | 20:CB:64:GLY:HA3   | 1.70        | 0.72     |
| 20:AB:96:LEU:H     | 20:AB:99:MET:HE3   | 1.53        | 0.72     |
| 49:DR:31:GLU:H     | 49:DR:63:VAL:CG2   | 2.02        | 0.72     |
| 23:DB:2720:U:H5''  | 28:DP:52:ARG:HH21  | 1.54        | 0.72     |
| 23:BB:2722:G:H4'   | 42:BN:4:ARG:HB2    | 1.70        | 0.72     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:CD:90:LEU:HA     | 3:CD:93:LEU:HD12   | 1.71        | 0.72     |
| 23:DB:2795:C:H2'   | 23:DB:2796:U:O4'   | 1.90        | 0.72     |
| 26:BD:111:GLY:H    | 26:BD:194:PRO:CG   | 2.02        | 0.72     |
| 20:CB:187:ASP:OD1  | 20:CB:203:ASP:HB3  | 1.90        | 0.72     |
| 3:CD:24:VAL:HG23   | 3:CD:25:ARG:H      | 1.54        | 0.72     |
| 23:DB:1060:U:C4    | 23:DB:1088:A:N6    | 2.58        | 0.72     |
| 23:BB:1076:C:H4'   | 24:BI:94:LYS:CE    | 2.19        | 0.72     |
| 23:DB:1080:A:H4'   | 24:DI:126:ARG:CD   | 2.19        | 0.72     |
| 23:DB:98:G:H2'     | 23:DB:99:U:H5''    | 1.71        | 0.72     |
| 23:DB:1558:C:H4'   | 23:DB:1559:U:H5'   | 1.69        | 0.72     |
| 2:CC:154:GLY:HA3   | 2:CC:162:ALA:HB1   | 1.70        | 0.72     |
| 23:DB:2052:A:O4'   | 26:DD:147:GLY:HA3  | 1.90        | 0.72     |
| 23:BB:1210:G:H5'   | 23:BB:1212:G:O4'   | 1.90        | 0.72     |
| 23:BB:580:U:H2'    | 23:BB:581:C:C6     | 2.24        | 0.72     |
| 4:AE:44:ARG:HA     | 4:AE:71:ILE:O      | 1.90        | 0.72     |
| 23:BB:858:G:N3     | 23:BB:2268:A:H2'   | 2.04        | 0.72     |
| 53:B6:32:ARG:NH1   | 53:B6:88:LEU:HD23  | 2.04        | 0.72     |
| 51:DZ:6:GLN:NE2    | 51:DZ:50:ARG:H     | 1.87        | 0.72     |
| 48:DG:17:LYS:HB3   | 48:DG:24:THR:H     | 1.54        | 0.72     |
| 13:AN:68:ARG:HH12  | 13:AN:70:HIS:HB2   | 1.54        | 0.72     |
| 1:AA:1361:G:H2'    | 1:AA:1362:A:H5''   | 1.72        | 0.72     |
| 24:DI:105:LEU:HD11 | 24:DI:139:VAL:HG21 | 1.69        | 0.72     |
| 26:BD:114:LYS:HB2  | 26:BD:116:LYS:HE3  | 1.72        | 0.72     |
| 1:AA:337:G:H2'     | 1:AA:338:A:C8      | 2.25        | 0.72     |
| 29:DE:194:LYS:O    | 29:DE:197:GLU:HB3  | 1.90        | 0.72     |
| 1:AA:552:U:H5'     | 11:AL:82:ARG:HH11  | 1.53        | 0.72     |
| 23:BB:1804:C:OP1   | 25:BC:256:THR:HB   | 1.90        | 0.72     |
| 3:AD:94:GLU:HG2    | 3:AD:185:PRO:HG3   | 1.72        | 0.72     |
| 1:CA:301:G:H2'     | 1:CA:302:G:H8      | 1.54        | 0.72     |
| 43:DO:76:LYS:O     | 43:DO:80:GLU:HG2   | 1.88        | 0.72     |
| 23:DB:2189:U:H2'   | 23:DB:2190:G:H5''  | 1.70        | 0.72     |
| 1:AA:301:G:H2'     | 1:AA:302:G:H8      | 1.54        | 0.72     |
| 42:BN:24:MET:HE3   | 42:BN:44:LEU:HB2   | 1.71        | 0.72     |
| 14:AO:24:SER:HB3   | 14:AO:27:VAL:HG23  | 1.71        | 0.72     |
| 52:DW:35:ILE:HG13  | 52:DW:57:THR:OG1   | 1.90        | 0.72     |
| 23:DB:1287:A:H3'   | 23:DB:1288:G:N2    | 2.04        | 0.72     |
| 5:CF:38:ARG:HH21   | 5:CF:63:ASN:HD21   | 1.38        | 0.72     |
| 27:BK:112:PHE:O    | 27:BK:115:ILE:HG22 | 1.90        | 0.72     |
| 49:DR:24:LYS:HA    | 49:DR:94:THR:HG23  | 1.71        | 0.72     |
| 15:AP:26:ASN:HD21  | 15:AP:31:ARG:HD3   | 1.53        | 0.72     |
| 41:BJ:24:THR:HA    | 41:BJ:63:ALA:HB3   | 1.70        | 0.71     |
| 26:DD:106:LYS:HB3  | 26:DD:206:ALA:H    | 1.54        | 0.71     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 22:DA:28:C:N4      | 22:DA:56:G:N1      | 2.38        | 0.71     |
| 48:DG:26:LYS:HG2   | 48:DG:27:GLY:N     | 2.04        | 0.71     |
| 29:DE:60:TRP:O     | 29:DE:61:ARG:HB2   | 1.89        | 0.71     |
| 3:AD:25:ARG:HD3    | 3:AD:26:ALA:N      | 2.04        | 0.71     |
| 23:BB:320:A:H4'    | 23:BB:322:A:N7     | 2.05        | 0.71     |
| 1:AA:1369:C:H2'    | 1:AA:1370:G:C8     | 2.25        | 0.71     |
| 27:BK:41:ILE:HG13  | 27:BK:42:THR:N     | 2.03        | 0.71     |
| 39:DX:20:ASN:N     | 39:DX:20:ASN:HD22  | 1.88        | 0.71     |
| 25:DC:32:LEU:HD22  | 25:DC:63:ILE:HG13  | 1.72        | 0.71     |
| 23:DB:357:C:H2'    | 23:DB:358:U:C6     | 2.25        | 0.71     |
| 41:BJ:23:LYS:HE3   | 41:BJ:142:ILE:HG12 | 1.72        | 0.71     |
| 16:AQ:13:SER:HB3   | 16:AQ:21:VAL:HB    | 1.70        | 0.71     |
| 23:BB:1796:U:H2'   | 23:BB:1797:G:H8    | 1.55        | 0.71     |
| 12:AM:89:ARG:NH2   | 12:AM:94:LEU:HD12  | 2.05        | 0.71     |
| 53:D6:52:LEU:HD11  | 53:D6:79:ILE:HG23  | 1.72        | 0.71     |
| 42:DN:102:PHE:H    | 42:DN:109:PRO:HA   | 1.53        | 0.71     |
| 23:DB:1125:G:H4'   | 32:D4:37:GLN:NE2   | 2.04        | 0.71     |
| 26:DD:34:VAL:HA    | 26:DD:50:VAL:HG12  | 1.71        | 0.71     |
| 48:BG:71:LEU:HA    | 48:BG:74:MET:SD    | 2.30        | 0.71     |
| 23:BB:581:C:H2'    | 23:BB:582:A:C8     | 2.25        | 0.71     |
| 16:CQ:13:SER:HB3   | 16:CQ:21:VAL:HB    | 1.72        | 0.71     |
| 38:BM:114:ARG:HH21 | 38:BM:114:ARG:HB2  | 1.54        | 0.71     |
| 23:DB:773:U:H5'    | 23:DB:774:G:OP2    | 1.89        | 0.71     |
| 23:BB:2073:C:H5''  | 25:BC:227:VAL:HG12 | 1.72        | 0.71     |
| 4:CE:44:ARG:HA     | 4:CE:71:ILE:O      | 1.90        | 0.71     |
| 36:B2:30:VAL:HA    | 36:B2:33:ARG:NH2   | 2.04        | 0.71     |
| 48:BG:9:VAL:HA     | 48:BG:48:THR:HG22  | 1.71        | 0.71     |
| 23:DB:855:G:H21    | 52:DW:23:LYS:CG    | 2.03        | 0.71     |
| 13:AN:5:MET:HB3    | 13:AN:62:ARG:HH12  | 1.55        | 0.71     |
| 47:BF:78:ILE:H     | 47:BF:79:ARG:HH11  | 1.38        | 0.71     |
| 1:CA:1361:G:H2'    | 1:CA:1362:A:H5''   | 1.70        | 0.71     |
| 10:CK:31:VAL:HG21  | 10:CK:66:ALA:HA    | 1.72        | 0.71     |
| 29:DE:143:LEU:HB3  | 29:DE:146:VAL:HG21 | 1.72        | 0.71     |
| 27:BK:102:PRO:HA   | 27:BK:120:PRO:HB3  | 1.71        | 0.71     |
| 1:AA:22:G:H2'      | 1:AA:23:C:C6       | 2.25        | 0.71     |
| 3:AD:116:LEU:HB3   | 3:AD:122:ILE:HD11  | 1.71        | 0.71     |
| 1:CA:674:G:H2'     | 1:CA:675:A:H8      | 1.54        | 0.71     |
| 1:AA:1011:C:H2'    | 1:AA:1012:A:H8     | 1.55        | 0.71     |
| 23:DB:1365:A:OP2   | 51:DZ:3:ARG:HB2    | 1.90        | 0.71     |
| 6:AG:78:ARG:HG2    | 6:AG:83:THR:HG22   | 1.72        | 0.71     |
| 1:AA:674:G:H2'     | 1:AA:675:A:H8      | 1.55        | 0.71     |
| 1:CA:493:A:H5'     | 1:CA:494:G:OP2     | 1.91        | 0.71     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 20:CB:202:ASN:HD22 | 20:CB:203:ASP:N   | 1.88        | 0.71     |
| 51:BZ:5:CYS:HB3    | 51:BZ:10:LYS:N    | 2.04        | 0.71     |
| 1:AA:522:C:H41     | 11:AL:49:ARG:HH22 | 1.38        | 0.71     |
| 29:BE:60:TRP:O     | 29:BE:61:ARG:HB2  | 1.90        | 0.71     |
| 13:AN:11:LYS:O     | 13:AN:15:LEU:HG   | 1.91        | 0.71     |
| 10:AK:28:ASN:HD21  | 10:AK:47:GLY:H    | 1.38        | 0.71     |
| 1:CA:33:A:H2'      | 1:CA:34:C:C6      | 2.25        | 0.71     |
| 1:CA:1057:G:H4'    | 2:CC:196:GLY:H    | 1.53        | 0.71     |
| 46:BU:26:ASN:HD22  | 46:BU:26:ASN:N    | 1.85        | 0.71     |
| 1:AA:33:A:H2'      | 1:AA:34:C:H6      | 1.54        | 0.71     |
| 8:CI:117:LEU:HD22  | 8:CI:123:ARG:HG2  | 1.72        | 0.71     |
| 23:DB:1274:A:N3    | 23:DB:1297:C:H1'  | 2.05        | 0.71     |
| 41:DJ:73:VAL:HG23  | 41:DJ:74:TYR:H    | 1.56        | 0.71     |
| 22:BA:28:C:N4      | 22:BA:56:G:N1     | 2.38        | 0.71     |
| 50:DT:2:ILE:HB     | 50:DT:3:ARG:HD3   | 1.72        | 0.71     |
| 40:BH:108:VAL:HG12 | 40:BH:109:GLU:N   | 2.04        | 0.71     |
| 23:DB:784:G:O2'    | 23:DB:785:G:H5''  | 1.90        | 0.71     |
| 15:CP:40:ASN:HD21  | 15:CP:43:ALA:N    | 1.89        | 0.71     |
| 23:DB:320:A:H4'    | 23:DB:322:A:N7    | 2.04        | 0.71     |
| 1:AA:957:U:H4'     | 18:AS:78:THR:HB   | 1.71        | 0.71     |
| 1:CA:1216:A:H5''   | 13:CN:4:SER:HB3   | 1.69        | 0.71     |
| 41:BJ:3:THR:HG21   | 44:BQ:60:TRP:HE1  | 1.55        | 0.71     |
| 48:BG:26:LYS:HG2   | 48:BG:27:GLY:N    | 2.03        | 0.71     |
| 23:BB:1060:U:C4    | 23:BB:1088:A:N6   | 2.58        | 0.71     |
| 9:CJ:51:VAL:CG2    | 13:CN:80:ARG:HB2  | 2.21        | 0.71     |
| 23:DB:2741:A:H2'   | 23:DB:2742:G:O4'  | 1.89        | 0.71     |
| 23:BB:30:G:H2'     | 23:BB:31:C:C6     | 2.25        | 0.71     |
| 38:BM:19:GLY:HA2   | 38:BM:97:GLN:HB2  | 1.71        | 0.71     |
| 1:CA:41:G:H2'      | 1:CA:42:G:H8      | 1.55        | 0.71     |
| 14:AO:70:LEU:HD12  | 14:AO:78:TYR:HB2  | 1.71        | 0.71     |
| 12:CM:89:ARG:NH2   | 12:CM:94:LEU:HD12 | 2.04        | 0.71     |
| 23:BB:2615:U:H1'   | 31:B0:3:GLN:HB3   | 1.72        | 0.71     |
| 1:CA:195:A:H2'     | 1:CA:196:A:C8     | 2.25        | 0.71     |
| 1:CA:957:U:H4'     | 18:CS:78:THR:HB   | 1.71        | 0.71     |
| 2:CC:26:LYS:HG3    | 2:CC:27:GLU:H     | 1.56        | 0.71     |
| 10:CK:124:LYS:HA   | 21:CU:34:ARG:CB   | 2.18        | 0.71     |
| 53:B6:51:PRO:O     | 53:B6:55:ILE:HG22 | 1.91        | 0.71     |
| 38:BM:71:LYS:HD3   | 38:BM:95:LEU:HD13 | 1.73        | 0.71     |
| 40:DH:94:ILE:HG22  | 40:DH:122:LEU:HG  | 1.73        | 0.71     |
| 21:AU:24:LYS:HD2   | 21:AU:25:ALA:H    | 1.55        | 0.71     |
| 26:BD:186:LEU:HD11 | 28:BP:3:ILE:HG13  | 1.73        | 0.71     |
| 23:BB:2741:A:H2'   | 23:BB:2742:G:O4'  | 1.90        | 0.71     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2529:G:H5''  | 48:DG:174:LYS:HB2  | 1.72        | 0.71     |
| 23:BB:1138:G:H2'   | 23:BB:1139:G:O4'   | 1.91        | 0.71     |
| 42:DN:24:MET:HE3   | 42:DN:44:LEU:HB2   | 1.73        | 0.71     |
| 1:CA:927:G:H4'     | 1:CA:1503:A:N7     | 2.06        | 0.71     |
| 23:DB:1097:U:H2'   | 23:DB:1098:A:O4'   | 1.90        | 0.71     |
| 23:DB:2387:U:H1'   | 52:DW:38:ARG:CZ    | 2.21        | 0.71     |
| 21:CU:40:PRO:HA    | 21:CU:44:ARG:HD3   | 1.73        | 0.71     |
| 26:BD:105:LYS:HD2  | 26:BD:177:VAL:HG22 | 1.72        | 0.71     |
| 8:CI:5:TYR:HB2     | 8:CI:20:ILE:HB     | 1.72        | 0.71     |
| 18:CS:18:VAL:HG21  | 18:CS:43:MET:HB3   | 1.73        | 0.71     |
| 23:BB:571:U:H3'    | 49:BR:80:ARG:HH12  | 1.56        | 0.71     |
| 46:DU:11:ILE:HG22  | 46:DU:70:ALA:HB3   | 1.72        | 0.71     |
| 23:DB:2075:U:H2'   | 23:DB:2238:G:N2    | 2.06        | 0.71     |
| 39:BX:20:ASN:HD22  | 39:BX:20:ASN:N     | 1.89        | 0.71     |
| 1:AA:706:A:H4'     | 10:AK:30:ILE:HD11  | 1.72        | 0.71     |
| 23:DB:2602:A:H2'   | 23:DB:2602:A:N3    | 2.05        | 0.71     |
| 24:DI:85:ILE:HD13  | 24:DI:137:LEU:HD21 | 1.73        | 0.71     |
| 1:CA:320:A:H2'     | 1:CA:321:A:C8      | 2.25        | 0.71     |
| 25:BC:183:VAL:HG13 | 25:BC:185:ALA:H    | 1.55        | 0.71     |
| 25:DC:183:VAL:HG13 | 25:DC:185:ALA:H    | 1.55        | 0.71     |
| 40:BH:84:ALA:HA    | 40:BH:90:LEU:CA    | 2.21        | 0.71     |
| 50:BT:2:ILE:HB     | 50:BT:3:ARG:HD3    | 1.73        | 0.71     |
| 1:CA:522:C:H41     | 11:CL:49:ARG:HH22  | 1.38        | 0.71     |
| 23:BB:2264:C:H41   | 52:BW:11:ASN:ND2   | 1.89        | 0.71     |
| 23:DB:2107:G:H2'   | 23:DB:2108:A:C8    | 2.25        | 0.71     |
| 20:AB:60:ALA:HA    | 20:AB:64:GLY:HA3   | 1.71        | 0.71     |
| 49:DR:4:VAL:HG23   | 49:DR:39:LEU:H     | 1.55        | 0.71     |
| 4:AE:39:GLY:HA3    | 4:AE:116:VAL:HB    | 1.73        | 0.71     |
| 1:AA:1086:U:H3     | 1:AA:1099:G:H22    | 1.39        | 0.71     |
| 23:DB:858:G:N3     | 23:DB:2268:A:H2'   | 2.06        | 0.71     |
| 23:BB:2746:U:H4'   | 48:BG:137:LYS:HG3  | 1.71        | 0.71     |
| 28:BP:89:GLY:HA2   | 28:BP:112:ARG:N    | 2.06        | 0.71     |
| 2:AC:142:ARG:HH21  | 2:AC:143:LEU:HD21  | 1.54        | 0.71     |
| 23:BB:2602:A:N3    | 23:BB:2602:A:H2'   | 2.05        | 0.71     |
| 23:BB:2241:A:H2'   | 23:BB:2242:G:C8    | 2.26        | 0.71     |
| 52:BW:43:LYS:HB3   | 52:BW:58:LEU:HD11  | 1.73        | 0.71     |
| 22:DA:43:C:O2'     | 47:DF:91:ARG:HD2   | 1.91        | 0.71     |
| 1:CA:429:U:H3'     | 3:CD:8:LEU:HD23    | 1.71        | 0.71     |
| 51:BZ:71:LEU:HD13  | 51:BZ:76:GLU:HB3   | 1.72        | 0.71     |
| 29:BE:130:LYS:HB2  | 29:BE:133:LEU:HG   | 1.72        | 0.71     |
| 12:AM:38:ILE:HG13  | 12:AM:55:LEU:HD21  | 1.70        | 0.71     |
| 27:BK:71:ARG:HG3   | 27:BK:105:ARG:HH21 | 1.56        | 0.71     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 29:DE:130:LYS:HB2  | 29:DE:133:LEU:HG   | 1.71        | 0.71     |
| 14:CO:70:LEU:HD12  | 14:CO:78:TYR:HB2   | 1.71        | 0.71     |
| 28:DP:26:GLU:HB3   | 28:DP:84:SER:HB3   | 1.72        | 0.71     |
| 23:BB:1274:A:N3    | 23:BB:1297:C:H1'   | 2.05        | 0.71     |
| 19:CT:66:ILE:HG23  | 19:CT:70:LYS:HB3   | 1.73        | 0.71     |
| 52:BW:58:LEU:HD12  | 52:BW:79:ILE:HD12  | 1.73        | 0.70     |
| 23:DB:1790:C:H2'   | 23:DB:1791:A:C8    | 2.26        | 0.70     |
| 13:CN:11:LYS:O     | 13:CN:15:LEU:HG    | 1.92        | 0.70     |
| 38:DM:42:THR:HB    | 38:DM:45:GLN:HG3   | 1.73        | 0.70     |
| 23:DB:845:A:C2     | 23:DB:847:U:H1'    | 2.26        | 0.70     |
| 20:AB:113:LEU:HD12 | 20:AB:143:LEU:HB3  | 1.74        | 0.70     |
| 1:CA:1071:C:H2'    | 1:CA:1072:G:H8     | 1.55        | 0.70     |
| 26:BD:14:ILE:HG22  | 26:BD:22:ILE:O     | 1.90        | 0.70     |
| 23:BB:131:A:H2'    | 23:BB:132:G:H8     | 1.56        | 0.70     |
| 40:BH:78:VAL:HB    | 40:BH:143:ILE:HD12 | 1.73        | 0.70     |
| 23:BB:1458:U:C5'   | 23:BB:1459:G:H5'   | 2.21        | 0.70     |
| 40:DH:125:THR:HA   | 40:DH:146:VAL:HB   | 1.72        | 0.70     |
| 4:AE:15:ILE:HD12   | 4:AE:35:LEU:HG     | 1.73        | 0.70     |
| 34:D3:30:HIS:H     | 34:D3:32:LEU:HD21  | 1.56        | 0.70     |
| 23:BB:215:G:H4'    | 23:BB:216:A:H4'    | 1.73        | 0.70     |
| 23:DB:1550:C:H2'   | 23:DB:1551:A:H8    | 1.56        | 0.70     |
| 46:BU:11:ILE:HG22  | 46:BU:70:ALA:HB3   | 1.72        | 0.70     |
| 1:CA:474:G:H2'     | 1:CA:475:C:C6      | 2.26        | 0.70     |
| 1:CA:1011:C:H2'    | 1:CA:1012:A:C8     | 2.26        | 0.70     |
| 16:AQ:16:MET:HB2   | 16:AQ:19:SER:HB2   | 1.73        | 0.70     |
| 27:BK:87:LEU:HB2   | 27:BK:93:GLN:O     | 1.91        | 0.70     |
| 9:CJ:44:THR:HG23   | 9:CJ:69:THR:O      | 1.91        | 0.70     |
| 3:AD:90:LEU:HA     | 3:AD:93:LEU:HD12   | 1.73        | 0.70     |
| 1:CA:238:A:H2'     | 1:CA:239:U:H5''    | 1.73        | 0.70     |
| 23:DB:1099:G:H5''  | 24:DI:2:LYS:C      | 2.11        | 0.70     |
| 44:DQ:30:VAL:CG1   | 44:DQ:33:VAL:HG22  | 2.21        | 0.70     |
| 23:DB:138:U:O3'    | 23:DB:139:U:H3'    | 1.91        | 0.70     |
| 23:BB:162:U:H4'    | 23:BB:163:C:OP1    | 1.91        | 0.70     |
| 29:BE:175:ILE:HD11 | 29:BE:180:LEU:HD11 | 1.73        | 0.70     |
| 23:BB:721:A:H2'    | 23:BB:722:A:C8     | 2.26        | 0.70     |
| 1:CA:552:U:H5'     | 11:CL:82:ARG:HH11  | 1.56        | 0.70     |
| 23:BB:2297:A:H61   | 23:BB:2319:G:H1'   | 1.56        | 0.70     |
| 12:AM:2:ARG:HG3    | 12:AM:6:ILE:H      | 1.54        | 0.70     |
| 23:BB:2795:C:H2'   | 23:BB:2796:U:O4'   | 1.90        | 0.70     |
| 23:BB:2840:C:OP1   | 42:BN:50:PRO:HA    | 1.91        | 0.70     |
| 1:AA:532:A:N7      | 2:AC:192:TYR:HD2   | 1.87        | 0.70     |
| 52:BW:35:ILE:HG13  | 52:BW:57:THR:OG1   | 1.91        | 0.70     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 22:BA:43:C:O2'     | 47:BF:91:ARG:HD2   | 1.92        | 0.70     |
| 8:AI:47:VAL:HG23   | 8:AI:48:ARG:HG3    | 1.72        | 0.70     |
| 13:AN:71:GLY:O     | 13:AN:79:SER:HA    | 1.92        | 0.70     |
| 1:AA:946:A:H2'     | 1:AA:947:G:C8      | 2.26        | 0.70     |
| 23:BB:163:C:H2'    | 23:BB:164:C:O4'    | 1.92        | 0.70     |
| 9:CJ:52:LEU:HD21   | 9:CJ:59:LYS:HA     | 1.72        | 0.70     |
| 49:BR:78:ARG:HB3   | 49:BR:83:TYR:HB3   | 1.73        | 0.70     |
| 23:BB:1287:A:H3'   | 23:BB:1288:G:N2    | 2.05        | 0.70     |
| 1:AA:82:G:H2'      | 1:AA:84:U:C5       | 2.26        | 0.70     |
| 1:CA:1048:G:O3'    | 1:CA:1049:U:H3'    | 1.91        | 0.70     |
| 40:BH:18:GLN:NE2   | 40:BH:44:ILE:HG21  | 2.07        | 0.70     |
| 28:DP:31:VAL:HG12  | 28:DP:38:ARG:O     | 1.91        | 0.70     |
| 1:CA:9:G:H5'       | 4:CE:107:GLY:HA3   | 1.74        | 0.70     |
| 50:BT:59:ASN:O     | 50:BT:84:TYR:HB2   | 1.89        | 0.70     |
| 40:BH:122:LEU:HD12 | 40:BH:122:LEU:H    | 1.55        | 0.70     |
| 1:AA:1254:A:H5'    | 1:AA:1356:G:H4'    | 1.74        | 0.70     |
| 52:DW:43:LYS:HB3   | 52:DW:58:LEU:HD11  | 1.73        | 0.70     |
| 16:CQ:45:VAL:HG11  | 16:CQ:60:ILE:HG21  | 1.74        | 0.70     |
| 53:B6:95:LYS:HB3   | 53:B6:100:TYR:HE2  | 1.55        | 0.70     |
| 23:DB:636:G:H3'    | 37:DL:128:THR:CG2  | 2.20        | 0.70     |
| 48:DG:15:ASP:HB3   | 48:DG:25:ILE:HA    | 1.72        | 0.70     |
| 23:BB:1241:A:H2'   | 23:BB:1242:U:H5'   | 1.74        | 0.70     |
| 33:B1:26:LYS:HB2   | 33:B1:52:LYS:NZ    | 2.06        | 0.70     |
| 20:AB:31:PHE:HB2   | 20:AB:41:ASN:HA    | 1.72        | 0.70     |
| 23:DB:592:A:H2'    | 23:DB:593:U:C6     | 2.26        | 0.70     |
| 1:AA:41:G:H2'      | 1:AA:42:G:H8       | 1.54        | 0.70     |
| 23:BB:1654:A:O2'   | 26:BD:118:PHE:HB2  | 1.91        | 0.70     |
| 1:CA:337:G:H2'     | 1:CA:338:A:C8      | 2.26        | 0.70     |
| 19:AT:66:ILE:HG23  | 19:AT:70:LYS:HB3   | 1.71        | 0.70     |
| 23:BB:1485:U:H2'   | 23:BB:1486:U:C6    | 2.25        | 0.70     |
| 16:CQ:16:MET:HB2   | 16:CQ:19:SER:HB2   | 1.74        | 0.70     |
| 37:DL:90:VAL:HB    | 37:DL:122:VAL:HA   | 1.74        | 0.70     |
| 8:CI:47:VAL:HG23   | 8:CI:48:ARG:HG3    | 1.72        | 0.70     |
| 1:CA:1369:C:H2'    | 1:CA:1370:G:C8     | 2.26        | 0.70     |
| 23:DB:2734:A:H2'   | 23:DB:2735:G:H5'   | 1.74        | 0.70     |
| 38:DM:126:ILE:HG22 | 38:DM:127:LYS:H    | 1.56        | 0.70     |
| 42:BN:34:ILE:HB    | 42:BN:113:ILE:HG22 | 1.74        | 0.70     |
| 3:CD:116:LEU:HB3   | 3:CD:122:ILE:HD11  | 1.73        | 0.70     |
| 38:DM:19:GLY:N     | 38:DM:38:ARG:HH22  | 1.89        | 0.70     |
| 9:AJ:8:ILE:HB      | 9:AJ:74:VAL:HB     | 1.72        | 0.70     |
| 23:DB:276:U:H2'    | 23:DB:278:A:C2     | 2.27        | 0.70     |
| 1:AA:33:A:H2'      | 1:AA:34:C:C6       | 2.27        | 0.70     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 10:CK:105:ARG:NH2  | 21:CU:10:PRO:HB3   | 2.05        | 0.70     |
| 35:BV:9:ARG:NH2    | 35:BV:12:GLN:HA    | 2.06        | 0.70     |
| 23:BB:2591:C:H2'   | 23:BB:2592:G:C8    | 2.27        | 0.70     |
| 10:AK:110:THR:HG22 | 21:AU:4:LYS:HA     | 1.74        | 0.70     |
| 10:AK:126:ARG:HB2  | 21:AU:33:ARG:HD2   | 1.73        | 0.70     |
| 38:DM:19:GLY:HA2   | 38:DM:97:GLN:HB2   | 1.72        | 0.70     |
| 1:AA:1071:C:H2'    | 1:AA:1072:G:H8     | 1.56        | 0.70     |
| 23:DB:224:U:O4     | 23:DB:420:C:H5'    | 1.91        | 0.70     |
| 4:CE:76:ASN:HB2    | 4:CE:81:GLN:NE2    | 2.07        | 0.70     |
| 7:AH:11:THR:HG22   | 7:AH:14:ARG:HH12   | 1.56        | 0.70     |
| 52:BW:49:ASN:HB2   | 52:BW:61:LYS:H     | 1.56        | 0.70     |
| 37:BL:90:VAL:HB    | 37:BL:122:VAL:HA   | 1.74        | 0.70     |
| 48:DG:104:LEU:HB2  | 48:DG:112:VAL:HB   | 1.74        | 0.70     |
| 26:BD:34:VAL:HG12  | 26:BD:94:GLN:H     | 1.57        | 0.70     |
| 37:BL:30:THR:O     | 37:BL:33:ARG:HG2   | 1.91        | 0.70     |
| 27:DK:112:PHE:O    | 27:DK:115:ILE:HG22 | 1.92        | 0.70     |
| 1:AA:1273:C:H2'    | 1:AA:1274:A:O4'    | 1.92        | 0.70     |
| 27:DK:60:ALA:HA    | 27:DK:87:LEU:HD23  | 1.74        | 0.70     |
| 7:CH:51:GLU:HG2    | 7:CH:52:GLY:H      | 1.56        | 0.70     |
| 23:BB:558:U:OP1    | 41:BJ:113:PRO:HG2  | 1.91        | 0.70     |
| 23:DB:264:C:O2'    | 23:DB:265:A:H5''   | 1.92        | 0.70     |
| 11:AL:98:ARG:HA    | 11:AL:103:CYS:SG   | 2.31        | 0.70     |
| 4:AE:52:ALA:HB2    | 4:AE:61:LYS:HE2    | 1.74        | 0.70     |
| 1:AA:1048:G:O3'    | 1:AA:1049:U:H3'    | 1.91        | 0.70     |
| 15:AP:40:ASN:HD21  | 15:AP:43:ALA:N     | 1.89        | 0.70     |
| 23:BB:98:G:H2'     | 23:BB:99:U:H5''    | 1.73        | 0.70     |
| 9:AJ:24:GLU:HG2    | 9:AJ:90:LEU:HD21   | 1.74        | 0.70     |
| 53:B6:60:ALA:HA    | 53:B6:66:LEU:HA    | 1.72        | 0.70     |
| 35:DV:72:VAL:HG12  | 35:DV:94:ALA:H     | 1.55        | 0.70     |
| 23:DB:2379:G:H2'   | 23:DB:2380:C:C6    | 2.27        | 0.70     |
| 35:DV:9:ARG:NH2    | 35:DV:12:GLN:HA    | 2.07        | 0.70     |
| 1:CA:335:C:H2'     | 1:CA:336:A:C8      | 2.27        | 0.70     |
| 50:DT:59:ASN:O     | 50:DT:84:TYR:HB2   | 1.91        | 0.70     |
| 1:AA:9:G:H5'       | 4:AE:107:GLY:HA3   | 1.74        | 0.70     |
| 39:BX:34:SER:HB2   | 39:BX:36:GLN:OE1   | 1.92        | 0.70     |
| 23:DB:616:A:H3'    | 23:DB:617:G:H8     | 1.55        | 0.70     |
| 23:BB:49:A:H5''    | 23:BB:51:G:O4'     | 1.91        | 0.70     |
| 1:CA:1137:C:H1'    | 1:CA:1138:G:C2     | 2.26        | 0.70     |
| 23:BB:2356:U:H5''  | 52:BW:16:GLU:HG3   | 1.73        | 0.70     |
| 35:DV:42:LEU:H     | 35:DV:42:LEU:HD23  | 1.57        | 0.70     |
| 23:DB:2328:A:H2'   | 23:DB:2329:U:C6    | 2.27        | 0.70     |
| 20:AB:202:ASN:HD22 | 20:AB:203:ASP:N    | 1.89        | 0.70     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1139:G:O2'  | 23:BB:1140:C:H5'   | 1.92        | 0.70     |
| 46:BU:35:VAL:HB   | 46:BU:38:ILE:HG21  | 1.72        | 0.70     |
| 29:BE:194:LYS:O   | 29:BE:197:GLU:HB3  | 1.91        | 0.70     |
| 23:DB:1210:G:H5'  | 23:DB:1212:G:O4'   | 1.91        | 0.70     |
| 1:AA:1479:C:H2'   | 1:AA:1480:A:H8     | 1.57        | 0.70     |
| 23:BB:264:C:O2'   | 23:BB:265:A:H5''   | 1.91        | 0.70     |
| 36:D2:30:VAL:HA   | 36:D2:33:ARG:NH2   | 2.07        | 0.70     |
| 8:CI:9:GLY:HA2    | 8:CI:80:HIS:CD2    | 2.27        | 0.70     |
| 37:BL:90:VAL:HB   | 37:BL:122:VAL:HG12 | 1.74        | 0.69     |
| 47:BF:107:VAL:O   | 47:BF:110:ILE:HG22 | 1.92        | 0.69     |
| 47:BF:105:ILE:O   | 47:BF:109:ARG:HB2  | 1.91        | 0.69     |
| 1:AA:922:G:H4'    | 4:AE:24:VAL:HA     | 1.74        | 0.69     |
| 23:BB:968:C:H2'   | 23:BB:969:G:C8     | 2.26        | 0.69     |
| 23:BB:2444:G:P    | 29:BE:63:LYS:HD2   | 2.32        | 0.69     |
| 44:BQ:104:ALA:HA  | 49:BR:46:GLU:OE1   | 1.92        | 0.69     |
| 23:DB:968:C:H2'   | 23:DB:969:G:C8     | 2.26        | 0.69     |
| 49:DR:8:GLY:HA3   | 49:DR:23:GLU:HB2   | 1.74        | 0.69     |
| 20:CB:95:TRP:HH2  | 20:CB:100:LEU:HB2  | 1.55        | 0.69     |
| 49:BR:31:GLU:H    | 49:BR:63:VAL:HG22  | 1.56        | 0.69     |
| 49:DR:68:ARG:NH1  | 49:DR:90:ARG:HD3   | 2.06        | 0.69     |
| 23:DB:2591:C:H2'  | 23:DB:2592:G:C8    | 2.26        | 0.69     |
| 23:BB:836:G:H2'   | 23:BB:837:C:C6     | 2.26        | 0.69     |
| 34:B3:30:HIS:H    | 34:B3:32:LEU:HD21  | 1.56        | 0.69     |
| 40:BH:73:ASN:N    | 40:BH:73:ASN:HD22  | 1.89        | 0.69     |
| 26:BD:148:GLN:HG3 | 26:BD:152:PRO:HG2  | 1.73        | 0.69     |
| 15:CP:40:ASN:HD21 | 15:CP:43:ALA:H     | 1.39        | 0.69     |
| 1:CA:195:A:H1'    | 1:CA:222:C:O2'     | 1.92        | 0.69     |
| 23:BB:645:C:H4'   | 23:BB:646:U:OP2    | 1.92        | 0.69     |
| 43:BO:47:VAL:HG12 | 43:BO:48:LEU:H     | 1.57        | 0.69     |
| 35:BV:29:ILE:HG13 | 35:BV:88:HIS:HE1   | 1.57        | 0.69     |
| 23:BB:1583:A:H5'' | 23:BB:1584:U:OP1   | 1.91        | 0.69     |
| 27:BK:53:LYS:H    | 27:BK:53:LYS:HD3   | 1.55        | 0.69     |
| 3:AD:84:ASN:ND2   | 4:AE:101:GLY:HA3   | 2.07        | 0.69     |
| 49:BR:19:THR:HB   | 49:BR:97:LYS:HA    | 1.74        | 0.69     |
| 26:BD:30:GLU:HG3  | 26:BD:52:THR:HG22  | 1.74        | 0.69     |
| 47:DF:107:VAL:O   | 47:DF:110:ILE:HG22 | 1.93        | 0.69     |
| 23:BB:2144:G:H2'  | 23:BB:2146:C:OP2   | 1.92        | 0.69     |
| 23:BB:1550:C:H2'  | 23:BB:1551:A:H8    | 1.57        | 0.69     |
| 11:AL:20:VAL:HG12 | 11:AL:93:ARG:HB3   | 1.74        | 0.69     |
| 20:AB:95:TRP:HH2  | 20:AB:100:LEU:HB2  | 1.57        | 0.69     |
| 1:AA:673:A:H2'    | 1:AA:674:G:C8      | 2.27        | 0.69     |
| 23:DB:1138:G:H2'  | 23:DB:1139:G:O4'   | 1.92        | 0.69     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 35:DV:29:ILE:HG13  | 35:DV:88:HIS:HE1   | 1.57        | 0.69     |
| 23:DB:721:A:H2'    | 23:DB:722:A:H8     | 1.57        | 0.69     |
| 23:BB:64:A:H2'     | 23:BB:65:U:C6      | 2.27        | 0.69     |
| 43:BO:24:THR:HG22  | 43:BO:42:PRO:HD3   | 1.74        | 0.69     |
| 27:BK:35:VAL:HG23  | 27:BK:36:GLY:N     | 2.04        | 0.69     |
| 30:DY:15:ARG:O     | 30:DY:20:LYS:HE3   | 1.93        | 0.69     |
| 18:AS:42:ASN:ND2   | 18:AS:43:MET:HG2   | 2.07        | 0.69     |
| 9:AJ:51:VAL:CG2    | 13:AN:80:ARG:HB2   | 2.22        | 0.69     |
| 23:BB:1178:C:H2'   | 23:BB:1179:G:H8    | 1.56        | 0.69     |
| 38:BM:126:ILE:HG22 | 38:BM:127:LYS:H    | 1.57        | 0.69     |
| 38:BM:19:GLY:N     | 38:BM:38:ARG:HH22  | 1.90        | 0.69     |
| 23:BB:784:G:O2'    | 23:BB:785:G:H5''   | 1.93        | 0.69     |
| 23:BB:118:A:OP2    | 23:BB:119:A:H2'    | 1.92        | 0.69     |
| 1:AA:238:A:H2'     | 1:AA:239:U:H5''    | 1.73        | 0.69     |
| 52:DW:58:LEU:HD12  | 52:DW:79:ILE:HD12  | 1.73        | 0.69     |
| 53:B6:69:GLN:NE2   | 53:B6:98:ALA:HB2   | 2.07        | 0.69     |
| 23:BB:1012:U:O4    | 41:BJ:30:THR:HG21  | 1.91        | 0.69     |
| 23:BB:670:A:H5''   | 37:BL:42:SER:HB2   | 1.73        | 0.69     |
| 18:CS:4:LEU:HD11   | 18:CS:9:PHE:HB3    | 1.72        | 0.69     |
| 49:DR:78:ARG:HB3   | 49:DR:83:TYR:HB3   | 1.73        | 0.69     |
| 35:DV:79:ARG:NH1   | 38:DM:134:THR:HG21 | 2.07        | 0.69     |
| 1:AA:22:G:H2'      | 1:AA:23:C:H6       | 1.56        | 0.69     |
| 26:DD:34:VAL:HB    | 26:DD:48:ILE:HD11  | 1.74        | 0.69     |
| 16:CQ:16:MET:CB    | 16:CQ:19:SER:HB2   | 2.22        | 0.69     |
| 1:CA:1163:A:H2'    | 1:CA:1164:G:H8     | 1.56        | 0.69     |
| 23:DB:1149:G:H2'   | 23:DB:1150:C:C6    | 2.26        | 0.69     |
| 49:BR:68:ARG:NH1   | 49:BR:90:ARG:HD3   | 2.07        | 0.69     |
| 3:AD:192:ALA:HB3   | 3:AD:194:ILE:HG22  | 1.72        | 0.69     |
| 23:BB:1935:G:H1'   | 23:BB:1964:G:N2    | 2.07        | 0.69     |
| 23:BB:2078:C:H2'   | 23:BB:2079:U:C6    | 2.28        | 0.69     |
| 20:AB:163:ILE:HG23 | 20:AB:164:ASP:N    | 2.04        | 0.69     |
| 52:DW:51:GLY:HA3   | 52:DW:59:PHE:CB    | 2.22        | 0.69     |
| 40:BH:79:THR:HA    | 40:BH:145:ASN:HB2  | 1.75        | 0.69     |
| 38:BM:71:LYS:HE3   | 38:BM:73:ILE:HD11  | 1.75        | 0.69     |
| 24:DI:9:LYS:HG2    | 24:DI:57:VAL:HG13  | 1.75        | 0.69     |
| 34:D3:31:ILE:HD11  | 34:D3:34:LYS:HD3   | 1.74        | 0.69     |
| 48:BG:167:VAL:HG23 | 48:BG:168:VAL:H    | 1.56        | 0.69     |
| 42:DN:34:ILE:HB    | 42:DN:113:ILE:HG22 | 1.75        | 0.69     |
| 23:DB:1199:U:H5'   | 44:DQ:4:LYS:HD3    | 1.75        | 0.69     |
| 27:BK:60:ALA:HA    | 27:BK:87:LEU:HD23  | 1.74        | 0.69     |
| 23:DB:125:A:H3'    | 23:DB:126:A:H5''   | 1.74        | 0.69     |
| 23:BB:274:C:H2'    | 23:BB:275:C:O4'    | 1.92        | 0.69     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 9:CJ:37:ARG:NE     | 9:CJ:37:ARG:HA     | 2.07        | 0.69     |
| 3:CD:169:TRP:CE2   | 3:CD:185:PRO:HB3   | 2.28        | 0.69     |
| 23:DB:37:C:O2'     | 29:DE:45:ALA:HA    | 1.93        | 0.69     |
| 29:BE:48:THR:HG22  | 29:BE:86:ALA:HB3   | 1.75        | 0.69     |
| 8:AI:48:ARG:HA     | 8:AI:51:LEU:HD12   | 1.74        | 0.69     |
| 51:BZ:6:GLN:NE2    | 51:BZ:50:ARG:H     | 1.90        | 0.69     |
| 9:AJ:52:LEU:HD21   | 9:AJ:59:LYS:HA     | 1.73        | 0.69     |
| 2:AC:8:GLY:HA3     | 13:AN:88:MET:SD    | 2.32        | 0.69     |
| 23:BB:2732:G:H3'   | 23:BB:2733:A:H5'   | 1.74        | 0.69     |
| 23:BB:592:A:H2'    | 23:BB:593:U:C6     | 2.27        | 0.69     |
| 1:CA:1347:G:H22    | 1:CA:1373:G:H2'    | 1.58        | 0.69     |
| 13:CN:87:ALA:HB2   | 13:CN:92:ILE:HD12  | 1.75        | 0.69     |
| 49:BR:8:GLY:HA3    | 49:BR:23:GLU:HB2   | 1.75        | 0.69     |
| 23:DB:1854:A:N6    | 23:DB:1888:G:H1'   | 2.08        | 0.69     |
| 1:AA:1137:C:H1'    | 1:AA:1138:G:C2     | 2.27        | 0.69     |
| 23:DB:1727:C:H2'   | 23:DB:1728:C:H6    | 1.57        | 0.69     |
| 47:BF:34:THR:HG22  | 47:BF:89:THR:HG22  | 1.74        | 0.69     |
| 53:B6:58:VAL:HG22  | 53:B6:68:VAL:HG13  | 1.75        | 0.69     |
| 44:DQ:57:ARG:NH1   | 44:DQ:61:ILE:HD11  | 2.06        | 0.69     |
| 38:DM:71:LYS:HD3   | 38:DM:95:LEU:HD13  | 1.73        | 0.69     |
| 23:DB:2732:G:H3'   | 23:DB:2733:A:H5'   | 1.74        | 0.69     |
| 3:AD:160:LEU:H     | 3:AD:160:LEU:HD13  | 1.57        | 0.69     |
| 18:AS:48:ILE:HG22  | 18:AS:49:ALA:H     | 1.56        | 0.69     |
| 45:DS:26:GLY:H     | 45:DS:71:VAL:HG13  | 1.57        | 0.69     |
| 20:CB:27:LYS:HA    | 20:CB:30:ILE:HD12  | 1.74        | 0.69     |
| 49:BR:4:VAL:HG23   | 49:BR:39:LEU:H     | 1.58        | 0.69     |
| 29:BE:109:LEU:HD13 | 29:BE:180:LEU:HD13 | 1.75        | 0.69     |
| 26:DD:148:GLN:HG3  | 26:DD:152:PRO:HG2  | 1.75        | 0.69     |
| 23:DB:361:G:O2'    | 23:DB:362:A:H5'    | 1.92        | 0.69     |
| 41:DJ:117:ALA:HA   | 41:DJ:120:ARG:HD2  | 1.74        | 0.69     |
| 49:BR:31:GLU:H     | 49:BR:63:VAL:CG2   | 2.05        | 0.69     |
| 23:DB:721:A:H2'    | 23:DB:722:A:C8     | 2.28        | 0.69     |
| 39:DX:17:GLU:OE1   | 39:DX:21:LEU:HD11  | 1.93        | 0.69     |
| 1:AA:17:U:H2'      | 1:AA:18:C:C6       | 2.27        | 0.69     |
| 23:BB:1149:G:H2'   | 23:BB:1150:C:C6    | 2.27        | 0.69     |
| 6:AG:108:ARG:HA    | 6:AG:115:MET:HE1   | 1.73        | 0.69     |
| 2:CC:96:VAL:HB     | 2:CC:97:PRO:HD2    | 1.75        | 0.69     |
| 38:DM:41:LEU:HB2   | 38:DM:94:ALA:HB3   | 1.73        | 0.69     |
| 6:CG:58:LEU:H      | 6:CG:58:LEU:HD23   | 1.58        | 0.69     |
| 23:DB:354:A:H2'    | 23:DB:355:U:C6     | 2.27        | 0.69     |
| 23:DB:1666:G:O3'   | 27:DK:6:THR:HG23   | 1.92        | 0.69     |
| 26:BD:5:VAL:H      | 26:BD:32:ASN:ND2   | 1.85        | 0.69     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 16:CQ:46:HIS:HB2   | 16:CQ:70:LYS:HE2   | 1.75        | 0.69     |
| 40:BH:84:ALA:HB2   | 40:BH:147:VAL:O    | 1.93        | 0.69     |
| 1:CA:16:A:O2'      | 1:CA:17:U:H5'      | 1.93        | 0.69     |
| 23:DB:2283:C:H5''  | 23:DB:2389:G:O2'   | 1.93        | 0.69     |
| 1:CA:22:G:H2'      | 1:CA:23:C:H6       | 1.58        | 0.69     |
| 26:DD:24:VAL:HG21  | 26:DD:188:LEU:HB3  | 1.75        | 0.69     |
| 23:DB:117:G:H5'    | 23:DB:126:A:H8     | 1.57        | 0.69     |
| 23:DB:1935:G:H1'   | 23:DB:1964:G:N2    | 2.06        | 0.69     |
| 23:BB:1131:G:N2    | 23:BB:2024:G:H21   | 1.90        | 0.69     |
| 23:BB:455:C:N3     | 23:BB:472:A:H2'    | 2.07        | 0.69     |
| 23:BB:2346:A:H3'   | 23:BB:2347:C:H5''  | 1.72        | 0.69     |
| 40:BH:124:THR:O    | 40:BH:125:THR:HB   | 1.91        | 0.69     |
| 23:DB:974:G:OP2    | 49:DR:78:ARG:HD3   | 1.93        | 0.69     |
| 48:DG:148:ARG:HB2  | 48:DG:152:ARG:NH2  | 2.08        | 0.69     |
| 45:BS:27:LYS:O     | 45:BS:32:ALA:HB2   | 1.91        | 0.69     |
| 11:CL:20:VAL:HG12  | 11:CL:93:ARG:HB3   | 1.74        | 0.69     |
| 4:AE:76:ASN:HB2    | 4:AE:81:GLN:NE2    | 2.08        | 0.69     |
| 45:DS:25:ARG:HE    | 45:DS:73:LYS:NZ    | 1.91        | 0.69     |
| 33:D1:46:VAL:HG22  | 33:D1:47:ILE:H     | 1.57        | 0.69     |
| 1:AA:493:A:H5'     | 1:AA:494:G:OP2     | 1.92        | 0.69     |
| 23:DB:2557:G:H2'   | 23:DB:2558:C:C6    | 2.28        | 0.69     |
| 47:BF:161:SER:OG   | 47:BF:164:GLU:HG3  | 1.93        | 0.69     |
| 38:BM:40:ARG:HD3   | 38:BM:93:VAL:HG21  | 1.73        | 0.69     |
| 29:BE:148:ILE:HD13 | 29:BE:187:VAL:HG21 | 1.74        | 0.69     |
| 6:AG:58:LEU:HD23   | 6:AG:58:LEU:H      | 1.58        | 0.69     |
| 23:DB:1098:A:OP2   | 24:DI:3:LYS:HG2    | 1.92        | 0.68     |
| 47:BF:64:PRO:HA    | 47:BF:88:VAL:CG2   | 2.23        | 0.68     |
| 27:BK:43:ILE:HG22  | 27:BK:54:LYS:HA    | 1.76        | 0.68     |
| 23:BB:170:U:H2'    | 23:BB:171:U:C6     | 2.28        | 0.68     |
| 23:DB:1199:U:H2'   | 23:DB:1200:C:C6    | 2.28        | 0.68     |
| 23:DB:170:U:H2'    | 23:DB:171:U:C6     | 2.28        | 0.68     |
| 19:CT:61:ALA:HA    | 19:CT:67:HIS:H     | 1.58        | 0.68     |
| 23:BB:152:A:H2'    | 23:BB:153:U:C6     | 2.27        | 0.68     |
| 3:CD:103:ARG:HH21  | 3:CD:110:ARG:HH22  | 1.39        | 0.68     |
| 23:BB:1812:U:H2'   | 23:BB:1813:G:H8    | 1.58        | 0.68     |
| 22:BA:13:G:H2'     | 22:BA:14:U:H5''    | 1.75        | 0.68     |
| 10:AK:31:VAL:HG21  | 10:AK:66:ALA:HA    | 1.75        | 0.68     |
| 23:DB:163:C:H2'    | 23:DB:164:C:O4'    | 1.94        | 0.68     |
| 1:AA:1347:G:H22    | 1:AA:1373:G:H2'    | 1.58        | 0.68     |
| 1:CA:235:C:H2'     | 1:CA:236:A:H8      | 1.57        | 0.68     |
| 15:AP:40:ASN:HD21  | 15:AP:43:ALA:H     | 1.42        | 0.68     |
| 7:CH:28:SER:OG     | 7:CH:56:PRO:HB2    | 1.93        | 0.68     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 6:CG:108:ARG:HA    | 6:CG:115:MET:HE1   | 1.74        | 0.68     |
| 13:AN:17:ASP:O     | 13:AN:21:ALA:HB3   | 1.94        | 0.68     |
| 23:DB:645:C:H4'    | 23:DB:646:U:OP2    | 1.92        | 0.68     |
| 39:BX:17:GLU:OE1   | 39:BX:21:LEU:HD11  | 1.92        | 0.68     |
| 26:BD:111:GLY:H    | 26:BD:194:PRO:HG2  | 1.58        | 0.68     |
| 23:DB:630:G:N2     | 23:DB:632:A:H3'    | 2.07        | 0.68     |
| 41:DJ:36:LEU:HD11  | 41:DJ:122:LEU:HB2  | 1.75        | 0.68     |
| 13:CN:71:GLY:O     | 13:CN:79:SER:HA    | 1.93        | 0.68     |
| 47:BF:103:ILE:HD11 | 47:BF:174:PHE:HA   | 1.75        | 0.68     |
| 29:BE:143:LEU:HB3  | 29:BE:146:VAL:HG21 | 1.74        | 0.68     |
| 36:B2:21:ARG:HH21  | 36:B2:43:THR:HG21  | 1.58        | 0.68     |
| 35:BV:28:ALA:HA    | 35:BV:88:HIS:ND1   | 2.09        | 0.68     |
| 35:DV:28:ALA:HA    | 35:DV:88:HIS:ND1   | 2.08        | 0.68     |
| 23:DB:1727:C:H2'   | 23:DB:1728:C:C6    | 2.28        | 0.68     |
| 1:AA:636:U:H2'     | 1:AA:637:C:C6      | 2.29        | 0.68     |
| 1:AA:484:G:H4'     | 1:AA:485:U:H5''    | 1.76        | 0.68     |
| 23:DB:152:A:H2'    | 23:DB:153:U:C6     | 2.29        | 0.68     |
| 23:DB:836:G:H2'    | 23:DB:837:C:C6     | 2.27        | 0.68     |
| 23:BB:121:G:H2'    | 23:BB:122:G:H8     | 1.57        | 0.68     |
| 37:BL:47:ARG:HG2   | 37:BL:50:PHE:HB2   | 1.75        | 0.68     |
| 38:DM:71:LYS:HE3   | 38:DM:73:ILE:HD11  | 1.73        | 0.68     |
| 44:BQ:60:TRP:O     | 44:BQ:64:ILE:HG12  | 1.94        | 0.68     |
| 50:DT:11:LEU:H     | 50:DT:11:LEU:HD22  | 1.57        | 0.68     |
| 2:CC:26:LYS:HE2    | 2:CC:27:GLU:HG3    | 1.74        | 0.68     |
| 1:AA:1048:G:H4'    | 13:AN:2:LYS:NZ     | 2.08        | 0.68     |
| 23:BB:947:A:HO2'   | 23:BB:984:A:H2     | 1.40        | 0.68     |
| 28:DP:20:ARG:HG3   | 28:DP:21:PRO:HD2   | 1.74        | 0.68     |
| 16:CQ:24:ILE:HD11  | 16:CQ:43:LEU:HD13  | 1.74        | 0.68     |
| 33:B1:46:VAL:HG22  | 33:B1:47:ILE:H     | 1.57        | 0.68     |
| 2:CC:59:PRO:HG2    | 2:CC:62:SER:OG     | 1.93        | 0.68     |
| 2:AC:96:VAL:HB     | 2:AC:97:PRO:HD2    | 1.75        | 0.68     |
| 48:DG:155:PRO:HA   | 48:DG:170:THR:HG22 | 1.74        | 0.68     |
| 23:DB:64:A:H2'     | 23:DB:65:U:C6      | 2.28        | 0.68     |
| 37:DL:90:VAL:HB    | 37:DL:122:VAL:HG12 | 1.74        | 0.68     |
| 26:BD:51:THR:HG21  | 26:BD:76:GLY:HA3   | 1.74        | 0.68     |
| 23:BB:1060:U:O2    | 23:BB:1088:A:N7    | 2.27        | 0.68     |
| 47:DF:105:ILE:O    | 47:DF:109:ARG:HB2  | 1.94        | 0.68     |
| 39:DX:7:ARG:NH1    | 39:DX:7:ARG:HB2    | 2.08        | 0.68     |
| 23:DB:2886:A:H3'   | 23:DB:2887:A:H8    | 1.58        | 0.68     |
| 23:BB:848:C:H2'    | 23:BB:849:A:C8     | 2.29        | 0.68     |
| 23:DB:581:C:H2'    | 23:DB:582:A:C8     | 2.27        | 0.68     |
| 10:AK:28:ASN:ND2   | 10:AK:46:ALA:HB3   | 2.07        | 0.68     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:AD:169:TRP:CE2   | 3:AD:185:PRO:HB3   | 2.27        | 0.68     |
| 23:BB:1700:A:H2'   | 23:BB:1701:A:H5'   | 1.75        | 0.68     |
| 23:DB:1597:A:H5''  | 23:DB:1598:A:H5'   | 1.73        | 0.68     |
| 1:AA:195:A:H1'     | 1:AA:222:C:O2'     | 1.93        | 0.68     |
| 1:AA:474:G:H2'     | 1:AA:475:C:C6      | 2.29        | 0.68     |
| 43:DO:24:THR:HG22  | 43:DO:42:PRO:HD3   | 1.75        | 0.68     |
| 1:CA:859:G:H2'     | 1:CA:860:A:C8      | 2.28        | 0.68     |
| 25:DC:86:ARG:NH1   | 25:DC:86:ARG:HB3   | 2.08        | 0.68     |
| 23:DB:49:A:H5''    | 23:DB:51:G:O4'     | 1.94        | 0.68     |
| 40:DH:96:THR:HG23  | 40:DH:97:ARG:H     | 1.58        | 0.68     |
| 40:DH:96:THR:HG23  | 40:DH:97:ARG:HD3   | 1.75        | 0.68     |
| 23:DB:1386:C:H2'   | 23:DB:1387:A:C8    | 2.29        | 0.68     |
| 40:BH:100:ALA:HB1  | 40:BH:132:PHE:HE1  | 1.58        | 0.68     |
| 8:AI:20:ILE:HD13   | 8:AI:85:ALA:HB3    | 1.74        | 0.68     |
| 40:DH:80:ILE:HD11  | 40:DH:146:VAL:HG13 | 1.75        | 0.68     |
| 40:DH:94:ILE:O     | 40:DH:122:LEU:HB2  | 1.93        | 0.68     |
| 18:CS:47:THR:HG23  | 18:CS:60:PHE:HE1   | 1.59        | 0.68     |
| 23:DB:2471:A:O2'   | 23:DB:2472:G:H8    | 1.77        | 0.68     |
| 23:BB:2751:G:H5'   | 48:BG:2:ARG:CD     | 2.23        | 0.68     |
| 45:BS:24:ILE:HG23  | 45:BS:32:ALA:HB1   | 1.76        | 0.68     |
| 1:AA:203:G:H1'     | 1:AA:465:A:H61     | 1.58        | 0.68     |
| 23:BB:721:A:H2'    | 23:BB:722:A:H8     | 1.58        | 0.68     |
| 3:CD:94:GLU:HG2    | 3:CD:185:PRO:HG3   | 1.76        | 0.68     |
| 23:BB:2379:G:H2'   | 23:BB:2380:C:C6    | 2.28        | 0.68     |
| 24:BI:105:LEU:HD11 | 24:BI:139:VAL:HG11 | 1.75        | 0.68     |
| 23:DB:96:C:H4'     | 39:DX:41:HIS:ND1   | 2.08        | 0.68     |
| 5:CF:16:GLU:CD     | 5:CF:16:GLU:H      | 1.97        | 0.68     |
| 23:DB:919:U:H2'    | 23:DB:920:A:C8     | 2.28        | 0.68     |
| 44:DQ:91:ARG:HG2   | 44:DQ:93:ILE:HG22  | 1.75        | 0.68     |
| 23:BB:142:A:H2'    | 23:BB:143:C:C6     | 2.29        | 0.68     |
| 4:AE:89:THR:HG21   | 4:AE:134:ASN:ND2   | 2.08        | 0.68     |
| 53:D6:177:GLU:O    | 53:D6:181:GLN:HG3  | 1.93        | 0.68     |
| 37:DL:30:THR:O     | 37:DL:33:ARG:HG2   | 1.92        | 0.68     |
| 13:CN:24:ALA:O     | 13:CN:27:LYS:HG2   | 1.93        | 0.68     |
| 39:BX:7:ARG:NH1    | 39:BX:7:ARG:HB2    | 2.09        | 0.68     |
| 48:DG:71:LEU:HA    | 48:DG:74:MET:SD    | 2.33        | 0.68     |
| 23:BB:90:U:H3'     | 23:BB:91:A:C5'     | 2.24        | 0.68     |
| 16:AQ:16:MET:CB    | 16:AQ:19:SER:HB2   | 2.24        | 0.68     |
| 19:AT:66:ILE:HG13  | 19:AT:70:LYS:HE3   | 1.74        | 0.68     |
| 27:DK:87:LEU:HB2   | 27:DK:93:GLN:O     | 1.93        | 0.68     |
| 23:DB:1853:A:N1    | 23:DB:2087:G:H1'   | 2.08        | 0.68     |
| 35:DV:53:LYS:NZ    | 35:DV:53:LYS:HA    | 2.08        | 0.68     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:2557:G:H2'   | 23:BB:2558:C:C6    | 2.28        | 0.68     |
| 1:CA:707:U:H2'     | 1:CA:708:C:C6      | 2.29        | 0.68     |
| 22:DA:13:G:H2'     | 22:DA:14:U:H5''    | 1.76        | 0.68     |
| 23:DB:281:C:H2'    | 23:DB:282:A:C8     | 2.29        | 0.68     |
| 26:DD:33:ARG:CZ    | 26:DD:74:GLU:HB3   | 2.23        | 0.68     |
| 1:AA:1423:G:H2'    | 1:AA:1424:U:H6     | 1.59        | 0.68     |
| 37:BL:123:ARG:HA   | 37:BL:143:GLU:CB   | 2.22        | 0.68     |
| 26:BD:34:VAL:CG1   | 26:BD:94:GLN:H     | 2.05        | 0.68     |
| 1:AA:812:G:O2'     | 1:AA:813:U:H6      | 1.73        | 0.68     |
| 23:DB:141:G:N3     | 23:DB:141:G:H3'    | 2.07        | 0.68     |
| 38:BM:19:GLY:H     | 38:BM:38:ARG:HH12  | 1.39        | 0.68     |
| 23:BB:2630:G:H2'   | 23:BB:2631:G:H8    | 1.58        | 0.68     |
| 23:BB:2328:A:H2'   | 23:BB:2329:U:C6    | 2.28        | 0.68     |
| 23:BB:1021:A:H61   | 23:BB:1142:A:N6    | 1.92        | 0.68     |
| 23:DB:848:C:H2'    | 23:DB:849:A:C8     | 2.29        | 0.68     |
| 44:DQ:104:ALA:HA   | 49:DR:46:GLU:OE1   | 1.94        | 0.68     |
| 44:DQ:10:ARG:HB2   | 44:DQ:10:ARG:NH1   | 2.08        | 0.68     |
| 23:BB:125:A:H5'    | 36:B2:19:ARG:HG3   | 1.76        | 0.68     |
| 28:DP:52:ARG:HH11  | 28:DP:52:ARG:HG2   | 1.59        | 0.68     |
| 1:CA:193:C:H2'     | 1:CA:194:C:C6      | 2.29        | 0.68     |
| 46:BU:72:PHE:HA    | 46:BU:78:LYS:O     | 1.94        | 0.68     |
| 23:DB:1469:A:H2'   | 23:DB:1470:A:H8    | 1.58        | 0.68     |
| 23:BB:1827:U:O2'   | 23:BB:1828:G:H5'   | 1.94        | 0.68     |
| 5:AF:53:LYS:HA     | 5:AF:53:LYS:HE2    | 1.75        | 0.68     |
| 23:BB:1854:A:N6    | 23:BB:1888:G:H1'   | 2.09        | 0.68     |
| 2:AC:129:PHE:HE2   | 2:AC:165:GLU:HG2   | 1.56        | 0.68     |
| 52:BW:24:ARG:HD2   | 52:BW:65:LYS:HG2   | 1.76        | 0.68     |
| 48:BG:68:ARG:HH12  | 48:BG:72:ASN:HD22  | 1.40        | 0.68     |
| 21:CU:36:PHE:HA    | 21:CU:39:LYS:HE3   | 1.76        | 0.68     |
| 48:DG:68:ARG:HH12  | 48:DG:72:ASN:HD22  | 1.42        | 0.68     |
| 3:CD:160:LEU:H     | 3:CD:160:LEU:HD13  | 1.58        | 0.68     |
| 38:BM:35:ALA:HB3   | 38:BM:99:GLY:N     | 2.07        | 0.68     |
| 33:D1:34:GLU:HB3   | 33:D1:49:LYS:HD3   | 1.76        | 0.68     |
| 16:AQ:45:VAL:HG11  | 16:AQ:60:ILE:HG21  | 1.76        | 0.68     |
| 13:AN:87:ALA:HB2   | 13:AN:92:ILE:HD12  | 1.74        | 0.68     |
| 42:DN:65:LEU:HD11  | 42:DN:69:ARG:CZ    | 2.24        | 0.68     |
| 34:B3:31:ILE:HD11  | 34:B3:34:LYS:HD3   | 1.74        | 0.68     |
| 1:CA:1137:C:O2'    | 1:CA:1138:G:H5''   | 1.94        | 0.68     |
| 23:DB:1241:A:H2'   | 23:DB:1242:U:H5'   | 1.76        | 0.68     |
| 3:CD:192:ALA:HB3   | 3:CD:194:ILE:HG22  | 1.76        | 0.68     |
| 29:DE:175:ILE:HD11 | 29:DE:180:LEU:HD11 | 1.76        | 0.68     |
| 1:AA:621:A:H2'     | 1:AA:622:A:C8      | 2.28        | 0.68     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:919:U:H2'   | 23:BB:920:A:C8     | 2.29        | 0.67     |
| 40:BH:90:LEU:HD11 | 40:BH:146:VAL:CG1  | 2.22        | 0.67     |
| 1:CA:1302:C:OP2   | 12:CM:16:ILE:HD11  | 1.94        | 0.67     |
| 44:BQ:91:ARG:HG2  | 44:BQ:93:ILE:HG22  | 1.75        | 0.67     |
| 16:AQ:59:GLU:O    | 16:AQ:75:VAL:HG22  | 1.93        | 0.67     |
| 38:DM:42:THR:O    | 38:DM:44:ARG:N     | 2.28        | 0.67     |
| 39:DX:48:ARG:O    | 39:DX:51:ALA:HB3   | 1.94        | 0.67     |
| 29:DE:48:THR:HG22 | 29:DE:86:ALA:HB3   | 1.76        | 0.67     |
| 1:AA:602:A:O2'    | 1:AA:603:U:H5'     | 1.93        | 0.67     |
| 1:AA:848:C:H2'    | 1:AA:849:G:O4'     | 1.94        | 0.67     |
| 5:AF:80:PHE:CZ    | 25:BC:123:ILE:HG12 | 2.28        | 0.67     |
| 12:CM:2:ARG:HG3   | 12:CM:6:ILE:H      | 1.59        | 0.67     |
| 1:CA:147:G:H2'    | 1:CA:148:G:H8      | 1.58        | 0.67     |
| 23:BB:2269:G:H4'  | 52:BW:19:ARG:NH1   | 2.09        | 0.67     |
| 52:BW:49:ASN:HB2  | 52:BW:60:ALA:HA    | 1.76        | 0.67     |
| 8:CI:26:LYS:N     | 8:CI:61:ASP:HB3    | 2.09        | 0.67     |
| 43:BO:34:HIS:HB3  | 43:BO:36:TYR:HE2   | 1.58        | 0.67     |
| 23:BB:594:U:H2'   | 23:BB:595:C:H6     | 1.60        | 0.67     |
| 23:BB:2443:C:H2'  | 23:BB:2444:G:C8    | 2.30        | 0.67     |
| 43:BO:62:LEU:HD11 | 43:BO:70:ALA:HA    | 1.77        | 0.67     |
| 1:CA:22:G:H2'     | 1:CA:23:C:C6       | 2.28        | 0.67     |
| 5:AF:6:ILE:HG23   | 5:AF:62:MET:HB3    | 1.77        | 0.67     |
| 23:DB:115:C:O2'   | 23:DB:116:C:H5'    | 1.94        | 0.67     |
| 1:CA:1521:C:H2'   | 1:CA:1522:U:C6     | 2.29        | 0.67     |
| 6:CG:56:SER:HB3   | 6:CG:59:GLU:HG3    | 1.75        | 0.67     |
| 23:DB:540:C:H2'   | 23:DB:541:A:H8     | 1.57        | 0.67     |
| 1:CA:1477:U:H2'   | 1:CA:1478:U:C6     | 2.29        | 0.67     |
| 45:DS:31:GLN:O    | 45:DS:35:ILE:HG12  | 1.94        | 0.67     |
| 1:AA:780:A:O2'    | 1:AA:781:A:H5''    | 1.94        | 0.67     |
| 23:DB:1485:U:H2'  | 23:DB:1486:U:C6    | 2.29        | 0.67     |
| 52:DW:18:LYS:HA   | 52:DW:36:ILE:HG12  | 1.75        | 0.67     |
| 40:BH:128:HIS:CE1 | 40:BH:130:VAL:HG13 | 2.29        | 0.67     |
| 51:DZ:5:CYS:CB    | 51:DZ:10:LYS:H     | 2.07        | 0.67     |
| 41:DJ:17:VAL:HG22 | 41:DJ:55:ILE:HD11  | 1.76        | 0.67     |
| 1:AA:429:U:H3'    | 3:AD:8:LEU:HD23    | 1.76        | 0.67     |
| 23:DB:162:U:H4'   | 23:DB:163:C:OP1    | 1.92        | 0.67     |
| 9:CJ:8:ILE:HB     | 9:CJ:74:VAL:HB     | 1.74        | 0.67     |
| 26:DD:148:GLN:O   | 26:DD:149:ASN:HB2  | 1.94        | 0.67     |
| 23:DB:30:G:H2'    | 23:DB:31:C:C6      | 2.28        | 0.67     |
| 26:BD:148:GLN:HB2 | 26:BD:152:PRO:HG2  | 1.76        | 0.67     |
| 1:AA:335:C:H2'    | 1:AA:336:A:C8      | 2.29        | 0.67     |
| 51:DZ:11:ARG:HB3  | 51:DZ:12:PRO:HD2   | 1.77        | 0.67     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 40:BH:41:LYS:HA   | 40:BH:44:ILE:HG13  | 1.76        | 0.67     |
| 28:DP:31:VAL:O    | 28:DP:32:VAL:HB    | 1.93        | 0.67     |
| 23:DB:717:C:H3'   | 23:DB:718:A:H5''   | 1.76        | 0.67     |
| 23:DB:742:A:H2'   | 23:DB:743:A:H8     | 1.60        | 0.67     |
| 23:BB:1579:A:H2'  | 23:BB:1580:A:C8    | 2.30        | 0.67     |
| 1:CA:802:A:H2'    | 1:CA:803:G:O4'     | 1.95        | 0.67     |
| 27:DK:35:VAL:HG12 | 27:DK:69:VAL:HG22  | 1.76        | 0.67     |
| 51:DZ:5:CYS:HB2   | 51:DZ:10:LYS:HB3   | 1.76        | 0.67     |
| 33:B1:34:GLU:HB3  | 33:B1:49:LYS:HD3   | 1.75        | 0.67     |
| 23:DB:1060:U:O2   | 23:DB:1088:A:N7    | 2.27        | 0.67     |
| 40:DH:88:GLY:O    | 40:DH:124:THR:HA   | 1.94        | 0.67     |
| 48:BG:148:ARG:HB2 | 48:BG:152:ARG:NH2  | 2.09        | 0.67     |
| 23:BB:181:A:H2'   | 23:BB:182:A:H8     | 1.56        | 0.67     |
| 46:DU:34:ILE:HG12 | 46:DU:63:ALA:HB2   | 1.75        | 0.67     |
| 23:DB:1469:A:H2'  | 23:DB:1470:A:C8    | 2.30        | 0.67     |
| 23:BB:609:A:H2'   | 23:BB:610:C:O4'    | 1.94        | 0.67     |
| 41:DJ:23:LYS:HE3  | 41:DJ:142:ILE:HG12 | 1.76        | 0.67     |
| 1:CA:806:C:H2'    | 1:CA:807:A:C8      | 2.29        | 0.67     |
| 23:DB:1509:A:H5'  | 23:DB:1510:G:H5'   | 1.75        | 0.67     |
| 23:BB:1735:A:H2'  | 23:BB:1736:U:C6    | 2.30        | 0.67     |
| 1:CA:834:U:H2'    | 1:CA:835:U:C6      | 2.30        | 0.67     |
| 6:AG:14:ASP:HB3   | 6:AG:18:GLY:H      | 1.58        | 0.67     |
| 1:CA:484:G:H4'    | 1:CA:485:U:H5''    | 1.76        | 0.67     |
| 23:DB:1373:A:H2'  | 23:DB:1374:G:O4'   | 1.95        | 0.67     |
| 46:DU:48:VAL:C    | 46:DU:53:GLN:HG3   | 2.15        | 0.67     |
| 26:BD:33:ARG:CZ   | 26:BD:74:GLU:HB3   | 2.24        | 0.67     |
| 26:DD:105:LYS:H   | 26:DD:106:LYS:HZ3  | 1.42        | 0.67     |
| 3:AD:25:ARG:HB2   | 3:AD:25:ARG:HH11   | 1.60        | 0.67     |
| 18:AS:49:ALA:HA   | 18:AS:57:VAL:O     | 1.95        | 0.67     |
| 23:BB:2886:A:H3'  | 23:BB:2887:A:H8    | 1.57        | 0.67     |
| 13:CN:26:LEU:HD11 | 13:CN:44:VAL:HG22  | 1.76        | 0.67     |
| 23:BB:364:C:H2'   | 23:BB:365:U:H6     | 1.55        | 0.67     |
| 23:BB:1309:G:OP1  | 36:B2:9:VAL:HG12   | 1.94        | 0.67     |
| 2:AC:26:LYS:HE2   | 2:AC:27:GLU:HG3    | 1.75        | 0.67     |
| 46:DU:70:ALA:HB1  | 46:DU:79:ALA:CB    | 2.24        | 0.67     |
| 4:CE:39:GLY:HA3   | 4:CE:116:VAL:HB    | 1.75        | 0.67     |
| 3:CD:103:ARG:HH21 | 3:CD:110:ARG:NH2   | 1.93        | 0.67     |
| 23:DB:2341:G:H2'  | 23:DB:2342:C:C6    | 2.30        | 0.67     |
| 1:CA:1273:C:H2'   | 1:CA:1274:A:O4'    | 1.93        | 0.67     |
| 25:DC:244:VAL:HB  | 25:DC:249:VAL:H    | 1.59        | 0.67     |
| 49:DR:72:VAL:HG23 | 49:DR:89:HIS:HB3   | 1.74        | 0.67     |
| 22:DA:25:U:OP1    | 22:DA:25:U:H3'     | 1.94        | 0.67     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DC:149:LYS:HD3  | 25:DC:152:GLN:HE22 | 1.60        | 0.67     |
| 47:DF:64:PRO:HA    | 47:DF:88:VAL:CG2   | 2.24        | 0.67     |
| 53:B6:77:LYS:CE    | 53:B6:94:ASN:HD21  | 2.02        | 0.67     |
| 7:CH:6:ILE:HB      | 7:CH:76:ARG:NH1    | 2.10        | 0.67     |
| 49:BR:5:PHE:O      | 49:BR:11:GLN:HA    | 1.95        | 0.67     |
| 51:BZ:40:VAL:HG22  | 51:BZ:45:ARG:O     | 1.95        | 0.67     |
| 24:DI:73:PRO:HG2   | 24:DI:78:LEU:HD21  | 1.75        | 0.67     |
| 13:AN:24:ALA:O     | 13:AN:27:LYS:HG2   | 1.94        | 0.67     |
| 23:BB:974:G:OP2    | 49:BR:78:ARG:HD3   | 1.95        | 0.67     |
| 24:BI:25:PRO:O     | 24:BI:29:GLN:HG2   | 1.95        | 0.67     |
| 2:CC:116:ALA:O     | 2:CC:119:ILE:HG22  | 1.95        | 0.67     |
| 1:AA:195:A:H2'     | 1:AA:196:A:C8      | 2.28        | 0.67     |
| 23:DB:1872:A:H2'   | 23:DB:1873:G:O4'   | 1.95        | 0.67     |
| 23:DB:414:C:H2'    | 23:DB:415:A:C8     | 2.30        | 0.67     |
| 2:AC:122:GLN:HB3   | 2:AC:127:VAL:HG21  | 1.77        | 0.67     |
| 23:DB:1390:U:O2'   | 23:DB:1391:U:H5'   | 1.94        | 0.67     |
| 10:AK:124:LYS:HA   | 21:AU:34:ARG:CB    | 2.20        | 0.67     |
| 52:BW:18:LYS:HA    | 52:BW:36:ILE:HG12  | 1.74        | 0.67     |
| 40:BH:65:ALA:O     | 40:BH:68:ARG:HD2   | 1.94        | 0.67     |
| 52:DW:24:ARG:HD2   | 52:DW:65:LYS:HG2   | 1.75        | 0.67     |
| 41:DJ:3:THR:HG21   | 44:DQ:60:TRP:HE1   | 1.59        | 0.67     |
| 26:DD:105:LYS:HD2  | 26:DD:177:VAL:HG22 | 1.77        | 0.67     |
| 47:DF:103:ILE:HD11 | 47:DF:174:PHE:HA   | 1.75        | 0.67     |
| 18:AS:27:LYS:HG3   | 18:AS:28:LYS:HD2   | 1.75        | 0.67     |
| 23:DB:1283:G:N2    | 23:DB:1286:A:H5'   | 2.08        | 0.67     |
| 23:DB:362:A:N3     | 23:DB:362:A:H2'    | 2.10        | 0.67     |
| 23:BB:1778:U:H2'   | 23:BB:1784:A:N6    | 2.09        | 0.67     |
| 8:AI:9:GLY:HA2     | 8:AI:80:HIS:CD2    | 2.28        | 0.67     |
| 1:CA:621:A:H2'     | 1:CA:622:A:C8      | 2.30        | 0.67     |
| 9:CJ:24:GLU:HG2    | 9:CJ:90:LEU:HD21   | 1.76        | 0.67     |
| 57:DB:3574:HOH:O   | 25:DC:230:PRO:HA   | 1.93        | 0.67     |
| 25:BC:32:LEU:O     | 25:BC:63:ILE:HG12  | 1.94        | 0.67     |
| 1:CA:848:C:H2'     | 1:CA:849:G:O4'     | 1.95        | 0.67     |
| 23:DB:365:U:H2'    | 23:DB:366:C:C6     | 2.29        | 0.67     |
| 29:DE:22:ASP:O     | 29:DE:107:SER:HB2  | 1.95        | 0.67     |
| 28:BP:31:VAL:HG12  | 28:BP:38:ARG:O     | 1.94        | 0.67     |
| 24:BI:10:LEU:HD13  | 24:BI:12:VAL:HG13  | 1.75        | 0.67     |
| 10:CK:126:ARG:HB2  | 21:CU:33:ARG:HD2   | 1.76        | 0.67     |
| 52:DW:49:ASN:HB2   | 52:DW:60:ALA:HA    | 1.76        | 0.67     |
| 8:CI:48:ARG:HA     | 8:CI:51:LEU:HD12   | 1.77        | 0.67     |
| 51:DZ:33:LEU:HA    | 51:DZ:52:SER:HA    | 1.77        | 0.67     |
| 23:DB:2305:U:H5"   | 47:DF:130:GLY:HA3  | 1.75        | 0.67     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 7:AH:6:ILE:HB      | 7:AH:76:ARG:NH1    | 2.09        | 0.67     |
| 43:BO:51:ALA:HB3   | 43:BO:78:VAL:HG22  | 1.77        | 0.67     |
| 18:CS:42:ASN:ND2   | 18:CS:43:MET:HG2   | 2.09        | 0.67     |
| 23:BB:2749:A:H3'   | 23:BB:2750:A:H5''  | 1.77        | 0.67     |
| 23:DB:27:G:N2      | 23:DB:512:G:H2'    | 2.09        | 0.67     |
| 13:CN:26:LEU:HG    | 13:CN:30:ILE:HD13  | 1.75        | 0.67     |
| 23:BB:2645:G:H3'   | 23:BB:2646:C:H5'   | 1.76        | 0.67     |
| 49:DR:39:LEU:HA    | 49:DR:53:PHE:HA    | 1.77        | 0.67     |
| 23:DB:90:U:H3'     | 23:DB:91:A:C5'     | 2.25        | 0.67     |
| 19:CT:66:ILE:HG13  | 19:CT:70:LYS:HE3   | 1.76        | 0.67     |
| 1:CA:335:C:H2'     | 1:CA:336:A:H8      | 1.60        | 0.67     |
| 29:DE:109:LEU:HD13 | 29:DE:180:LEU:HD13 | 1.75        | 0.67     |
| 23:BB:1597:A:H5''  | 23:BB:1598:A:H5'   | 1.76        | 0.67     |
| 23:BB:704:G:H2'    | 23:BB:726:G:H22    | 1.59        | 0.67     |
| 1:AA:926:G:N2      | 1:AA:1505:G:H2'    | 2.09        | 0.67     |
| 20:CB:63:LYS:HA    | 20:CB:224:ARG:HH11 | 1.60        | 0.67     |
| 40:BH:27:ARG:H     | 40:BH:31:VAL:CG2   | 2.08        | 0.67     |
| 41:BJ:17:VAL:HG22  | 41:BJ:55:ILE:HD11  | 1.77        | 0.67     |
| 48:DG:15:ASP:CB    | 48:DG:26:LYS:H     | 2.07        | 0.67     |
| 34:D3:40:LYS:HA    | 34:D3:43:LEU:HD12  | 1.76        | 0.67     |
| 1:CA:17:U:H2'      | 1:CA:18:C:H6       | 1.57        | 0.67     |
| 12:AM:10:ASP:HA    | 12:AM:44:ILE:HD13  | 1.77        | 0.67     |
| 1:AA:1320:C:OP2    | 18:AS:2:ARG:HA     | 1.94        | 0.67     |
| 23:DB:1790:C:O2'   | 25:DC:207:ALA:HB2  | 1.94        | 0.67     |
| 16:AQ:46:HIS:HB2   | 16:AQ:70:LYS:HE2   | 1.76        | 0.67     |
| 23:BB:1172:C:H3'   | 23:BB:1173:U:C6    | 2.29        | 0.67     |
| 23:DB:848:C:H2'    | 23:DB:849:A:H8     | 1.59        | 0.67     |
| 13:CN:27:LYS:HG3   | 13:CN:28:ALA:H     | 1.60        | 0.67     |
| 23:DB:2591:C:H2'   | 23:DB:2592:G:H8    | 1.60        | 0.67     |
| 23:DB:1139:G:O2'   | 23:DB:1140:C:H5'   | 1.94        | 0.67     |
| 23:BB:2091:C:H1'   | 51:BZ:34:HIS:CD2   | 2.30        | 0.67     |
| 1:CA:1254:A:H5'    | 1:CA:1356:G:H4'    | 1.75        | 0.67     |
| 28:BP:20:ARG:HG3   | 28:BP:21:PRO:HD2   | 1.75        | 0.67     |
| 38:BM:42:THR:HB    | 38:BM:45:GLN:HG3   | 1.75        | 0.67     |
| 16:AQ:24:ILE:HD11  | 16:AQ:43:LEU:HD13  | 1.76        | 0.67     |
| 53:D6:81:LYS:HA    | 53:D6:84:ARG:NH2   | 2.09        | 0.67     |
| 53:B6:55:ILE:HG23  | 53:B6:56:ALA:N     | 2.08        | 0.67     |
| 29:DE:58:LYS:C     | 29:DE:60:TRP:H     | 1.98        | 0.67     |
| 47:BF:78:ILE:H     | 47:BF:79:ARG:NH1   | 1.93        | 0.67     |
| 18:CS:27:LYS:HG3   | 18:CS:28:LYS:HD2   | 1.77        | 0.67     |
| 23:BB:1176:U:H3'   | 23:BB:1177:G:H8    | 1.59        | 0.67     |
| 32:D4:24:ARG:HG2   | 32:D4:36:ARG:HG3   | 1.77        | 0.67     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 18:CS:5:LYS:C      | 18:CS:6:LYS:HD2    | 2.15        | 0.67     |
| 23:BB:27:G:N2      | 23:BB:512:G:H2'    | 2.09        | 0.67     |
| 20:AB:57:ASN:HB2   | 20:AB:219:THR:O    | 1.95        | 0.67     |
| 23:BB:1727:C:H2'   | 23:BB:1728:C:H6    | 1.60        | 0.67     |
| 23:DB:1558:C:H4'   | 23:DB:1559:U:C5'   | 2.25        | 0.67     |
| 49:BR:28:ALA:O     | 49:BR:63:VAL:HG21  | 1.95        | 0.67     |
| 9:CJ:37:ARG:NH1    | 9:CJ:77:VAL:HG21   | 2.10        | 0.67     |
| 28:BP:31:VAL:O     | 28:BP:32:VAL:HB    | 1.95        | 0.67     |
| 23:BB:2484:G:OP1   | 38:BM:44:ARG:HD3   | 1.95        | 0.67     |
| 7:AH:51:GLU:HG2    | 7:AH:52:GLY:H      | 1.59        | 0.67     |
| 26:DD:14:ILE:HG22  | 26:DD:22:ILE:O     | 1.95        | 0.67     |
| 23:BB:2720:U:H5''  | 28:BP:52:ARG:HH21  | 1.60        | 0.67     |
| 1:CA:736:C:H2'     | 1:CA:737:C:C6      | 2.30        | 0.67     |
| 20:CB:185:ILE:HA   | 20:CB:199:ILE:HB   | 1.77        | 0.67     |
| 53:B6:18:LEU:HD21  | 53:B6:171:LYS:HD2  | 1.77        | 0.67     |
| 47:BF:62:GLN:HG3   | 47:BF:91:ARG:NH1   | 2.10        | 0.66     |
| 6:AG:149:ALA:N     | 10:AK:55:ARG:HH21  | 1.91        | 0.66     |
| 16:CQ:59:GLU:O     | 16:CQ:75:VAL:HG22  | 1.95        | 0.66     |
| 53:B6:42:LYS:HB3   | 53:B6:49:HIS:O     | 1.95        | 0.66     |
| 47:DF:78:ILE:H     | 47:DF:79:ARG:HH11  | 1.41        | 0.66     |
| 43:DO:34:HIS:HB3   | 43:DO:36:TYR:HE2   | 1.60        | 0.66     |
| 47:DF:37:MET:HE1   | 47:DF:149:ARG:HD2  | 1.77        | 0.66     |
| 4:AE:113:VAL:HG11  | 4:AE:136:VAL:HG23  | 1.77        | 0.66     |
| 12:CM:109:LYS:HD3  | 12:CM:113:LYS:HE3  | 1.77        | 0.66     |
| 1:CA:922:G:H4'     | 4:CE:24:VAL:HA     | 1.76        | 0.66     |
| 18:CS:43:MET:O     | 18:CS:46:LEU:HB2   | 1.95        | 0.66     |
| 25:DC:204:LEU:HD23 | 25:DC:209:ALA:HB1  | 1.76        | 0.66     |
| 3:CD:171:GLU:HB2   | 3:CD:180:THR:HB    | 1.77        | 0.66     |
| 29:DE:109:LEU:HD12 | 29:DE:112:LEU:HD12 | 1.76        | 0.66     |
| 20:AB:20:ARG:CZ    | 20:AB:20:ARG:HA    | 2.24        | 0.66     |
| 30:BY:40:THR:O     | 30:BY:43:ILE:HG23  | 1.95        | 0.66     |
| 45:BS:43:ALA:HA    | 45:BS:46:LEU:HD12  | 1.75        | 0.66     |
| 2:AC:6:PRO:HA      | 2:AC:9:ILE:HG22    | 1.76        | 0.66     |
| 1:AA:147:G:H2'     | 1:AA:148:G:H8      | 1.59        | 0.66     |
| 9:CJ:9:ARG:CB      | 9:CJ:99:GLN:HB3    | 2.23        | 0.66     |
| 40:BH:134:VAL:HG13 | 40:BH:135:HIS:H    | 1.59        | 0.66     |
| 5:AF:64:VAL:HG12   | 5:AF:65:GLU:H      | 1.59        | 0.66     |
| 45:DS:27:LYS:O     | 45:DS:32:ALA:HB2   | 1.95        | 0.66     |
| 30:DY:2:LYS:H      | 30:DY:2:LYS:HD3    | 1.59        | 0.66     |
| 23:DB:594:U:H2'    | 23:DB:595:C:H6     | 1.60        | 0.66     |
| 23:DB:38:A:O2'     | 29:DE:43:THR:HA    | 1.95        | 0.66     |
| 1:AA:634:C:H2'     | 1:AA:635:A:H8      | 1.59        | 0.66     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:2001:C:H4'  | 23:BB:2689:U:O2'  | 1.95        | 0.66     |
| 3:CD:84:ASN:ND2   | 4:CE:101:GLY:HA3  | 2.09        | 0.66     |
| 20:AB:185:ILE:HA  | 20:AB:199:ILE:HB  | 1.77        | 0.66     |
| 1:CA:1461:G:H2'   | 1:CA:1462:C:H6    | 1.59        | 0.66     |
| 20:CB:20:ARG:CZ   | 20:CB:20:ARG:HA   | 2.25        | 0.66     |
| 23:DB:21:A:H2'    | 23:DB:22:C:C6     | 2.30        | 0.66     |
| 2:CC:6:PRO:HA     | 2:CC:9:ILE:HG22   | 1.77        | 0.66     |
| 23:BB:296:U:H2'   | 23:BB:297:G:H8    | 1.59        | 0.66     |
| 23:DB:1176:U:H2'  | 23:DB:1177:G:C8   | 2.30        | 0.66     |
| 23:DB:704:G:H2'   | 23:DB:726:G:H22   | 1.60        | 0.66     |
| 13:CN:17:ASP:O    | 13:CN:21:ALA:HB3  | 1.94        | 0.66     |
| 25:DC:94:LEU:HD13 | 25:DC:100:ARG:HD3 | 1.76        | 0.66     |
| 41:BJ:43:GLU:O    | 41:BJ:45:THR:N    | 2.28        | 0.66     |
| 34:B3:40:LYS:HA   | 34:B3:43:LEU:HD12 | 1.77        | 0.66     |
| 42:DN:85:PRO:HA   | 42:DN:88:ALA:HB2  | 1.77        | 0.66     |
| 13:AN:27:LYS:HG3  | 13:AN:28:ALA:H    | 1.60        | 0.66     |
| 1:AA:1237:C:H3'   | 1:AA:1336:C:H41   | 1.58        | 0.66     |
| 23:BB:1558:C:H4'  | 23:BB:1559:U:C5'  | 2.24        | 0.66     |
| 1:AA:108:G:O6     | 19:AT:9:ARG:HG2   | 1.96        | 0.66     |
| 1:AA:269:C:H2'    | 1:AA:270:A:H8     | 1.58        | 0.66     |
| 26:BD:113:SER:HB3 | 26:BD:167:ASN:N   | 2.10        | 0.66     |
| 23:BB:2591:C:H2'  | 23:BB:2592:G:H8   | 1.59        | 0.66     |
| 1:AA:16:A:O2'     | 1:AA:17:U:H5'     | 1.94        | 0.66     |
| 35:BV:53:LYS:HA   | 35:BV:53:LYS:NZ   | 2.10        | 0.66     |
| 40:BH:2:GLN:O     | 40:BH:3:VAL:HG22  | 1.96        | 0.66     |
| 3:CD:97:LEU:HB2   | 3:CD:134:TYR:HB3  | 1.76        | 0.66     |
| 1:CA:1314:C:H41   | 18:CS:3:SER:HB3   | 1.60        | 0.66     |
| 48:BG:104:LEU:HB2 | 48:BG:112:VAL:HB  | 1.78        | 0.66     |
| 44:DQ:60:TRP:O    | 44:DQ:64:ILE:HG12 | 1.94        | 0.66     |
| 5:AF:29:ILE:HG22  | 5:AF:34:GLY:HA3   | 1.77        | 0.66     |
| 44:BQ:57:ARG:NH1  | 44:BQ:61:ILE:HD11 | 2.10        | 0.66     |
| 23:BB:594:U:H2'   | 23:BB:595:C:C6    | 2.31        | 0.66     |
| 11:CL:85:ARG:HA   | 11:CL:93:ARG:HA   | 1.78        | 0.66     |
| 10:CK:28:ASN:ND2  | 10:CK:46:ALA:HB3  | 2.09        | 0.66     |
| 23:BB:1727:C:H2'  | 23:BB:1728:C:C6   | 2.30        | 0.66     |
| 23:DB:1080:A:H4'  | 24:DI:126:ARG:HD3 | 1.77        | 0.66     |
| 1:CA:108:G:O6     | 19:CT:9:ARG:HG2   | 1.95        | 0.66     |
| 1:CA:336:A:O2'    | 1:CA:337:G:H5'    | 1.95        | 0.66     |
| 1:CA:1521:C:H2'   | 1:CA:1522:U:H6    | 1.61        | 0.66     |
| 39:DX:34:SER:HB2  | 39:DX:36:GLN:OE1  | 1.96        | 0.66     |
| 4:AE:106:ALA:HB1  | 4:AE:110:MET:HB3  | 1.78        | 0.66     |
| 49:DR:2:TYR:HB2   | 49:DR:42:ALA:HB2  | 1.78        | 0.66     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:224:U:O4    | 23:BB:420:C:H5'    | 1.95        | 0.66     |
| 23:DB:1583:A:H5'' | 23:DB:1584:U:OP1   | 1.95        | 0.66     |
| 16:CQ:8:GLN:HA    | 16:CQ:59:GLU:HA    | 1.78        | 0.66     |
| 51:DZ:71:LEU:HD13 | 51:DZ:76:GLU:HB3   | 1.75        | 0.66     |
| 25:BC:67:LYS:HD3  | 25:BC:150:GLY:HA2  | 1.76        | 0.66     |
| 23:DB:1458:U:C5'  | 23:DB:1459:G:H5'   | 2.26        | 0.66     |
| 26:DD:113:SER:HB3 | 26:DD:167:ASN:N    | 2.10        | 0.66     |
| 23:BB:848:C:H2'   | 23:BB:849:A:H8     | 1.60        | 0.66     |
| 20:CB:83:ALA:O    | 20:CB:88:GLN:HB2   | 1.96        | 0.66     |
| 23:DB:2080:A:OP1  | 51:DZ:20:HIS:HB3   | 1.95        | 0.66     |
| 15:AP:25:ARG:HD3  | 15:AP:25:ARG:H     | 1.60        | 0.66     |
| 12:AM:87:GLY:HA2  | 12:AM:90:HIS:HD2   | 1.60        | 0.66     |
| 1:CA:1163:A:H2'   | 1:CA:1164:G:C8     | 2.31        | 0.66     |
| 38:BM:42:THR:O    | 38:BM:44:ARG:N     | 2.29        | 0.66     |
| 1:CA:517:G:H22    | 1:CA:533:A:P       | 2.18        | 0.66     |
| 37:DL:47:ARG:HG2  | 37:DL:50:PHE:HB2   | 1.75        | 0.66     |
| 1:CA:634:C:H2'    | 1:CA:635:A:H8      | 1.61        | 0.66     |
| 41:BJ:105:VAL:O   | 41:BJ:109:LEU:HG   | 1.96        | 0.66     |
| 53:B6:3:LEU:HD12  | 53:B6:143:LEU:HD23 | 1.78        | 0.66     |
| 2:AC:119:ILE:HG21 | 2:AC:197:VAL:HG11  | 1.78        | 0.66     |
| 23:DB:1735:A:H2'  | 23:DB:1736:U:C6    | 2.31        | 0.66     |
| 23:DB:2138:G:H2'  | 23:DB:2139:U:O4'   | 1.96        | 0.66     |
| 40:BH:27:ARG:HH11 | 51:BZ:64:ILE:HD11  | 1.61        | 0.66     |
| 41:BJ:58:ASN:HA   | 41:BJ:127:GLY:CA   | 2.26        | 0.66     |
| 41:DJ:58:ASN:HA   | 41:DJ:127:GLY:CA   | 2.25        | 0.66     |
| 47:BF:71:LYS:HG2  | 47:BF:73:VAL:H     | 1.61        | 0.66     |
| 47:DF:102:LEU:HA  | 47:DF:106:ALA:HB2  | 1.78        | 0.66     |
| 21:AU:3:ILE:HG21  | 21:AU:19:LYS:HG3   | 1.76        | 0.66     |
| 29:DE:29:HIS:NE2  | 37:DL:8:PRO:HG3    | 2.10        | 0.66     |
| 2:CC:8:GLY:HA3    | 13:CN:88:MET:SD    | 2.35        | 0.66     |
| 28:BP:52:ARG:HH11 | 28:BP:52:ARG:HG2   | 1.59        | 0.66     |
| 1:CA:602:A:O2'    | 1:CA:603:U:H5'     | 1.96        | 0.66     |
| 23:DB:609:A:H2'   | 23:DB:610:C:O4'    | 1.95        | 0.66     |
| 11:CL:14:LYS:HG2  | 11:CL:15:VAL:N     | 2.11        | 0.66     |
| 20:AB:83:ALA:O    | 20:AB:88:GLN:HB2   | 1.96        | 0.66     |
| 42:DN:97:ILE:HD12 | 42:DN:98:LEU:N     | 2.11        | 0.66     |
| 23:BB:1390:U:O2'  | 23:BB:1391:U:H5'   | 1.95        | 0.66     |
| 23:DB:2027:G:O2'  | 23:DB:2028:U:H5'   | 1.95        | 0.66     |
| 1:CA:1027:C:H2'   | 1:CA:1028:C:C6     | 2.31        | 0.66     |
| 23:BB:1872:A:H2'  | 23:BB:1873:G:O4'   | 1.96        | 0.66     |
| 6:CG:14:ASP:HB3   | 6:CG:18:GLY:H      | 1.58        | 0.66     |
| 23:BB:526:A:N6    | 23:BB:2626:C:H4'   | 2.11        | 0.66     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1532:U:C2     | 1:AA:1534:A:H5'    | 2.30        | 0.66     |
| 23:BB:2066:C:O2'   | 23:BB:2067:G:H5'   | 1.95        | 0.66     |
| 44:BQ:30:VAL:CG1   | 44:BQ:33:VAL:HG22  | 2.25        | 0.66     |
| 48:DG:17:LYS:HA    | 48:DG:17:LYS:HZ2   | 1.61        | 0.66     |
| 47:DF:101:ARG:CZ   | 47:DF:138:PRO:HB2  | 2.26        | 0.66     |
| 23:DB:1033:U:H5    | 32:D4:15:LYS:HE3   | 1.60        | 0.66     |
| 23:DB:982:C:O2     | 23:DB:982:C:H5'    | 1.96        | 0.66     |
| 23:BB:547:A:H3'    | 23:BB:548:G:C8     | 2.29        | 0.66     |
| 53:B6:114:LEU:O    | 53:B6:118:VAL:HG23 | 1.95        | 0.66     |
| 1:AA:1002:G:H2'    | 1:AA:1003:G:O4'    | 1.95        | 0.66     |
| 1:AA:1137:C:O2'    | 1:AA:1138:G:H5''   | 1.96        | 0.66     |
| 23:DB:1173:U:H2'   | 23:DB:1174:U:C6    | 2.30        | 0.66     |
| 1:CA:1314:C:N4     | 18:CS:3:SER:HB3    | 2.10        | 0.66     |
| 1:CA:135:C:O2      | 15:CP:1:MET:HB2    | 1.95        | 0.66     |
| 1:AA:1329:A:OP1    | 12:AM:28:ARG:HB2   | 1.96        | 0.66     |
| 49:BR:2:TYR:HB2    | 49:BR:42:ALA:HB2   | 1.77        | 0.66     |
| 23:BB:1469:A:H2'   | 23:BB:1470:A:H8    | 1.60        | 0.66     |
| 41:DJ:64:VAL:O     | 41:DJ:68:LYS:HD2   | 1.96        | 0.66     |
| 5:CF:64:VAL:HG12   | 5:CF:65:GLU:H      | 1.61        | 0.66     |
| 53:B6:51:PRO:HG2   | 53:B6:53:ASN:OD1   | 1.96        | 0.66     |
| 8:CI:59:LYS:HB3    | 8:CI:60:LEU:HD23   | 1.78        | 0.66     |
| 47:DF:71:LYS:HG2   | 47:DF:73:VAL:H     | 1.61        | 0.66     |
| 25:BC:94:LEU:HB2   | 25:BC:100:ARG:HD3  | 1.78        | 0.66     |
| 3:CD:25:ARG:HH11   | 3:CD:26:ALA:N      | 1.91        | 0.66     |
| 46:DU:95:PHE:CE1   | 46:DU:102:ILE:HB   | 2.27        | 0.66     |
| 23:BB:1023:U:H2'   | 23:BB:1024:G:H5'   | 1.77        | 0.66     |
| 20:AB:120:SER:HA   | 20:AB:125:PHE:CB   | 2.26        | 0.66     |
| 1:AA:17:U:H2'      | 1:AA:18:C:H6       | 1.61        | 0.66     |
| 1:CA:636:U:H2'     | 1:CA:637:C:C6      | 2.31        | 0.66     |
| 1:AA:868:C:H2'     | 1:AA:869:G:O4'     | 1.94        | 0.66     |
| 42:DN:90:ARG:HB3   | 42:DN:94:TYR:CE1   | 2.31        | 0.66     |
| 50:DT:54:GLU:HG3   | 50:DT:90:GLY:H     | 1.61        | 0.66     |
| 49:DR:34:GLU:HG2   | 49:DR:60:LYS:HG2   | 1.77        | 0.66     |
| 21:AU:36:PHE:HA    | 21:AU:39:LYS:HE3   | 1.76        | 0.66     |
| 12:CM:44:ILE:HA    | 12:CM:47:LEU:HD12  | 1.77        | 0.66     |
| 23:DB:1021:A:H61   | 23:DB:1142:A:N6    | 1.94        | 0.66     |
| 31:B0:21:LEU:HD13  | 45:BS:23:LEU:HD11  | 1.78        | 0.66     |
| 32:D4:7:VAL:HG13   | 32:D4:8:LYS:H      | 1.60        | 0.66     |
| 48:DG:167:VAL:HG23 | 48:DG:168:VAL:H    | 1.60        | 0.66     |
| 23:DB:1796:U:H2'   | 23:DB:1797:G:C8    | 2.30        | 0.66     |
| 26:DD:34:VAL:CG1   | 26:DD:94:GLN:H     | 2.09        | 0.66     |
| 23:BB:1387:A:H2'   | 23:BB:1388:G:H8    | 1.60        | 0.66     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:2241:A:H2'  | 23:DB:2242:G:C8    | 2.31        | 0.66     |
| 23:DB:2153:C:H2'  | 23:DB:2154:A:C8    | 2.31        | 0.66     |
| 23:BB:1594:U:H2'  | 23:BB:1595:C:C6    | 2.29        | 0.66     |
| 20:AB:26:MET:SD   | 20:AB:192:PRO:HD3  | 2.36        | 0.66     |
| 40:DH:2:GLN:O     | 40:DH:3:VAL:HG22   | 1.95        | 0.66     |
| 1:AA:1009:U:H1'   | 1:AA:1021:A:C2     | 2.31        | 0.66     |
| 27:BK:63:VAL:HG21 | 27:BK:85:VAL:HG23  | 1.76        | 0.66     |
| 11:AL:17:LYS:N    | 11:AL:17:LYS:HE3   | 2.11        | 0.66     |
| 1:CA:408:A:OP1    | 3:CD:111:ALA:HB3   | 1.95        | 0.66     |
| 40:DH:27:ARG:H    | 40:DH:31:VAL:CG2   | 2.09        | 0.66     |
| 6:AG:149:ALA:CB   | 10:AK:55:ARG:HE    | 2.01        | 0.66     |
| 26:DD:111:GLY:H   | 26:DD:194:PRO:CG   | 2.08        | 0.66     |
| 38:DM:35:ALA:HB2  | 38:DM:100:LYS:H    | 1.60        | 0.66     |
| 48:BG:15:ASP:CB   | 48:BG:26:LYS:H     | 2.07        | 0.66     |
| 23:BB:1203:U:H4'  | 37:BL:3:LEU:HD12   | 1.78        | 0.66     |
| 26:DD:148:GLN:HB2 | 26:DD:152:PRO:HG2  | 1.76        | 0.66     |
| 23:DB:1080:A:H2'  | 23:DB:1081:U:C6    | 2.30        | 0.66     |
| 26:BD:148:GLN:O   | 26:BD:149:ASN:HB2  | 1.96        | 0.66     |
| 25:BC:158:GLY:N   | 25:BC:194:VAL:HG13 | 2.11        | 0.66     |
| 29:DE:154:ASP:OD2 | 29:DE:157:LEU:HB3  | 1.96        | 0.66     |
| 23:DB:62:U:H3'    | 23:DB:63:A:H8      | 1.61        | 0.66     |
| 1:CA:235:C:H2'    | 1:CA:236:A:C8      | 2.31        | 0.66     |
| 45:DS:95:ARG:HG3  | 45:DS:97:LEU:HD13  | 1.78        | 0.66     |
| 23:DB:2377:A:H2'  | 23:DB:2378:A:C8    | 2.31        | 0.66     |
| 3:AD:2:ARG:NH1    | 3:AD:114:ARG:HG3   | 2.11        | 0.66     |
| 41:BJ:73:VAL:HG23 | 41:BJ:74:TYR:H     | 1.61        | 0.66     |
| 47:DF:161:SER:OG  | 47:DF:164:GLU:HG3  | 1.94        | 0.66     |
| 41:DJ:136:GLN:N   | 41:DJ:137:PRO:HD3  | 2.11        | 0.65     |
| 23:BB:107:G:O2'   | 23:BB:108:G:H5'    | 1.96        | 0.65     |
| 20:CB:44:LYS:C    | 20:CB:47:PRO:HD2   | 2.16        | 0.65     |
| 23:BB:2039:U:H2'  | 23:BB:2040:G:C8    | 2.28        | 0.65     |
| 23:BB:1283:G:N2   | 23:BB:1286:A:H5'   | 2.09        | 0.65     |
| 23:DB:1437:C:H2'  | 23:DB:1438:U:H6    | 1.61        | 0.65     |
| 23:DB:62:U:O2'    | 23:DB:63:A:H5'     | 1.96        | 0.65     |
| 3:CD:53:GLN:HA    | 3:CD:198:LEU:HD22  | 1.78        | 0.65     |
| 1:AA:193:C:H2'    | 1:AA:194:C:C6      | 2.31        | 0.65     |
| 1:CA:868:C:H2'    | 1:CA:869:G:O4'     | 1.96        | 0.65     |
| 23:BB:1853:A:N1   | 23:BB:2087:G:H1'   | 2.11        | 0.65     |
| 1:CA:780:A:O2'    | 1:CA:781:A:H5''    | 1.95        | 0.65     |
| 23:BB:2022:U:O2'  | 23:BB:2617:U:H5'   | 1.96        | 0.65     |
| 1:CA:1086:U:H3    | 1:CA:1099:G:H22    | 1.43        | 0.65     |
| 33:D1:3:GLY:O     | 33:D1:4:ILE:HG12   | 1.96        | 0.65     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 20:AB:63:LYS:HA   | 20:AB:224:ARG:HH11 | 1.60        | 0.65     |
| 2:CC:104:GLU:HG2  | 2:CC:105:VAL:H     | 1.61        | 0.65     |
| 23:BB:2246:G:H2'  | 23:BB:2247:A:C8    | 2.31        | 0.65     |
| 8:AI:5:TYR:HB2    | 8:AI:20:ILE:HB     | 1.77        | 0.65     |
| 25:DC:94:LEU:HB2  | 25:DC:100:ARG:HD3  | 1.77        | 0.65     |
| 32:B4:2:LYS:HG2   | 32:B4:4:ARG:NE     | 2.12        | 0.65     |
| 32:D4:3:VAL:HG23  | 32:D4:4:ARG:H      | 1.61        | 0.65     |
| 23:DB:2884:U:O2   | 31:D0:49:ARG:HG2   | 1.97        | 0.65     |
| 40:DH:73:ASN:OD1  | 40:DH:140:ALA:HB1  | 1.95        | 0.65     |
| 36:D2:21:ARG:HD2  | 36:D2:43:THR:HG21  | 1.77        | 0.65     |
| 23:DB:181:A:H2'   | 23:DB:182:A:H8     | 1.59        | 0.65     |
| 23:DB:2529:G:H4'  | 48:DG:174:LYS:HG3  | 1.77        | 0.65     |
| 23:BB:2841:C:H2'  | 23:BB:2842:G:C8    | 2.30        | 0.65     |
| 39:DX:56:LEU:C    | 39:DX:58:ASN:H     | 2.00        | 0.65     |
| 1:AA:860:A:H2'    | 1:AA:861:G:O4'     | 1.96        | 0.65     |
| 38:BM:30:SER:HA   | 38:BM:133:LYS:HB2  | 1.78        | 0.65     |
| 23:DB:1594:U:H2'  | 23:DB:1595:C:C6    | 2.31        | 0.65     |
| 1:AA:408:A:OP1    | 3:AD:111:ALA:HB3   | 1.97        | 0.65     |
| 15:CP:57:ILE:O    | 15:CP:61:VAL:HG23  | 1.96        | 0.65     |
| 23:BB:1739:A:H2'  | 23:BB:1740:G:O4'   | 1.96        | 0.65     |
| 37:BL:74:THR:HA   | 37:BL:107:PHE:O    | 1.95        | 0.65     |
| 23:DB:2875:C:H2'  | 23:DB:2876:G:H8    | 1.61        | 0.65     |
| 12:CM:28:ARG:NH2  | 12:CM:62:PHE:HB2   | 2.11        | 0.65     |
| 49:BR:34:GLU:HG2  | 49:BR:60:LYS:HG2   | 1.79        | 0.65     |
| 23:DB:2748:A:H4'  | 48:DG:3:VAL:HG21   | 1.78        | 0.65     |
| 40:BH:116:ARG:NH1 | 40:BH:139:PHE:HB2  | 2.12        | 0.65     |
| 53:B6:77:LYS:O    | 53:B6:81:LYS:HG2   | 1.96        | 0.65     |
| 1:AA:764:C:C2'    | 1:AA:765:G:H5'     | 2.26        | 0.65     |
| 18:AS:5:LYS:C     | 18:AS:6:LYS:HD2    | 2.17        | 0.65     |
| 23:BB:1177:G:H2'  | 23:BB:1178:C:C6    | 2.32        | 0.65     |
| 22:DA:32:U:H1'    | 22:DA:52:A:N7      | 2.11        | 0.65     |
| 44:DQ:104:ALA:HA  | 49:DR:46:GLU:CD    | 2.15        | 0.65     |
| 1:CA:203:G:H1'    | 1:CA:465:A:H61     | 1.60        | 0.65     |
| 23:DB:1174:U:H1'  | 23:DB:1176:U:C2    | 2.30        | 0.65     |
| 7:AH:55:LYS:HZ1   | 7:AH:55:LYS:HA     | 1.62        | 0.65     |
| 23:BB:2243:U:H2'  | 23:BB:2244:U:C6    | 2.30        | 0.65     |
| 22:DA:37:C:H2'    | 22:DA:38:C:O4'     | 1.97        | 0.65     |
| 1:CA:57:G:H2'     | 1:CA:58:C:C6       | 2.32        | 0.65     |
| 39:BX:48:ARG:O    | 39:BX:51:ALA:HB3   | 1.96        | 0.65     |
| 1:AA:802:A:H2'    | 1:AA:803:G:O4'     | 1.95        | 0.65     |
| 23:DB:2385:C:H2'  | 23:DB:2386:A:C8    | 2.32        | 0.65     |
| 40:BH:114:GLU:HB3 | 40:BH:134:VAL:HA   | 1.79        | 0.65     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:2443:C:H2'  | 23:DB:2444:G:H8    | 1.61        | 0.65     |
| 24:DI:72:THR:HG22 | 24:DI:115:ASP:OD2  | 1.96        | 0.65     |
| 47:BF:2:LYS:HD2   | 47:BF:100:GLU:HG2  | 1.79        | 0.65     |
| 1:CA:764:C:C2'    | 1:CA:765:G:H5'     | 2.26        | 0.65     |
| 12:CM:78:ARG:O    | 12:CM:82:LEU:HB2   | 1.96        | 0.65     |
| 18:AS:18:VAL:CG2  | 18:AS:43:MET:HB3   | 2.26        | 0.65     |
| 13:AN:53:ASP:HA   | 13:AN:58:ARG:CD    | 2.26        | 0.65     |
| 23:BB:982:C:O2    | 23:BB:982:C:H5'    | 1.96        | 0.65     |
| 13:CN:53:ASP:HA   | 13:CN:58:ARG:CD    | 2.25        | 0.65     |
| 3:AD:116:LEU:HD21 | 3:AD:153:ARG:HD2   | 1.78        | 0.65     |
| 11:AL:85:ARG:HA   | 11:AL:93:ARG:HA    | 1.78        | 0.65     |
| 40:DH:113:SER:N   | 40:DH:132:PHE:HE1  | 1.94        | 0.65     |
| 2:AC:116:ALA:O    | 2:AC:119:ILE:HG22  | 1.96        | 0.65     |
| 1:AA:736:C:H2'    | 1:AA:737:C:C6      | 2.31        | 0.65     |
| 1:CA:577:G:O2'    | 1:CA:578:C:H5'     | 1.97        | 0.65     |
| 53:B6:14:MET:HB3  | 53:B6:168:PHE:CD2  | 2.32        | 0.65     |
| 23:BB:345:A:H1'   | 23:BB:346:A:C2     | 2.31        | 0.65     |
| 23:BB:321:U:H1'   | 29:BE:162:ARG:HH11 | 1.61        | 0.65     |
| 45:DS:29:VAL:HA   | 45:DS:32:ALA:HB3   | 1.78        | 0.65     |
| 24:DI:27:LEU:HD12 | 24:DI:32:VAL:HG11  | 1.76        | 0.65     |
| 24:DI:25:PRO:O    | 24:DI:29:GLN:HG3   | 1.96        | 0.65     |
| 49:DR:49:ILE:HD13 | 49:DR:53:PHE:H     | 1.60        | 0.65     |
| 36:D2:21:ARG:HH21 | 36:D2:43:THR:HG21  | 1.60        | 0.65     |
| 1:AA:336:A:O2'    | 1:AA:337:G:H5'     | 1.97        | 0.65     |
| 23:BB:717:C:H3'   | 23:BB:718:A:H5''   | 1.77        | 0.65     |
| 1:AA:239:U:H4'    | 1:AA:239:U:OP1     | 1.96        | 0.65     |
| 29:BE:46:GLN:HG3  | 29:BE:87:ALA:HB3   | 1.79        | 0.65     |
| 1:AA:781:A:H2'    | 1:AA:782:A:H5'     | 1.76        | 0.65     |
| 23:DB:2710:C:H2'  | 23:DB:2711:A:H8    | 1.60        | 0.65     |
| 1:AA:68:G:H5'     | 1:AA:171:A:H1'     | 1.78        | 0.65     |
| 9:AJ:37:ARG:NE    | 9:AJ:37:ARG:HA     | 2.11        | 0.65     |
| 27:DK:24:VAL:HG13 | 27:DK:33:ALA:HB2   | 1.78        | 0.65     |
| 23:DB:811:U:OP2   | 37:DL:20:GLY:HA2   | 1.97        | 0.65     |
| 27:DK:63:VAL:HG21 | 27:DK:85:VAL:HG23  | 1.76        | 0.65     |
| 25:DC:41:GLY:HA3  | 25:DC:53:ILE:HG21  | 1.78        | 0.65     |
| 47:DF:65:LEU:HD23 | 47:DF:87:LYS:HD2   | 1.78        | 0.65     |
| 27:DK:47:ILE:CG1  | 27:DK:48:PRO:HD2   | 2.24        | 0.65     |
| 8:AI:64:ILE:HD12  | 8:AI:64:ILE:H      | 1.61        | 0.65     |
| 25:BC:128:THR:HA  | 25:BC:190:THR:CA   | 2.25        | 0.65     |
| 13:AN:25:GLU:HB2  | 13:AN:29:ILE:HD11  | 1.78        | 0.65     |
| 2:CC:72:PRO:O     | 2:CC:76:ILE:HG12   | 1.96        | 0.65     |
| 32:B4:7:VAL:HB    | 32:B4:36:ARG:O     | 1.97        | 0.65     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 21:CU:3:ILE:HG21  | 21:CU:19:LYS:HG3   | 1.76        | 0.65     |
| 23:DB:1460:U:H4'  | 23:DB:1461:C:O5'   | 1.97        | 0.65     |
| 49:BR:49:ILE:HD13 | 49:BR:53:PHE:H     | 1.59        | 0.65     |
| 23:DB:2897:U:H2'  | 23:DB:2898:U:C6    | 2.32        | 0.65     |
| 1:CA:270:A:H2'    | 1:CA:271:C:H6      | 1.59        | 0.65     |
| 23:BB:773:U:H4'   | 25:BC:45:ASN:O     | 1.97        | 0.65     |
| 3:AD:171:GLU:HB2  | 3:AD:180:THR:HB    | 1.78        | 0.65     |
| 23:DB:857:G:C2'   | 23:DB:858:G:H5'    | 2.27        | 0.65     |
| 23:BB:121:G:H2'   | 23:BB:122:G:C8     | 2.31        | 0.65     |
| 23:DB:1178:C:H2'  | 23:DB:1179:G:C8    | 2.32        | 0.65     |
| 6:CG:21:LEU:HG    | 6:CG:22:LEU:H      | 1.61        | 0.65     |
| 3:CD:2:ARG:NH1    | 3:CD:114:ARG:HG3   | 2.12        | 0.65     |
| 23:BB:1993:U:H4'  | 26:BD:133:THR:HG22 | 1.78        | 0.65     |
| 39:DX:39:GLN:HB3  | 39:DX:42:LEU:HD13  | 1.77        | 0.65     |
| 23:BB:2579:C:O2'  | 26:BD:136:ASN:HA   | 1.97        | 0.65     |
| 23:DB:2630:G:H2'  | 23:DB:2631:G:H8    | 1.62        | 0.65     |
| 1:CA:501:C:H2'    | 1:CA:502:A:H8      | 1.62        | 0.65     |
| 9:AJ:22:THR:OG1   | 9:AJ:72:ARG:HG3    | 1.96        | 0.65     |
| 23:BB:2216:G:H2'  | 23:BB:2217:G:H8    | 1.62        | 0.65     |
| 6:CG:102:TRP:HZ3  | 6:CG:137:ARG:HB2   | 1.62        | 0.65     |
| 40:DH:62:LEU:HG   | 40:DH:66:ASN:ND2   | 2.11        | 0.65     |
| 1:AA:1521:C:H2'   | 1:AA:1522:U:C6     | 2.32        | 0.65     |
| 23:DB:1739:A:H2'  | 23:DB:1740:G:O4'   | 1.96        | 0.65     |
| 25:BC:86:ARG:NH1  | 25:BC:86:ARG:HB3   | 2.11        | 0.65     |
| 48:BG:84:LYS:HG3  | 48:BG:131:VAL:CA   | 2.27        | 0.65     |
| 44:DQ:27:ARG:HA   | 44:DQ:33:VAL:HG23  | 1.79        | 0.65     |
| 26:BD:34:VAL:HA   | 26:BD:50:VAL:HG12  | 1.77        | 0.65     |
| 41:BJ:136:GLN:N   | 41:BJ:137:PRO:HD3  | 2.11        | 0.65     |
| 41:DJ:43:GLU:O    | 41:DJ:45:THR:N     | 2.29        | 0.65     |
| 23:DB:851:C:O4'   | 30:DY:46:MET:HG2   | 1.96        | 0.65     |
| 26:DD:34:VAL:HG12 | 26:DD:94:GLN:H     | 1.61        | 0.65     |
| 20:CB:57:ASN:HB2  | 20:CB:219:THR:O    | 1.97        | 0.65     |
| 23:BB:1790:C:H2'  | 23:BB:1791:A:C8    | 2.32        | 0.65     |
| 45:BS:6:LYS:HB3   | 45:BS:104:THR:HA   | 1.78        | 0.65     |
| 23:BB:1386:C:H2'  | 23:BB:1387:A:C8    | 2.32        | 0.65     |
| 23:BB:1469:A:H2'  | 23:BB:1470:A:C8    | 2.32        | 0.65     |
| 1:CA:524:G:H2'    | 1:CA:525:C:C6      | 2.32        | 0.65     |
| 1:AA:6:G:H4'      | 1:AA:298:A:H4'     | 1.79        | 0.65     |
| 15:CP:76:LYS:NZ   | 15:CP:80:LYS:HD3   | 2.11        | 0.65     |
| 23:BB:2229:U:H2'  | 23:BB:2230:G:H8    | 1.62        | 0.65     |
| 1:AA:1163:A:H2'   | 1:AA:1164:G:H8     | 1.62        | 0.65     |
| 22:DA:111:U:H2'   | 22:DA:112:G:C8     | 2.32        | 0.65     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 2:AC:81:GLU:HG3    | 2:AC:82:ASP:N      | 2.11        | 0.65     |
| 37:DL:123:ARG:HA   | 37:DL:143:GLU:CB   | 2.21        | 0.65     |
| 53:D6:77:LYS:O     | 53:D6:81:LYS:HG3   | 1.96        | 0.65     |
| 1:AA:920:U:H2'     | 1:AA:921:U:H6      | 1.62        | 0.65     |
| 1:AA:1316:G:N2     | 1:AA:1318:A:H3'    | 2.11        | 0.65     |
| 32:B4:7:VAL:HG13   | 32:B4:8:LYS:H      | 1.60        | 0.65     |
| 45:BS:22:ASP:HA    | 45:BS:25:ARG:NH1   | 2.12        | 0.65     |
| 36:B2:21:ARG:HD2   | 36:B2:43:THR:HG21  | 1.78        | 0.65     |
| 1:CA:1478:U:H2'    | 1:CA:1479:C:C6     | 2.32        | 0.65     |
| 1:CA:781:A:H2'     | 1:CA:782:A:H5'     | 1.78        | 0.65     |
| 1:AA:859:G:H2'     | 1:AA:860:A:C8      | 2.31        | 0.65     |
| 23:BB:2246:G:H2'   | 23:BB:2247:A:H8    | 1.61        | 0.65     |
| 23:BB:2567:G:H2'   | 23:BB:2568:U:C6    | 2.32        | 0.65     |
| 23:BB:1192:G:O2'   | 23:BB:1193:G:H5'   | 1.96        | 0.65     |
| 1:CA:394:G:H2'     | 1:CA:395:C:H6      | 1.59        | 0.65     |
| 23:DB:2852:G:H2'   | 23:DB:2853:C:C6    | 2.31        | 0.65     |
| 23:DB:1813:G:N3    | 25:DC:49:THR:HG21  | 2.11        | 0.65     |
| 3:AD:97:LEU:HB2    | 3:AD:134:TYR:HB3   | 1.77        | 0.65     |
| 1:AA:806:C:H2'     | 1:AA:807:A:C8      | 2.32        | 0.65     |
| 23:BB:2461:A:H2'   | 23:BB:2462:C:C6    | 2.32        | 0.65     |
| 40:DH:31:VAL:O     | 40:DH:32:PRO:C     | 2.34        | 0.65     |
| 23:DB:1827:U:O2'   | 23:DB:1828:G:H5'   | 1.97        | 0.65     |
| 23:DB:1012:U:O4    | 41:DJ:30:THR:HG21  | 1.97        | 0.65     |
| 25:BC:196:ASN:ND2  | 25:BC:199:HIS:HB2  | 2.11        | 0.65     |
| 16:AQ:46:HIS:HB2   | 16:AQ:66:LEU:HD13  | 1.79        | 0.65     |
| 23:BB:1171:G:C4    | 23:BB:1172:C:H1'   | 2.32        | 0.65     |
| 21:CU:24:LYS:HD2   | 21:CU:25:ALA:N     | 2.12        | 0.65     |
| 24:DI:42:ASN:HA    | 24:DI:45:THR:OG1   | 1.96        | 0.65     |
| 49:DR:28:ALA:O     | 49:DR:63:VAL:HG21  | 1.96        | 0.65     |
| 46:DU:72:PHE:HA    | 46:DU:78:LYS:O     | 1.97        | 0.65     |
| 23:BB:2820:A:OP1   | 42:BN:4:ARG:HA     | 1.97        | 0.65     |
| 39:BX:17:GLU:HB3   | 39:BX:53:VAL:HG11  | 1.77        | 0.65     |
| 1:CA:1524:C:H2'    | 1:CA:1525:G:C8     | 2.32        | 0.65     |
| 23:DB:1181:U:H2'   | 23:DB:1182:G:H8    | 1.60        | 0.65     |
| 23:BB:1593:A:H2'   | 23:BB:1594:U:C6    | 2.31        | 0.65     |
| 4:CE:106:ALA:HB1   | 4:CE:110:MET:HB3   | 1.77        | 0.65     |
| 1:AA:793:U:O2      | 1:AA:1516:G:H4'    | 1.97        | 0.65     |
| 20:CB:172:ILE:HG22 | 20:CB:176:ASN:HD21 | 1.61        | 0.65     |
| 23:DB:2461:A:H2'   | 23:DB:2462:C:C6    | 2.32        | 0.65     |
| 39:BX:39:GLN:HB3   | 39:BX:42:LEU:HD13  | 1.78        | 0.65     |
| 25:DC:239:PHE:O    | 25:DC:241:LYS:HG3  | 1.96        | 0.65     |
| 22:BA:25:U:OP1     | 22:BA:25:U:H3'     | 1.96        | 0.65     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1192:G:O2'   | 23:DB:1193:G:H5'   | 1.96        | 0.65     |
| 25:DC:67:LYS:HD3   | 25:DC:150:GLY:HA2  | 1.77        | 0.65     |
| 23:BB:21:A:H2'     | 23:BB:22:C:C6      | 2.32        | 0.65     |
| 40:BH:90:LEU:HD21  | 40:BH:146:VAL:HG11 | 1.79        | 0.65     |
| 1:AA:1314:C:N4     | 18:AS:3:SER:HB3    | 2.12        | 0.65     |
| 23:DB:1788:C:O2'   | 23:DB:1789:A:H5'   | 1.97        | 0.65     |
| 23:DB:594:U:H2'    | 23:DB:595:C:C6     | 2.31        | 0.65     |
| 15:CP:25:ARG:HD3   | 15:CP:25:ARG:H     | 1.61        | 0.65     |
| 46:DU:78:LYS:HD3   | 46:DU:79:ALA:H     | 1.61        | 0.65     |
| 23:DB:559:G:H21    | 44:DQ:51:GLN:NE2   | 1.95        | 0.65     |
| 46:BU:70:ALA:HB1   | 46:BU:79:ALA:CB    | 2.27        | 0.65     |
| 23:DB:1150:C:H2'   | 23:DB:1151:A:H8    | 1.61        | 0.65     |
| 15:AP:57:ILE:O     | 15:AP:61:VAL:HG23  | 1.97        | 0.65     |
| 49:DR:19:THR:HB    | 49:DR:97:LYS:HA    | 1.78        | 0.65     |
| 5:CF:53:LYS:HE2    | 5:CF:53:LYS:HA     | 1.79        | 0.65     |
| 40:BH:57:LYS:HG3   | 40:BH:58:LEU:N     | 2.12        | 0.65     |
| 23:DB:1355:G:O2'   | 23:DB:1356:G:H5'   | 1.97        | 0.65     |
| 10:CK:110:THR:HG22 | 21:CU:4:LYS:HA     | 1.79        | 0.65     |
| 23:BB:664:G:H2'    | 23:BB:665:U:H6     | 1.62        | 0.65     |
| 46:BU:48:VAL:C     | 46:BU:53:GLN:HG3   | 2.16        | 0.65     |
| 23:BB:2710:C:H2'   | 23:BB:2711:A:H8    | 1.62        | 0.65     |
| 23:DB:1571:A:H2'   | 23:DB:1572:A:C8    | 2.32        | 0.65     |
| 23:DB:1821:A:H2'   | 23:DB:1822:C:C6    | 2.31        | 0.64     |
| 25:DC:64:VAL:HG11  | 25:DC:66:PHE:CE2   | 2.32        | 0.64     |
| 5:CF:29:ILE:HG22   | 5:CF:34:GLY:HA3    | 1.79        | 0.64     |
| 16:CQ:46:HIS:HB2   | 16:CQ:66:LEU:HD13  | 1.78        | 0.64     |
| 46:BU:85:ARG:HD3   | 46:BU:86:PHE:N     | 2.12        | 0.64     |
| 23:DB:27:G:H1'     | 23:DB:513:A:N6     | 2.12        | 0.64     |
| 27:DK:43:ILE:HG22  | 27:DK:54:LYS:HA    | 1.78        | 0.64     |
| 23:BB:593:U:H2'    | 23:BB:594:U:C6     | 2.33        | 0.64     |
| 1:AA:1239:A:H62    | 1:AA:1299:A:H62    | 1.44        | 0.64     |
| 1:CA:1002:G:H2'    | 1:CA:1003:G:O4'    | 1.96        | 0.64     |
| 1:AA:270:A:H2'     | 1:AA:271:C:H6      | 1.61        | 0.64     |
| 1:CA:108:G:C6      | 19:CT:9:ARG:HG2    | 2.32        | 0.64     |
| 23:DB:321:U:H1'    | 29:DE:162:ARG:HH11 | 1.62        | 0.64     |
| 23:BB:2135:A:H3'   | 23:BB:2136:G:H8    | 1.62        | 0.64     |
| 1:AA:264:C:O2'     | 16:AQ:65:PRO:HG2   | 1.98        | 0.64     |
| 1:CA:147:G:H2'     | 1:CA:148:G:C8      | 2.31        | 0.64     |
| 1:AA:147:G:H2'     | 1:AA:148:G:C8      | 2.32        | 0.64     |
| 23:DB:1812:U:H2'   | 23:DB:1813:G:H8    | 1.60        | 0.64     |
| 23:DB:1684:G:H2'   | 23:DB:1685:C:H6    | 1.61        | 0.64     |
| 3:CD:148:ALA:O     | 3:CD:151:GLN:HB2   | 1.97        | 0.64     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 37:BL:143:GLU:CG   | 37:BL:144:GLU:H    | 2.10        | 0.64     |
| 26:BD:34:VAL:HB    | 26:BD:48:ILE:HD11  | 1.78        | 0.64     |
| 25:DC:14:HIS:O     | 25:DC:203:VAL:HG11 | 1.97        | 0.64     |
| 37:BL:19:LEU:O     | 37:BL:21:ARG:HG2   | 1.97        | 0.64     |
| 45:BS:25:ARG:HE    | 45:BS:73:LYS:NZ    | 1.95        | 0.64     |
| 49:DR:66:HIS:ND1   | 49:DR:94:THR:HG22  | 2.12        | 0.64     |
| 28:DP:20:ARG:O     | 28:DP:46:VAL:HG21  | 1.98        | 0.64     |
| 23:DB:742:A:H2'    | 23:DB:743:A:C8     | 2.33        | 0.64     |
| 6:CG:21:LEU:H      | 6:CG:21:LEU:HD23   | 1.62        | 0.64     |
| 23:DB:309:A:H4'    | 46:DU:15:GLY:HA3   | 1.79        | 0.64     |
| 23:BB:2097:A:H2'   | 23:BB:2098:U:C6    | 2.32        | 0.64     |
| 25:DC:219:VAL:HG12 | 25:DC:224:MET:HE2  | 1.78        | 0.64     |
| 1:AA:394:G:H2'     | 1:AA:395:C:H6      | 1.60        | 0.64     |
| 1:CA:371:A:O2'     | 1:CA:372:C:H5'     | 1.97        | 0.64     |
| 19:CT:43:LYS:HE2   | 19:CT:44:ALA:H     | 1.61        | 0.64     |
| 1:AA:797:C:O2'     | 1:AA:798:U:H5'     | 1.98        | 0.64     |
| 1:CA:1009:U:H1'    | 1:CA:1021:A:C2     | 2.32        | 0.64     |
| 23:BB:693:A:H2'    | 23:BB:694:U:C6     | 2.32        | 0.64     |
| 3:AD:88:ASN:O      | 3:AD:92:LEU:HD23   | 1.97        | 0.64     |
| 7:AH:28:SER:OG     | 7:AH:56:PRO:HB2    | 1.96        | 0.64     |
| 6:AG:66:GLU:HA     | 6:AG:69:ARG:HD2    | 1.79        | 0.64     |
| 25:BC:94:LEU:HD13  | 25:BC:100:ARG:HD3  | 1.79        | 0.64     |
| 51:DZ:40:VAL:HG22  | 51:DZ:45:ARG:O     | 1.98        | 0.64     |
| 3:CD:25:ARG:NH1    | 3:CD:26:ALA:H      | 1.92        | 0.64     |
| 47:BF:102:LEU:HA   | 47:BF:106:ALA:HB2  | 1.78        | 0.64     |
| 4:CE:15:ILE:HD12   | 4:CE:35:LEU:HG     | 1.79        | 0.64     |
| 23:BB:27:G:H1'     | 23:BB:513:A:N6     | 2.13        | 0.64     |
| 35:BV:40:ILE:HD13  | 35:BV:40:ILE:N     | 2.12        | 0.64     |
| 23:BB:170:U:H2'    | 23:BB:171:U:H6     | 1.60        | 0.64     |
| 23:DB:1443:U:H2'   | 23:DB:1444:G:H8    | 1.62        | 0.64     |
| 23:DB:1550:C:H2'   | 23:DB:1551:A:C8    | 2.32        | 0.64     |
| 40:DH:67:ALA:O     | 40:DH:70:GLU:HG3   | 1.96        | 0.64     |
| 24:DI:126:ARG:HB3  | 24:DI:126:ARG:HH11 | 1.62        | 0.64     |
| 23:BB:1442:U:H2'   | 23:BB:1443:U:C6    | 2.32        | 0.64     |
| 45:DS:6:LYS:HB3    | 45:DS:104:THR:HA   | 1.79        | 0.64     |
| 23:DB:170:U:H2'    | 23:DB:171:U:H6     | 1.62        | 0.64     |
| 23:BB:1778:U:H2'   | 23:BB:1784:A:H62   | 1.61        | 0.64     |
| 11:AL:106:VAL:HG23 | 11:AL:116:TYR:HB3  | 1.79        | 0.64     |
| 6:AG:21:LEU:H      | 6:AG:21:LEU:HD23   | 1.63        | 0.64     |
| 23:DB:1866:A:H2'   | 23:DB:1867:G:O4'   | 1.97        | 0.64     |
| 19:CT:60:GLN:HB3   | 19:CT:65:LEU:HD23  | 1.77        | 0.64     |
| 23:DB:521:U:H2'    | 23:DB:522:A:C8     | 2.33        | 0.64     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1000:A:H2'  | 23:BB:1001:A:C8    | 2.32        | 0.64     |
| 45:BS:95:ARG:HG3  | 45:BS:97:LEU:HD13  | 1.79        | 0.64     |
| 33:B1:3:GLY:O     | 33:B1:4:ILE:HG12   | 1.98        | 0.64     |
| 1:CA:678:U:H2'    | 1:CA:679:C:C6      | 2.33        | 0.64     |
| 1:AA:1053:G:N7    | 1:AA:1200:C:H5''   | 2.11        | 0.64     |
| 52:DW:49:ASN:HB3  | 52:DW:81:ILE:CG1   | 2.28        | 0.64     |
| 29:DE:58:LYS:HZ2  | 29:DE:58:LYS:H     | 1.43        | 0.64     |
| 12:CM:12:LYS:HB3  | 12:CM:16:ILE:HG23  | 1.79        | 0.64     |
| 53:B6:111:ARG:O   | 53:B6:115:VAL:HG23 | 1.97        | 0.64     |
| 29:BE:136:GLN:NE2 | 29:BE:139:LYS:HD3  | 2.12        | 0.64     |
| 24:BI:129:GLU:HB3 | 24:BI:133:ARG:NH1  | 2.11        | 0.64     |
| 45:BS:26:GLY:H    | 45:BS:71:VAL:HG13  | 1.60        | 0.64     |
| 24:DI:41:PHE:O    | 24:DI:45:THR:HG23  | 1.98        | 0.64     |
| 48:BG:30:GLY:CA   | 48:BG:78:VAL:HA    | 2.28        | 0.64     |
| 2:CC:119:ILE:HG21 | 2:CC:197:VAL:HG11  | 1.79        | 0.64     |
| 46:DU:35:VAL:HB   | 46:DU:38:ILE:CG2   | 2.27        | 0.64     |
| 1:CA:1011:C:H2'   | 1:CA:1012:A:H8     | 1.61        | 0.64     |
| 1:CA:255:G:H2'    | 1:CA:256:U:C6      | 2.33        | 0.64     |
| 4:CE:81:GLN:H     | 4:CE:146:MET:HE3   | 1.61        | 0.64     |
| 23:BB:557:C:H2'   | 23:BB:558:U:C6     | 2.33        | 0.64     |
| 39:DX:21:LEU:HA   | 39:DX:25:GLN:HE21  | 1.62        | 0.64     |
| 44:BQ:101:ASP:HB2 | 49:BR:2:TYR:OH     | 1.98        | 0.64     |
| 23:DB:2841:C:H2'  | 23:DB:2842:G:C8    | 2.31        | 0.64     |
| 39:BX:56:LEU:C    | 39:BX:58:ASN:H     | 2.01        | 0.64     |
| 23:DB:2066:C:O2'  | 23:DB:2067:G:H5'   | 1.96        | 0.64     |
| 23:DB:2635:A:H5'  | 26:DD:79:LEU:HD23  | 1.80        | 0.64     |
| 24:BI:7:TYR:HB2   | 24:BI:58:ILE:O     | 1.97        | 0.64     |
| 20:CB:52:ALA:O    | 20:CB:56:LEU:HB2   | 1.98        | 0.64     |
| 23:DB:1915:U:O5'  | 23:DB:1915:U:H6    | 1.81        | 0.64     |
| 23:DB:664:G:H2'   | 23:DB:665:U:H6     | 1.61        | 0.64     |
| 52:DW:23:LYS:C    | 52:DW:66:VAL:HB    | 2.18        | 0.64     |
| 41:DJ:18:VAL:HG12 | 41:DJ:54:ILE:HD11  | 1.79        | 0.64     |
| 41:BJ:44:TYR:CD2  | 44:BQ:59:LEU:HD21  | 2.31        | 0.64     |
| 23:BB:2849:U:H4'  | 23:BB:2850:A:C5'   | 2.28        | 0.64     |
| 32:B4:3:VAL:HG23  | 32:B4:4:ARG:H      | 1.62        | 0.64     |
| 16:AQ:8:GLN:HA    | 16:AQ:59:GLU:HA    | 1.80        | 0.64     |
| 23:DB:819:A:H5'   | 23:DB:973:A:N1     | 2.13        | 0.64     |
| 23:BB:2884:U:O2   | 31:B0:49:ARG:HG2   | 1.98        | 0.64     |
| 15:AP:68:SER:OG   | 15:AP:71:VAL:HG12  | 1.98        | 0.64     |
| 23:BB:1447:C:H2'  | 23:BB:1448:G:C8    | 2.33        | 0.64     |
| 1:CA:1239:A:H62   | 1:CA:1299:A:H62    | 1.44        | 0.64     |
| 14:CO:26:GLU:HA   | 14:CO:81:LEU:HD11  | 1.78        | 0.64     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 22:BA:75:G:H1      | 22:BA:102:G:H22   | 1.42        | 0.64     |
| 26:BD:113:SER:HB2  | 26:BD:168:GLU:H   | 1.61        | 0.64     |
| 19:AT:61:ALA:HA    | 19:AT:67:HIS:H    | 1.60        | 0.64     |
| 23:DB:125:A:H3'    | 23:DB:126:A:C5'   | 2.28        | 0.64     |
| 39:BX:21:LEU:HA    | 39:BX:25:GLN:HE21 | 1.62        | 0.64     |
| 23:DB:1387:A:H2'   | 23:DB:1388:G:H8   | 1.62        | 0.64     |
| 37:DL:3:LEU:O      | 37:DL:5:THR:HG23  | 1.98        | 0.64     |
| 29:DE:46:GLN:HG3   | 29:DE:87:ALA:HB3  | 1.77        | 0.64     |
| 12:CM:6:ILE:O      | 12:CM:8:ILE:HG23  | 1.97        | 0.64     |
| 23:BB:75:G:H4'     | 39:BX:48:ARG:HH22 | 1.62        | 0.64     |
| 45:BS:84:ARG:HB3   | 45:BS:96:ILE:HG23 | 1.79        | 0.64     |
| 23:BB:1889:A:H2'   | 23:BB:1890:A:C8   | 2.33        | 0.64     |
| 14:CO:11:ILE:HD11  | 14:CO:30:ALA:HB1  | 1.80        | 0.64     |
| 23:DB:1406:U:H2'   | 23:DB:1407:G:H8   | 1.61        | 0.64     |
| 23:DB:1042:G:H2'   | 23:DB:1043:C:C6   | 2.31        | 0.64     |
| 9:CJ:22:THR:OG1    | 9:CJ:72:ARG:HG3   | 1.97        | 0.64     |
| 23:BB:1355:G:O2'   | 23:BB:1356:G:H5'  | 1.96        | 0.64     |
| 23:BB:2027:G:O2'   | 23:BB:2028:U:H5'  | 1.97        | 0.64     |
| 23:BB:753:A:H2'    | 23:BB:754:U:C6    | 2.32        | 0.64     |
| 49:BR:72:VAL:HG23  | 49:BR:89:HIS:HB3  | 1.80        | 0.64     |
| 43:DO:47:VAL:HG12  | 43:DO:48:LEU:H    | 1.61        | 0.64     |
| 23:BB:328:U:H4'    | 46:BU:65:GLN:NE2  | 2.13        | 0.64     |
| 23:DB:2415:G:H4'   | 37:DL:66:PHE:HB2  | 1.79        | 0.64     |
| 50:DT:68:LYS:O     | 50:DT:69:ARG:HB3  | 1.98        | 0.64     |
| 52:BW:23:LYS:HZ3   | 52:BW:24:ARG:HG3  | 1.62        | 0.64     |
| 23:BB:1821:A:H2'   | 23:BB:1822:C:C6   | 2.32        | 0.64     |
| 37:DL:123:ARG:HH11 | 37:DL:123:ARG:HB3 | 1.63        | 0.64     |
| 25:BC:116:GLN:HG2  | 25:BC:117:SER:H   | 1.62        | 0.64     |
| 30:DY:40:THR:O     | 30:DY:43:ILE:HG23 | 1.98        | 0.64     |
| 51:BZ:33:LEU:HA    | 51:BZ:52:SER:HA   | 1.79        | 0.64     |
| 30:BY:15:ARG:O     | 30:BY:20:LYS:HE3  | 1.97        | 0.64     |
| 1:CA:1225:A:H3'    | 1:CA:1226:C:C6    | 2.32        | 0.64     |
| 18:AS:43:MET:O     | 18:AS:46:LEU:HB2  | 1.96        | 0.64     |
| 29:DE:149:ILE:HG23 | 29:DE:188:MET:HA  | 1.78        | 0.64     |
| 48:DG:30:GLY:CA    | 48:DG:78:VAL:HA   | 2.27        | 0.64     |
| 40:DH:113:SER:HB2  | 40:DH:132:PHE:HZ  | 1.62        | 0.64     |
| 42:DN:90:ARG:HB3   | 42:DN:94:TYR:HE1  | 1.61        | 0.64     |
| 23:DB:1593:A:H2'   | 23:DB:1594:U:C6   | 2.33        | 0.64     |
| 2:CC:81:GLU:HG3    | 2:CC:82:ASP:N     | 2.13        | 0.64     |
| 23:BB:1166:G:H2'   | 23:BB:1167:C:C6   | 2.33        | 0.64     |
| 1:AA:407:U:O2'     | 3:AD:112:GLU:HG3  | 1.97        | 0.64     |
| 23:DB:1381:G:C2'   | 23:DB:1382:G:H5'  | 2.27        | 0.64     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:296:U:H2'   | 23:DB:297:G:H8     | 1.62        | 0.64     |
| 23:DB:937:C:H2'   | 23:DB:938:G:H8     | 1.63        | 0.64     |
| 44:DQ:30:VAL:HG11 | 44:DQ:33:VAL:HG22  | 1.79        | 0.64     |
| 41:DJ:44:TYR:CD2  | 44:DQ:59:LEU:HD21  | 2.33        | 0.64     |
| 50:BT:1:MET:HG3   | 50:BT:2:ILE:H      | 1.61        | 0.64     |
| 46:BU:3:LYS:HD3   | 46:BU:82:VAL:HG21  | 1.79        | 0.64     |
| 22:BA:28:C:C4     | 22:BA:56:G:N1      | 2.66        | 0.64     |
| 4:CE:113:VAL:HG11 | 4:CE:136:VAL:HG23  | 1.80        | 0.64     |
| 45:BS:29:VAL:HA   | 45:BS:32:ALA:HB3   | 1.80        | 0.64     |
| 23:DB:2884:U:H2'  | 23:DB:2885:G:C8    | 2.32        | 0.64     |
| 1:CA:269:C:H2'    | 1:CA:270:A:H8      | 1.61        | 0.64     |
| 1:AA:108:G:C6     | 19:AT:9:ARG:HG2    | 2.32        | 0.64     |
| 23:BB:1486:U:H2'  | 23:BB:1487:U:H6    | 1.63        | 0.64     |
| 1:CA:254:G:OP1    | 16:CQ:68:LYS:O     | 2.15        | 0.64     |
| 39:BX:1:MET:O     | 39:BX:5:GLU:HG2    | 1.98        | 0.64     |
| 6:CG:134:VAL:O    | 6:CG:138:GLU:HG3   | 1.97        | 0.64     |
| 1:AA:366:A:H1'    | 1:AA:395:C:O2      | 1.98        | 0.64     |
| 1:CA:678:U:H2'    | 1:CA:679:C:H6      | 1.62        | 0.64     |
| 50:DT:69:ARG:HG2  | 50:DT:73:ARG:O     | 1.98        | 0.64     |
| 1:AA:1007:U:H2'   | 1:AA:1008:U:C6     | 2.33        | 0.64     |
| 43:DO:9:ARG:HG3   | 43:DO:10:ARG:N     | 2.13        | 0.64     |
| 23:DB:1259:G:H2'  | 23:DB:1260:A:H8    | 1.63        | 0.64     |
| 7:CH:94:VAL:HG23  | 7:CH:101:ALA:HB2   | 1.80        | 0.64     |
| 51:BZ:11:ARG:HB3  | 51:BZ:12:PRO:HD2   | 1.79        | 0.64     |
| 1:AA:1225:A:H3'   | 1:AA:1226:C:C6     | 2.32        | 0.64     |
| 11:CL:79:ILE:HG22 | 11:CL:103:CYS:HB2  | 1.80        | 0.64     |
| 52:BW:35:ILE:HG12 | 52:BW:35:ILE:O     | 1.97        | 0.64     |
| 23:BB:18:U:H2'    | 23:BB:19:A:H8      | 1.63        | 0.64     |
| 44:DQ:86:SER:CB   | 49:DR:51:VAL:HA    | 2.28        | 0.64     |
| 35:DV:62:THR:HB   | 35:DV:71:LYS:HG2   | 1.79        | 0.64     |
| 42:DN:8:ARG:HH21  | 42:DN:39:PRO:HB3   | 1.62        | 0.64     |
| 44:BQ:63:ARG:HH21 | 44:BQ:64:ILE:HD11  | 1.61        | 0.64     |
| 29:DE:136:GLN:NE2 | 29:DE:139:LYS:HD3  | 2.12        | 0.64     |
| 23:BB:2751:G:N3   | 23:BB:2751:G:H2'   | 2.12        | 0.64     |
| 38:DM:30:SER:HA   | 38:DM:133:LYS:HB2  | 1.79        | 0.64     |
| 40:DH:4:ILE:HG22  | 40:DH:17:ASP:N     | 2.12        | 0.64     |
| 25:DC:158:GLY:N   | 25:DC:194:VAL:HG13 | 2.13        | 0.64     |
| 23:BB:1486:U:H2'  | 23:BB:1487:U:C6    | 2.32        | 0.64     |
| 23:DB:1486:U:H2'  | 23:DB:1487:U:C6    | 2.32        | 0.64     |
| 23:DB:18:U:H2'    | 23:DB:19:A:H8      | 1.62        | 0.64     |
| 23:DB:2246:G:H2'  | 23:DB:2247:A:C8    | 2.33        | 0.64     |
| 1:AA:57:G:H2'     | 1:AA:58:C:C6       | 2.33        | 0.64     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 19:AT:60:GLN:HB3   | 19:AT:65:LEU:HD23  | 1.79        | 0.64     |
| 20:CB:26:MET:SD    | 20:CB:192:PRO:HD3  | 2.38        | 0.64     |
| 2:AC:104:GLU:HG2   | 2:AC:105:VAL:H     | 1.62        | 0.64     |
| 22:BA:111:U:H2'    | 22:BA:112:G:C8     | 2.33        | 0.64     |
| 11:CL:35:ARG:NH1   | 53:D6:104:PRO:HB3  | 2.13        | 0.64     |
| 23:DB:2385:C:H2'   | 23:DB:2386:A:H8    | 1.61        | 0.64     |
| 23:BB:2019:A:H4'   | 44:BQ:33:VAL:HG11  | 1.78        | 0.64     |
| 44:BQ:27:ARG:HA    | 44:BQ:33:VAL:HG23  | 1.79        | 0.64     |
| 53:B6:42:LYS:HG2   | 53:B6:51:PRO:HB3   | 1.80        | 0.64     |
| 53:B6:75:ALA:O     | 53:B6:79:ILE:HD12  | 1.98        | 0.64     |
| 13:CN:65:GLN:HG2   | 13:CN:82:LYS:HE2   | 1.80        | 0.64     |
| 23:DB:1256:G:H21   | 29:DE:77:ILE:HG22  | 1.62        | 0.64     |
| 42:BN:8:ARG:HH21   | 42:BN:39:PRO:HB3   | 1.61        | 0.64     |
| 23:BB:2306:C:H3'   | 23:BB:2307:G:H5''  | 1.79        | 0.64     |
| 47:DF:8:LYS:HA     | 47:DF:12:VAL:HG21  | 1.80        | 0.64     |
| 23:DB:1789:A:P     | 25:DC:220:ARG:HD3  | 2.38        | 0.64     |
| 29:BE:109:LEU:HD12 | 29:BE:112:LEU:HD12 | 1.78        | 0.64     |
| 1:CA:1003:G:N2     | 1:CA:1005:A:H5'    | 2.12        | 0.64     |
| 23:BB:131:A:H2'    | 23:BB:132:G:C8     | 2.32        | 0.64     |
| 23:DB:1582:C:H2'   | 23:DB:1583:A:O4'   | 1.98        | 0.64     |
| 23:DB:1381:G:H2'   | 23:DB:1382:G:H5'   | 1.79        | 0.64     |
| 1:AA:1226:C:C4     | 12:AM:102:LYS:HB3  | 2.33        | 0.64     |
| 52:DW:77:LYS:NZ    | 52:DW:77:LYS:H     | 1.96        | 0.64     |
| 38:DM:108:VAL:HG13 | 38:DM:112:LEU:HB3  | 1.78        | 0.64     |
| 6:AG:135:LYS:HD3   | 6:AG:136:LYS:N     | 2.12        | 0.64     |
| 23:DB:1000:A:H2'   | 23:DB:1001:A:C8    | 2.32        | 0.64     |
| 1:AA:213:G:H3'     | 1:AA:214:C:H6      | 1.63        | 0.64     |
| 10:AK:16:SER:HA    | 10:AK:78:ILE:HA    | 1.80        | 0.64     |
| 6:CG:68:VAL:HG11   | 6:CG:133:ALA:HB1   | 1.79        | 0.64     |
| 26:DD:16:THR:O     | 28:DP:78:PRO:HG2   | 1.98        | 0.64     |
| 23:BB:2801:G:H2'   | 23:BB:2802:G:C8    | 2.33        | 0.64     |
| 25:BC:219:VAL:HG12 | 25:BC:224:MET:HE2  | 1.79        | 0.64     |
| 3:AD:148:ALA:O     | 3:AD:151:GLN:HB2   | 1.98        | 0.64     |
| 23:BB:857:G:C2'    | 23:BB:858:G:H5'    | 2.28        | 0.64     |
| 20:CB:163:ILE:HG23 | 20:CB:164:ASP:N    | 2.07        | 0.64     |
| 5:AF:36:ILE:HA     | 5:AF:64:VAL:HG13   | 1.80        | 0.64     |
| 26:DD:111:GLY:H    | 26:DD:194:PRO:HG2  | 1.62        | 0.64     |
| 47:DF:37:MET:SD    | 47:DF:52:ALA:HB1   | 2.38        | 0.64     |
| 23:BB:1460:U:H4'   | 23:BB:1461:C:O5'   | 1.98        | 0.64     |
| 18:AS:47:THR:HG23  | 18:AS:60:PHE:HE1   | 1.63        | 0.64     |
| 33:D1:26:LYS:HB2   | 33:D1:52:LYS:NZ    | 2.13        | 0.64     |
| 23:BB:2472:G:C2'   | 23:BB:2475:C:H42   | 2.11        | 0.64     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:97:G:H2'      | 1:AA:98:A:O4'      | 1.98        | 0.64     |
| 23:DB:873:C:H2'    | 23:DB:874:G:H8     | 1.63        | 0.64     |
| 23:BB:873:C:H4'    | 38:BM:64:TRP:NE1   | 2.13        | 0.64     |
| 1:AA:1391:U:H2'    | 1:AA:1392:G:H8     | 1.60        | 0.64     |
| 1:CA:239:U:OP1     | 1:CA:239:U:H4'     | 1.98        | 0.64     |
| 1:AA:1513:A:H2'    | 1:AA:1514:G:C8     | 2.33        | 0.64     |
| 25:DC:116:GLN:HG2  | 25:DC:117:SER:H    | 1.63        | 0.64     |
| 3:AD:60:VAL:HA     | 3:AD:63:ILE:HD12   | 1.80        | 0.64     |
| 23:DB:526:A:N6     | 23:DB:2626:C:H4'   | 2.13        | 0.64     |
| 42:DN:15:SER:O     | 42:DN:18:GLN:HB2   | 1.98        | 0.64     |
| 1:CA:1006:G:H2'    | 1:CA:1007:U:C6     | 2.33        | 0.64     |
| 45:BS:82:MET:HB2   | 45:BS:98:LYS:HB2   | 1.80        | 0.64     |
| 23:DB:543:G:H2'    | 23:DB:544:C:H4'    | 1.81        | 0.64     |
| 23:BB:2880:C:O4'   | 42:BN:91:ALA:HB3   | 1.98        | 0.64     |
| 20:CB:8:MET:CG     | 20:CB:9:LEU:H      | 2.11        | 0.64     |
| 11:AL:120:ARG:HG3  | 11:AL:121:PRO:HD2  | 1.79        | 0.64     |
| 50:BT:12:ARG:NH1   | 50:BT:12:ARG:HB3   | 2.12        | 0.64     |
| 1:CA:1404:C:H2'    | 1:CA:1405:G:C8     | 2.33        | 0.64     |
| 23:DB:2498:C:O2'   | 23:DB:2499:C:H5'   | 1.97        | 0.63     |
| 5:CF:3:HIS:CG      | 5:CF:92:THR:HG23   | 2.33        | 0.63     |
| 23:BB:100:U:C2'    | 23:BB:100:U:O2     | 2.42        | 0.63     |
| 23:BB:138:U:O5'    | 23:BB:138:U:H6     | 1.81        | 0.63     |
| 23:DB:2360:G:H4'   | 37:DL:61:LEU:HD11  | 1.79        | 0.63     |
| 51:BZ:71:LEU:O     | 51:BZ:74:ARG:HG2   | 1.97        | 0.63     |
| 23:BB:1060:U:OP2   | 24:BI:74:PRO:HA    | 1.98        | 0.63     |
| 23:BB:2471:A:O2'   | 23:BB:2472:G:H8    | 1.81        | 0.63     |
| 45:DS:24:ILE:HG23  | 45:DS:32:ALA:HB1   | 1.78        | 0.63     |
| 32:B4:24:ARG:HG2   | 32:B4:36:ARG:HG3   | 1.78        | 0.63     |
| 23:DB:2849:U:H4'   | 23:DB:2850:A:C5'   | 2.28        | 0.63     |
| 23:DB:2379:G:H2'   | 23:DB:2380:C:H6    | 1.63        | 0.63     |
| 7:AH:47:ASP:CG     | 7:AH:48:PHE:H      | 2.01        | 0.63     |
| 11:AL:66:ILE:HG21  | 11:AL:71:HIS:HB3   | 1.79        | 0.63     |
| 23:BB:1443:U:H2'   | 23:BB:1444:G:H8    | 1.63        | 0.63     |
| 46:BU:39:ASN:HB3   | 46:BU:62:ALA:HB3   | 1.80        | 0.63     |
| 46:BU:35:VAL:HB    | 46:BU:38:ILE:CG2   | 2.28        | 0.63     |
| 1:CA:1048:G:H4'    | 13:CN:2:LYS:NZ     | 2.12        | 0.63     |
| 23:BB:559:G:H21    | 44:BQ:51:GLN:NE2   | 1.94        | 0.63     |
| 36:D2:9:VAL:HG13   | 36:D2:10:LEU:N     | 2.13        | 0.63     |
| 23:DB:2139:U:O2'   | 23:DB:2140:G:H5'   | 1.97        | 0.63     |
| 20:AB:172:ILE:HG22 | 20:AB:176:ASN:HD21 | 1.62        | 0.63     |
| 45:BS:31:GLN:O     | 45:BS:35:ILE:HG12  | 1.97        | 0.63     |
| 25:BC:239:PHE:O    | 25:BC:241:LYS:HG3  | 1.98        | 0.63     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 14:AO:11:ILE:HD11 | 14:AO:30:ALA:HB1   | 1.81        | 0.63     |
| 1:AA:1029:U:H2'   | 1:AA:1031:C:N3     | 2.14        | 0.63     |
| 42:BN:15:SER:O    | 42:BN:18:GLN:HB2   | 1.98        | 0.63     |
| 5:AF:47:LEU:HD21  | 5:AF:57:ALA:HB3    | 1.79        | 0.63     |
| 11:CL:17:LYS:HE3  | 11:CL:17:LYS:N     | 2.13        | 0.63     |
| 52:BW:51:GLY:HA3  | 52:BW:59:PHE:CB    | 2.27        | 0.63     |
| 37:DL:143:GLU:CG  | 37:DL:144:GLU:H    | 2.09        | 0.63     |
| 27:BK:35:VAL:HG12 | 27:BK:69:VAL:HG22  | 1.79        | 0.63     |
| 53:D6:58:VAL:HG22 | 53:D6:68:VAL:HG22  | 1.80        | 0.63     |
| 53:D6:68:VAL:HG21 | 53:D6:99:LEU:HD12  | 1.80        | 0.63     |
| 26:DD:105:LYS:H   | 26:DD:106:LYS:NZ   | 1.95        | 0.63     |
| 48:BG:17:LYS:NZ   | 48:BG:18:ILE:H     | 1.95        | 0.63     |
| 23:DB:1060:U:O4   | 23:DB:1088:A:N6    | 2.31        | 0.63     |
| 12:CM:10:ASP:HA   | 12:CM:44:ILE:HD13  | 1.80        | 0.63     |
| 4:AE:28:ARG:NH2   | 4:AE:30:PHE:HA     | 2.13        | 0.63     |
| 23:BB:675:A:H5'   | 29:BE:60:TRP:HE1   | 1.63        | 0.63     |
| 50:DT:11:LEU:HD21 | 50:DT:46:ALA:HB1   | 1.80        | 0.63     |
| 23:BB:2897:U:H2'  | 23:BB:2898:U:C6    | 2.34        | 0.63     |
| 3:AD:53:GLN:HA    | 3:AD:198:LEU:HD22  | 1.78        | 0.63     |
| 6:AG:14:ASP:HB3   | 6:AG:19:SER:H      | 1.63        | 0.63     |
| 1:CA:1329:A:OP1   | 12:CM:28:ARG:HB2   | 1.97        | 0.63     |
| 1:CA:501:C:H2'    | 1:CA:502:A:C8      | 2.33        | 0.63     |
| 6:AG:134:VAL:O    | 6:AG:138:GLU:HG3   | 1.98        | 0.63     |
| 1:CA:793:U:O2     | 1:CA:1516:G:H4'    | 1.98        | 0.63     |
| 23:DB:200:U:H5''  | 51:DZ:22:LEU:O     | 1.98        | 0.63     |
| 23:BB:632:A:H2'   | 23:BB:633:A:C8     | 2.32        | 0.63     |
| 10:CK:16:SER:HA   | 10:CK:78:ILE:HA    | 1.79        | 0.63     |
| 25:BC:166:ARG:HB2 | 25:BC:171:VAL:HG22 | 1.79        | 0.63     |
| 23:BB:1666:G:O3'  | 27:BK:6:THR:HG23   | 1.97        | 0.63     |
| 1:AA:1141:C:H2'   | 1:AA:1142:G:H8     | 1.63        | 0.63     |
| 20:AB:128:LEU:HG  | 20:AB:132:GLU:HG2  | 1.80        | 0.63     |
| 24:BI:89:SER:HA   | 24:BI:97:VAL:HG21  | 1.80        | 0.63     |
| 38:BM:68:PHE:CG   | 38:BM:69:PRO:HD2   | 2.33        | 0.63     |
| 6:AG:4:ARG:NE     | 6:AG:6:ILE:HG23    | 2.14        | 0.63     |
| 53:D6:61:PRO:HD2  | 53:D6:66:LEU:HA    | 1.80        | 0.63     |
| 40:BH:82:SER:HB3  | 40:BH:92:GLY:O     | 1.99        | 0.63     |
| 12:AM:44:ILE:HA   | 12:AM:47:LEU:HD12  | 1.79        | 0.63     |
| 10:CK:58:THR:HB   | 10:CK:59:PRO:HD2   | 1.81        | 0.63     |
| 15:CP:4:ILE:HG12  | 15:CP:21:VAL:HG22  | 1.79        | 0.63     |
| 5:CF:66:ALA:HB1   | 5:CF:67:PRO:HD2    | 1.80        | 0.63     |
| 49:BR:39:LEU:HA   | 49:BR:53:PHE:HA    | 1.80        | 0.63     |
| 23:DB:1081:U:H5'  | 24:DI:126:ARG:NH1  | 2.13        | 0.63     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:1437:C:H2'  | 23:BB:1438:U:H6   | 1.60        | 0.63     |
| 1:CA:1343:G:H2'   | 1:CA:1344:C:C6    | 2.33        | 0.63     |
| 23:DB:1486:U:H2'  | 23:DB:1487:U:H6   | 1.63        | 0.63     |
| 1:AA:1006:G:H2'   | 1:AA:1007:U:H6    | 1.64        | 0.63     |
| 23:BB:630:G:N2    | 23:BB:632:A:H3'   | 2.14        | 0.63     |
| 23:DB:2540:C:H2'  | 23:DB:2541:A:C8   | 2.33        | 0.63     |
| 23:DB:1923:U:H2'  | 23:DB:1924:C:H6   | 1.64        | 0.63     |
| 23:BB:1373:A:H2'  | 23:BB:1374:G:O4'  | 1.98        | 0.63     |
| 23:DB:1636:U:H2'  | 23:DB:1637:A:H8   | 1.64        | 0.63     |
| 23:BB:2512:C:H2'  | 23:BB:2513:A:O4'  | 1.98        | 0.63     |
| 1:CA:87:C:H2'     | 1:CA:88:U:H5''    | 1.79        | 0.63     |
| 37:DL:74:THR:HA   | 37:DL:107:PHE:O   | 1.97        | 0.63     |
| 2:CC:122:GLN:HB3  | 2:CC:127:VAL:HG21 | 1.80        | 0.63     |
| 52:DW:23:LYS:HZ3  | 52:DW:24:ARG:HG3  | 1.61        | 0.63     |
| 8:AI:59:LYS:HB3   | 8:AI:60:LEU:HD23  | 1.78        | 0.63     |
| 7:AH:94:VAL:HG23  | 7:AH:101:ALA:HB2  | 1.79        | 0.63     |
| 42:BN:85:PRO:HA   | 42:BN:88:ALA:HB2  | 1.81        | 0.63     |
| 29:BE:154:ASP:OD2 | 29:BE:157:LEU:HB3 | 1.99        | 0.63     |
| 1:CA:413:G:H2'    | 1:CA:428:G:H21    | 1.62        | 0.63     |
| 4:CE:19:ARG:O     | 4:CE:20:VAL:HB    | 1.98        | 0.63     |
| 18:CS:62:THR:HG22 | 18:CS:63:ASP:H    | 1.62        | 0.63     |
| 31:B0:21:LEU:HD12 | 45:BS:19:LEU:O    | 1.98        | 0.63     |
| 23:DB:850:U:O2'   | 30:DY:22:THR:HG22 | 1.99        | 0.63     |
| 43:DO:62:LEU:HD11 | 43:DO:70:ALA:HA   | 1.79        | 0.63     |
| 23:BB:27:G:H1'    | 23:BB:513:A:H61   | 1.62        | 0.63     |
| 1:CA:1391:U:H2'   | 1:CA:1392:G:H8    | 1.63        | 0.63     |
| 14:CO:25:THR:HB   | 14:CO:70:LEU:HD23 | 1.79        | 0.63     |
| 1:AA:235:C:H2'    | 1:AA:236:A:C8     | 2.34        | 0.63     |
| 39:DX:1:MET:O     | 39:DX:5:GLU:HG2   | 1.98        | 0.63     |
| 23:DB:1508:A:H2'  | 23:DB:1509:A:C2   | 2.34        | 0.63     |
| 9:AJ:37:ARG:NH1   | 9:AJ:77:VAL:HG21  | 2.14        | 0.63     |
| 1:CA:676:A:H2'    | 1:CA:677:U:C6     | 2.33        | 0.63     |
| 27:BK:24:VAL:HG13 | 27:BK:33:ALA:HB2  | 1.81        | 0.63     |
| 6:AG:24:LYS:O     | 6:AG:28:ILE:HG12  | 1.99        | 0.63     |
| 23:BB:1040:A:H2   | 23:BB:1115:G:H22  | 1.46        | 0.63     |
| 15:AP:5:ARG:HH21  | 15:AP:24:SER:HA   | 1.64        | 0.63     |
| 9:CJ:92:LEU:H     | 9:CJ:92:LEU:HD22  | 1.62        | 0.63     |
| 23:DB:1099:G:C8   | 24:DI:3:LYS:CA    | 2.79        | 0.63     |
| 47:DF:64:PRO:HA   | 47:DF:88:VAL:HG22 | 1.80        | 0.63     |
| 22:DA:28:C:C4     | 22:DA:56:G:N1     | 2.67        | 0.63     |
| 3:CD:25:ARG:HB2   | 3:CD:25:ARG:HH11  | 1.63        | 0.63     |
| 51:BZ:5:CYS:HB2   | 51:BZ:10:LYS:HB3  | 1.79        | 0.63     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 3:AD:25:ARG:NH1   | 3:AD:26:ALA:H      | 1.93        | 0.63     |
| 23:DB:2471:A:HO2' | 23:DB:2472:G:H8    | 1.47        | 0.63     |
| 23:BB:2884:U:H2'  | 23:BB:2885:G:C8    | 2.34        | 0.63     |
| 24:DI:121:ILE:N   | 24:DI:121:ILE:HD13 | 2.13        | 0.63     |
| 15:CP:68:SER:OG   | 15:CP:71:VAL:HG12  | 1.99        | 0.63     |
| 45:BS:24:ILE:HG12 | 45:BS:36:LEU:HD21  | 1.81        | 0.63     |
| 23:DB:2898:U:H2'  | 23:DB:2899:A:C8    | 2.34        | 0.63     |
| 44:BQ:10:ARG:HA   | 44:BQ:13:HIS:HB2   | 1.79        | 0.63     |
| 23:BB:1550:C:H2'  | 23:BB:1551:A:C8    | 2.32        | 0.63     |
| 42:BN:49:GLU:HB2  | 42:BN:50:PRO:HD3   | 1.81        | 0.63     |
| 3:CD:169:TRP:HB2  | 3:CD:183:ARG:HD2   | 1.81        | 0.63     |
| 23:BB:1993:U:H4'  | 26:BD:133:THR:CG2  | 2.28        | 0.63     |
| 11:CL:98:ARG:HA   | 11:CL:103:CYS:SG   | 2.38        | 0.63     |
| 11:CL:120:ARG:HG3 | 11:CL:121:PRO:HD2  | 1.79        | 0.63     |
| 11:AL:14:LYS:HG2  | 11:AL:15:VAL:N     | 2.14        | 0.63     |
| 23:BB:2377:A:H2'  | 23:BB:2378:A:C8    | 2.34        | 0.63     |
| 17:AR:41:SER:HB2  | 17:AR:51:GLN:HG2   | 1.79        | 0.63     |
| 53:D6:63:PRO:HD2  | 53:D6:64:ARG:NH1   | 2.14        | 0.63     |
| 1:CA:213:G:H3'    | 1:CA:214:C:H6      | 1.62        | 0.63     |
| 20:CB:23:ASN:HD22 | 20:CB:24:PRO:HD2   | 1.63        | 0.63     |
| 50:DT:12:ARG:NH1  | 50:DT:12:ARG:HB3   | 2.12        | 0.63     |
| 1:CA:880:C:H2'    | 1:CA:881:G:H8      | 1.64        | 0.63     |
| 1:CA:1053:G:N7    | 1:CA:1200:C:H5''   | 2.13        | 0.63     |
| 23:BB:2064:C:H2'  | 23:BB:2065:C:C6    | 2.32        | 0.63     |
| 41:DJ:45:THR:H    | 41:DJ:46:PRO:HD3   | 1.62        | 0.63     |
| 47:DF:78:ILE:H    | 47:DF:79:ARG:NH1   | 1.97        | 0.63     |
| 23:DB:2645:G:H3'  | 23:DB:2646:C:H5'   | 1.79        | 0.63     |
| 30:BY:12:ALA:HA   | 30:BY:15:ARG:HD3   | 1.81        | 0.63     |
| 23:BB:1060:U:O4   | 23:BB:1088:A:N6    | 2.31        | 0.63     |
| 46:DU:80:ASP:HB3  | 46:DU:96:LYS:N     | 2.13        | 0.63     |
| 1:CA:920:U:O2'    | 1:CA:1081:A:H4'    | 1.98        | 0.63     |
| 1:AA:1314:C:H41   | 18:AS:3:SER:HB3    | 1.63        | 0.63     |
| 33:D1:33:LEU:N    | 33:D1:51:ALA:HB3   | 2.12        | 0.63     |
| 23:DB:2039:U:H2'  | 23:DB:2040:G:C8    | 2.29        | 0.63     |
| 23:DB:1551:A:C3'  | 23:DB:1552:A:H5''  | 2.28        | 0.63     |
| 29:DE:158:PHE:HA  | 29:DE:169:VAL:HG21 | 1.81        | 0.63     |
| 23:BB:2230:G:H2'  | 23:BB:2231:U:C6    | 2.34        | 0.63     |
| 23:DB:2415:G:H2'  | 23:DB:2416:C:C6    | 2.34        | 0.63     |
| 1:CA:1053:G:C3'   | 1:CA:1054:C:H5'    | 2.27        | 0.63     |
| 1:AA:707:U:H2'    | 1:AA:708:C:C6      | 2.34        | 0.63     |
| 28:DP:24:THR:O    | 28:DP:25:VAL:HG22  | 1.99        | 0.63     |
| 25:BC:244:VAL:HB  | 25:BC:249:VAL:H    | 1.64        | 0.63     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:2216:G:H2'  | 23:DB:2217:G:H8    | 1.63        | 0.63     |
| 2:CC:142:ARG:HH21 | 2:CC:143:LEU:HD21  | 1.63        | 0.63     |
| 23:BB:1326:U:H2'  | 23:BB:1327:A:H8    | 1.63        | 0.63     |
| 1:CA:1141:C:H2'   | 1:CA:1142:G:H8     | 1.64        | 0.63     |
| 23:BB:506:G:H5''  | 23:BB:509:C:O2'    | 1.99        | 0.63     |
| 23:BB:2386:A:H2'  | 23:BB:2387:U:C6    | 2.34        | 0.63     |
| 23:BB:922:C:H1'   | 52:BW:22:VAL:HG21  | 1.79        | 0.63     |
| 52:BW:49:ASN:O    | 52:BW:50:VAL:HG13  | 1.99        | 0.63     |
| 52:DW:49:ASN:O    | 52:DW:50:VAL:HG13  | 1.98        | 0.63     |
| 18:CS:49:ALA:HA   | 18:CS:57:VAL:O     | 1.97        | 0.63     |
| 23:DB:873:C:H4'   | 38:DM:64:TRP:HE1   | 1.63        | 0.63     |
| 30:DY:18:LYS:O    | 30:DY:22:THR:HG23  | 1.99        | 0.63     |
| 3:AD:187:ARG:NH1  | 3:AD:191:SER:HA    | 2.13        | 0.63     |
| 1:CA:876:C:H1'    | 7:CH:11:THR:HG21   | 1.81        | 0.63     |
| 23:DB:2720:U:H5'' | 28:DP:52:ARG:NH2   | 2.13        | 0.63     |
| 1:AA:335:C:H2'    | 1:AA:336:A:H8      | 1.64        | 0.63     |
| 14:AO:26:GLU:HA   | 14:AO:81:LEU:HD11  | 1.80        | 0.63     |
| 23:DB:2557:G:H2'  | 23:DB:2558:C:H6    | 1.64        | 0.63     |
| 6:CG:66:GLU:HA    | 6:CG:69:ARG:HD2    | 1.79        | 0.63     |
| 20:CB:8:MET:SD    | 20:CB:9:LEU:N      | 2.72        | 0.63     |
| 45:DS:82:MET:HB2  | 45:DS:98:LYS:HB2   | 1.81        | 0.63     |
| 23:DB:693:A:H2'   | 23:DB:694:U:C6     | 2.34        | 0.63     |
| 23:BB:1259:G:H2'  | 23:BB:1260:A:H8    | 1.64        | 0.63     |
| 6:CG:135:LYS:HD3  | 6:CG:136:LYS:N     | 2.13        | 0.63     |
| 47:BF:32:LYS:HA   | 47:BF:95:MET:HG3   | 1.80        | 0.63     |
| 20:AB:14:HIS:HB2  | 20:AB:208:ALA:HB2  | 1.80        | 0.63     |
| 5:AF:3:HIS:CD2    | 5:AF:65:GLU:HG3    | 2.33        | 0.63     |
| 23:DB:632:A:H2'   | 23:DB:633:A:C8     | 2.32        | 0.63     |
| 13:CN:68:ARG:HB3  | 13:CN:68:ARG:NH1   | 2.10        | 0.63     |
| 44:BQ:90:ASP:O    | 44:BQ:94:LEU:HB2   | 1.98        | 0.63     |
| 1:AA:1271:A:H5'   | 1:AA:1314:C:H5''   | 1.81        | 0.63     |
| 32:D4:7:VAL:HB    | 32:D4:36:ARG:O     | 1.99        | 0.63     |
| 1:CA:1237:C:H3'   | 1:CA:1336:C:H41    | 1.63        | 0.63     |
| 31:D0:43:THR:OG1  | 31:D0:47:TYR:HB2   | 1.99        | 0.63     |
| 37:BL:102:GLY:O   | 37:BL:105:ILE:HG12 | 1.99        | 0.63     |
| 1:CA:806:C:H2'    | 1:CA:807:A:H8      | 1.64        | 0.63     |
| 8:AI:14:SER:HA    | 8:AI:68:GLY:O      | 1.99        | 0.63     |
| 30:BY:29:ARG:H    | 30:BY:33:HIS:CD2   | 2.17        | 0.63     |
| 23:BB:2875:C:H2'  | 23:BB:2876:G:H8    | 1.62        | 0.63     |
| 23:DB:269:C:H2'   | 23:DB:270:A:H8     | 1.63        | 0.63     |
| 29:BE:22:ASP:O    | 29:BE:107:SER:HB2  | 1.97        | 0.63     |
| 1:AA:135:C:O2     | 15:AP:1:MET:HB2    | 1.99        | 0.63     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 50:BT:69:ARG:HG2   | 50:BT:73:ARG:O    | 1.99        | 0.63     |
| 23:BB:1407:G:H2'   | 23:BB:1408:G:H8   | 1.64        | 0.63     |
| 52:BW:49:ASN:HB3   | 52:BW:81:ILE:CG1  | 2.29        | 0.63     |
| 23:DB:947:A:HO2'   | 23:DB:984:A:H2    | 1.47        | 0.63     |
| 52:DW:81:ILE:O     | 52:DW:81:ILE:HG13 | 1.99        | 0.63     |
| 1:AA:1148:U:O4'    | 8:AI:17:ARG:HD3   | 1.99        | 0.63     |
| 13:AN:60:ARG:HG3   | 13:AN:62:ARG:HG3  | 1.81        | 0.63     |
| 47:BF:111:ARG:HH22 | 47:BF:113:PHE:HB2 | 1.62        | 0.63     |
| 13:AN:26:LEU:HD11  | 13:AN:44:VAL:HG22 | 1.81        | 0.63     |
| 23:BB:1024:G:C3'   | 23:BB:1025:G:H5'' | 2.27        | 0.63     |
| 43:DO:63:LYS:HD3   | 43:DO:67:ASN:OD1  | 1.99        | 0.63     |
| 27:DK:118:LEU:O    | 27:DK:120:PRO:HD2 | 1.98        | 0.63     |
| 23:BB:1551:A:C3'   | 23:BB:1552:A:H5'' | 2.28        | 0.63     |
| 23:BB:62:U:H3'     | 23:BB:63:A:H8     | 1.62        | 0.63     |
| 1:AA:1524:C:H2'    | 1:AA:1525:G:C8    | 2.34        | 0.63     |
| 19:CT:57:VAL:HG23  | 19:CT:58:ASP:H    | 1.64        | 0.63     |
| 53:D6:63:PRO:HD2   | 53:D6:64:ARG:CZ   | 2.29        | 0.63     |
| 23:BB:2698:U:H2'   | 23:BB:2699:C:C6   | 2.34        | 0.63     |
| 23:DB:2776:A:H4'   | 23:DB:2777:G:H5'' | 1.79        | 0.63     |
| 23:DB:2064:C:H2'   | 23:DB:2065:C:C6   | 2.34        | 0.63     |
| 23:DB:2093:G:O5'   | 40:DH:24:GLY:HA3  | 1.99        | 0.63     |
| 1:AA:1027:C:H2'    | 1:AA:1028:C:C6    | 2.34        | 0.63     |
| 1:CA:451:A:H4'     | 1:CA:452:A:O4'    | 1.99        | 0.63     |
| 23:DB:1166:G:H2'   | 23:DB:1167:C:C6   | 2.34        | 0.63     |
| 9:CJ:80:THR:HB     | 9:CJ:83:THR:OG1   | 1.99        | 0.63     |
| 41:BJ:117:ALA:HA   | 41:BJ:120:ARG:HD2 | 1.79        | 0.63     |
| 1:AA:524:G:H2'     | 1:AA:525:C:C6     | 2.33        | 0.63     |
| 23:BB:1939:U:H6    | 23:BB:1939:U:H5'  | 1.64        | 0.63     |
| 5:AF:66:ALA:HB1    | 5:AF:67:PRO:HD2   | 1.80        | 0.63     |
| 1:AA:1461:G:H2'    | 1:AA:1462:C:H6    | 1.63        | 0.63     |
| 23:DB:1958:C:O2'   | 23:DB:1959:G:H5'  | 1.99        | 0.63     |
| 40:BH:31:VAL:O     | 40:BH:32:PRO:C    | 2.34        | 0.62     |
| 40:BH:31:VAL:CB    | 40:BH:32:PRO:CD   | 2.77        | 0.62     |
| 40:BH:134:VAL:HG13 | 40:BH:138:VAL:O   | 1.98        | 0.62     |
| 53:D6:36:ALA:HA    | 53:D6:39:LEU:CD2  | 2.29        | 0.62     |
| 20:CB:14:HIS:HB2   | 20:CB:208:ALA:HB2 | 1.79        | 0.62     |
| 47:DF:43:ILE:HB    | 47:DF:82:TYR:OH   | 1.98        | 0.62     |
| 30:DY:12:ALA:HA    | 30:DY:15:ARG:HD3  | 1.81        | 0.62     |
| 38:DM:35:ALA:CB    | 38:DM:100:LYS:H   | 2.12        | 0.62     |
| 3:CD:29:THR:HG22   | 3:CD:30:LYS:H     | 1.64        | 0.62     |
| 46:DU:85:ARG:HD3   | 46:DU:86:PHE:N    | 2.12        | 0.62     |
| 47:BF:37:MET:SD    | 47:BF:52:ALA:HB1  | 2.39        | 0.62     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 47:DF:102:LEU:HD22 | 47:DF:103:ILE:H   | 1.64        | 0.62     |
| 37:DL:19:LEU:O     | 37:DL:21:ARG:HG2  | 1.99        | 0.62     |
| 35:DV:40:ILE:N     | 35:DV:40:ILE:HD13 | 2.13        | 0.62     |
| 23:BB:2547:A:H2'   | 23:BB:2548:U:C6   | 2.34        | 0.62     |
| 24:DI:20:SER:O     | 24:DI:25:PRO:HD2  | 1.99        | 0.62     |
| 24:BI:20:SER:O     | 24:BI:25:PRO:HD2  | 1.99        | 0.62     |
| 46:DU:21:ARG:HD3   | 46:DU:72:PHE:CG   | 2.34        | 0.62     |
| 14:CO:78:TYR:CZ    | 14:CO:82:ILE:HD11 | 2.34        | 0.62     |
| 23:DB:2086:U:H2'   | 23:DB:2087:G:C8   | 2.33        | 0.62     |
| 1:CA:620:C:H2'     | 1:CA:621:A:C8     | 2.34        | 0.62     |
| 42:DN:49:GLU:HB2   | 42:DN:50:PRO:HD3  | 1.80        | 0.62     |
| 40:BH:47:PHE:HA    | 40:BH:50:ARG:NH2  | 2.14        | 0.62     |
| 23:DB:1684:G:H2'   | 23:DB:1685:C:C6   | 2.33        | 0.62     |
| 1:AA:1006:G:H2'    | 1:AA:1007:U:C6    | 2.33        | 0.62     |
| 52:DW:41:GLY:HA2   | 52:DW:44:PHE:CD2  | 2.34        | 0.62     |
| 1:AA:1377:A:H2'    | 6:AG:6:ILE:HD11   | 1.81        | 0.62     |
| 52:BW:41:GLY:HA2   | 52:BW:44:PHE:CD2  | 2.34        | 0.62     |
| 48:DG:54:ARG:HB3   | 48:DG:57:TYR:CD1  | 2.34        | 0.62     |
| 23:DB:1505:A:H2'   | 23:DB:1506:U:C6   | 2.34        | 0.62     |
| 23:BB:1381:G:H2'   | 23:BB:1382:G:H5'  | 1.79        | 0.62     |
| 1:CA:6:G:H4'       | 1:CA:298:A:H4'    | 1.81        | 0.62     |
| 41:BJ:124:VAL:HG23 | 41:BJ:125:TYR:H   | 1.64        | 0.62     |
| 42:BN:58:ASP:O     | 42:BN:59:SER:HB3  | 1.99        | 0.62     |
| 25:DC:128:THR:HA   | 25:DC:190:THR:CA  | 2.28        | 0.62     |
| 23:DB:573:U:O2'    | 23:DB:574:A:H3'   | 1.99        | 0.62     |
| 47:BF:64:PRO:HA    | 47:BF:88:VAL:HG22 | 1.81        | 0.62     |
| 21:AU:38:GLU:C     | 21:AU:40:PRO:HD2  | 2.19        | 0.62     |
| 33:B1:33:LEU:N     | 33:B1:51:ALA:HB3  | 2.12        | 0.62     |
| 1:AA:413:G:H2'     | 1:AA:428:G:H21    | 1.64        | 0.62     |
| 24:BI:11:GLN:HA    | 24:BI:55:PRO:HA   | 1.80        | 0.62     |
| 2:AC:72:PRO:O      | 2:AC:76:ILE:HG12  | 1.99        | 0.62     |
| 13:AN:26:LEU:HG    | 13:AN:30:ILE:HD13 | 1.80        | 0.62     |
| 53:D6:16:LYS:O     | 53:D6:20:VAL:HG23 | 1.98        | 0.62     |
| 27:BK:8:LEU:N      | 27:BK:8:LEU:HD12  | 2.14        | 0.62     |
| 44:DQ:10:ARG:HA    | 44:DQ:13:HIS:HB2  | 1.81        | 0.62     |
| 23:BB:1796:U:H2'   | 23:BB:1797:G:C8   | 2.34        | 0.62     |
| 1:AA:255:G:H2'     | 1:AA:256:U:C6     | 2.33        | 0.62     |
| 23:DB:1407:G:H2'   | 23:DB:1408:G:H8   | 1.64        | 0.62     |
| 19:AT:43:LYS:HE2   | 19:AT:44:ALA:H    | 1.63        | 0.62     |
| 1:AA:927:G:O2'     | 1:AA:928:G:H5'    | 1.99        | 0.62     |
| 23:BB:1904:G:H1'   | 23:BB:1927:A:N1   | 2.13        | 0.62     |
| 23:DB:2182:U:H2'   | 23:DB:2183:A:C8   | 2.34        | 0.62     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:2001:C:H4'  | 23:DB:2689:U:O2'   | 1.97        | 0.62     |
| 23:DB:2199:A:H5'  | 23:DB:2200:C:OP2   | 1.99        | 0.62     |
| 23:BB:2075:U:H2'  | 23:BB:2238:G:N2    | 2.14        | 0.62     |
| 10:AK:51:PHE:HB2  | 10:AK:55:ARG:HB3   | 1.81        | 0.62     |
| 26:BD:37:VAL:CG2  | 26:BD:91:THR:HA    | 2.29        | 0.62     |
| 38:BM:59:ARG:NH1  | 38:BM:60:GLN:HB3   | 2.10        | 0.62     |
| 12:AM:12:LYS:HB3  | 12:AM:16:ILE:HG23  | 1.81        | 0.62     |
| 23:DB:2393:U:H5'' | 37:DL:62:PRO:CG    | 2.28        | 0.62     |
| 29:DE:58:LYS:HE2  | 29:DE:60:TRP:HD1   | 1.64        | 0.62     |
| 46:BU:85:ARG:HA   | 46:BU:85:ARG:NE    | 2.12        | 0.62     |
| 47:BF:76:PHE:HD2  | 47:BF:78:ILE:HD13  | 1.65        | 0.62     |
| 47:DF:2:LYS:HD2   | 47:DF:100:GLU:HG2  | 1.80        | 0.62     |
| 25:DC:18:VAL:O    | 25:DC:18:VAL:HG13  | 1.98        | 0.62     |
| 24:DI:27:LEU:CD2  | 24:DI:27:LEU:H     | 2.12        | 0.62     |
| 25:BC:14:HIS:O    | 25:BC:203:VAL:HG11 | 1.99        | 0.62     |
| 27:DK:8:LEU:HD12  | 27:DK:8:LEU:N      | 2.13        | 0.62     |
| 43:BO:63:LYS:HD3  | 43:BO:67:ASN:OD1   | 1.99        | 0.62     |
| 23:BB:171:U:H2'   | 23:BB:172:A:C8     | 2.34        | 0.62     |
| 20:CB:125:PHE:HA  | 20:CB:127:LYS:NZ   | 2.14        | 0.62     |
| 23:BB:863:A:H2'   | 23:BB:864:G:C8     | 2.34        | 0.62     |
| 45:BS:6:LYS:HD3   | 45:BS:104:THR:HG23 | 1.81        | 0.62     |
| 6:AG:56:SER:HB3   | 6:AG:59:GLU:HG3    | 1.81        | 0.62     |
| 23:DB:664:G:H2'   | 23:DB:665:U:C6     | 2.34        | 0.62     |
| 1:CA:1006:G:H2'   | 1:CA:1007:U:H6     | 1.63        | 0.62     |
| 23:DB:547:A:N1    | 23:DB:548:G:H1'    | 2.15        | 0.62     |
| 20:AB:165:ALA:HA  | 20:AB:172:ILE:HD11 | 1.82        | 0.62     |
| 23:BB:2875:C:H2'  | 23:BB:2876:G:C8    | 2.35        | 0.62     |
| 26:DD:108:ASP:OD2 | 26:DD:173:GLN:HA   | 1.99        | 0.62     |
| 1:AA:1180:A:P     | 8:AI:98:ARG:HH22   | 2.22        | 0.62     |
| 23:BB:350:G:H2'   | 23:BB:351:C:C6     | 2.34        | 0.62     |
| 23:BB:2758:A:H2'  | 23:BB:2759:G:O4'   | 1.99        | 0.62     |
| 23:DB:2091:C:H1'  | 51:DZ:34:HIS:CD2   | 2.33        | 0.62     |
| 28:BP:24:THR:O    | 28:BP:25:VAL:HG22  | 1.99        | 0.62     |
| 1:AA:678:U:H2'    | 1:AA:679:C:C6      | 2.34        | 0.62     |
| 1:CA:1384:C:H2'   | 1:CA:1385:G:H8     | 1.64        | 0.62     |
| 16:CQ:80:LYS:H    | 16:CQ:80:LYS:HD2   | 1.64        | 0.62     |
| 23:BB:2019:A:H2   | 23:BB:2035:G:H22   | 1.47        | 0.62     |
| 53:D6:36:ALA:HA   | 53:D6:39:LEU:HD23  | 1.81        | 0.62     |
| 44:DQ:63:ARG:HH21 | 44:DQ:64:ILE:HD11  | 1.64        | 0.62     |
| 51:BZ:7:VAL:HG21  | 51:BZ:59:ILE:HD11  | 1.80        | 0.62     |
| 12:CM:47:LEU:HD13 | 12:CM:51:GLN:O     | 1.99        | 0.62     |
| 29:BE:58:LYS:C    | 29:BE:60:TRP:H     | 2.01        | 0.62     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 50:DT:1:MET:HG3    | 50:DT:2:ILE:H      | 1.64        | 0.62     |
| 23:DB:580:U:H2'    | 23:DB:581:C:H6     | 1.63        | 0.62     |
| 23:DB:557:C:H2'    | 23:DB:558:U:C6     | 2.35        | 0.62     |
| 50:BT:82:LYS:HD2   | 50:BT:84:TYR:HE1   | 1.64        | 0.62     |
| 50:DT:82:LYS:HD2   | 50:DT:84:TYR:HE1   | 1.64        | 0.62     |
| 1:AA:235:C:H2'     | 1:AA:236:A:H8      | 1.61        | 0.62     |
| 23:DB:1178:C:H2'   | 23:DB:1179:G:H8    | 1.63        | 0.62     |
| 40:DH:59:ALA:O     | 40:DH:62:LEU:HD22  | 1.99        | 0.62     |
| 6:AG:102:TRP:HZ3   | 6:AG:137:ARG:HB2   | 1.64        | 0.62     |
| 20:CB:8:MET:HB2    | 20:CB:11:ALA:HB3   | 1.82        | 0.62     |
| 1:CA:1515:G:O2'    | 1:CA:1516:G:H5'    | 1.99        | 0.62     |
| 38:BM:41:LEU:HB2   | 38:BM:94:ALA:HB3   | 1.80        | 0.62     |
| 9:CJ:29:ALA:O      | 9:CJ:32:THR:HG22   | 1.99        | 0.62     |
| 1:AA:481:G:HO2'    | 1:AA:482:A:H8      | 1.47        | 0.62     |
| 4:AE:19:ARG:O      | 4:AE:20:VAL:HB     | 1.99        | 0.62     |
| 23:DB:833:A:H1'    | 37:DL:52:GLY:H     | 1.62        | 0.62     |
| 23:BB:1913:A:H4'   | 23:BB:1914:C:H5''  | 1.81        | 0.62     |
| 9:AJ:92:LEU:H      | 9:AJ:92:LEU:HD22   | 1.64        | 0.62     |
| 40:DH:131:SER:HB2  | 40:DH:141:LYS:HG3  | 1.81        | 0.62     |
| 42:BN:65:LEU:HD11  | 42:BN:69:ARG:CZ    | 2.29        | 0.62     |
| 25:DC:140:VAL:HG12 | 25:DC:141:HIS:H    | 1.63        | 0.62     |
| 48:DG:84:LYS:HG3   | 48:DG:131:VAL:CA   | 2.28        | 0.62     |
| 26:BD:105:LYS:H    | 26:BD:106:LYS:NZ   | 1.97        | 0.62     |
| 51:DZ:7:VAL:HG21   | 51:DZ:59:ILE:HD11  | 1.80        | 0.62     |
| 25:BC:64:VAL:HG11  | 25:BC:66:PHE:CE2   | 2.35        | 0.62     |
| 3:AD:25:ARG:HH11   | 3:AD:26:ALA:N      | 1.93        | 0.62     |
| 10:AK:58:THR:HB    | 10:AK:59:PRO:HD2   | 1.80        | 0.62     |
| 18:CS:30:LEU:HD12  | 18:CS:48:ILE:HG12  | 1.81        | 0.62     |
| 9:AJ:55:PRO:HA     | 13:AN:80:ARG:HH22  | 1.64        | 0.62     |
| 1:AA:98:A:O2'      | 1:AA:99:C:H5'      | 1.99        | 0.62     |
| 37:DL:18:ARG:C     | 37:DL:19:LEU:HD12  | 2.20        | 0.62     |
| 23:BB:1080:A:O2'   | 24:BI:126:ARG:HB2  | 1.98        | 0.62     |
| 53:D6:1:MET:HB3    | 53:D6:143:LEU:HD11 | 1.79        | 0.62     |
| 23:DB:593:U:H2'    | 23:DB:594:U:C6     | 2.33        | 0.62     |
| 44:BQ:10:ARG:NH1   | 44:BQ:10:ARG:HB2   | 2.14        | 0.62     |
| 7:CH:11:THR:HA     | 7:CH:14:ARG:NH1    | 2.14        | 0.62     |
| 1:AA:1343:G:H2'    | 1:AA:1344:C:C6     | 2.34        | 0.62     |
| 23:DB:38:A:N3      | 29:DE:43:THR:HB    | 2.15        | 0.62     |
| 6:AG:41:ILE:HG21   | 6:AG:115:MET:HG3   | 1.82        | 0.62     |
| 1:AA:1423:G:H2'    | 1:AA:1424:U:C6     | 2.33        | 0.62     |
| 45:DS:84:ARG:HB3   | 45:DS:96:ILE:HG23  | 1.81        | 0.62     |
| 1:CA:676:A:H2'     | 1:CA:677:U:H6      | 1.64        | 0.62     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:1381:G:C2'   | 23:BB:1382:G:H5'   | 2.28        | 0.62     |
| 17:CR:41:SER:HB2   | 17:CR:51:GLN:HG2   | 1.80        | 0.62     |
| 23:DB:899:A:H3'    | 23:DB:900:A:C8     | 2.35        | 0.62     |
| 15:CP:5:ARG:HH21   | 15:CP:24:SER:HA    | 1.63        | 0.62     |
| 23:BB:540:C:H2'    | 23:BB:541:A:H8     | 1.64        | 0.62     |
| 23:DB:2194:U:H2'   | 23:DB:2195:U:H6    | 1.64        | 0.62     |
| 16:CQ:30:HIS:CE1   | 16:CQ:32:ILE:HG22  | 2.35        | 0.62     |
| 3:CD:58:GLN:O      | 3:CD:62:ARG:HG2    | 1.99        | 0.62     |
| 6:CG:24:LYS:O      | 6:CG:28:ILE:HG12   | 1.98        | 0.62     |
| 1:AA:532:A:N6      | 2:AC:191:THR:HB    | 2.14        | 0.62     |
| 52:BW:39:GLN:NE2   | 52:BW:43:LYS:HB2   | 2.14        | 0.62     |
| 53:D6:90:LEU:O     | 53:D6:92:PRO:HD3   | 2.00        | 0.62     |
| 44:DQ:63:ARG:NH2   | 44:DQ:96:ASP:HA    | 2.14        | 0.62     |
| 8:AI:62:LEU:HD22   | 8:AI:62:LEU:H      | 1.63        | 0.62     |
| 7:AH:76:ARG:HG3    | 7:AH:77:VAL:N      | 2.15        | 0.62     |
| 53:B6:128:ALA:O    | 53:B6:132:ILE:HG13 | 1.98        | 0.62     |
| 22:BA:24:G:N7      | 22:BA:56:G:H2'     | 2.15        | 0.62     |
| 29:DE:105:LEU:HA   | 29:DE:108:ILE:HG22 | 1.80        | 0.62     |
| 12:CM:78:ARG:HH22  | 18:CS:68:HIS:CE1   | 2.18        | 0.62     |
| 37:BL:18:ARG:C     | 37:BL:19:LEU:HD12  | 2.19        | 0.62     |
| 31:B0:43:THR:OG1   | 31:B0:47:TYR:HB2   | 1.99        | 0.62     |
| 23:DB:2380:C:H5'   | 43:DO:17:LYS:NZ    | 2.15        | 0.62     |
| 40:BH:4:ILE:HG22   | 40:BH:17:ASP:N     | 2.15        | 0.62     |
| 5:CF:1:MET:SD      | 5:CF:67:PRO:HD3    | 2.40        | 0.62     |
| 23:DB:2895:G:H2'   | 23:DB:2896:C:C6    | 2.34        | 0.62     |
| 23:DB:1440:U:H2'   | 23:DB:1441:G:H8    | 1.64        | 0.62     |
| 20:CB:113:LEU:HD12 | 20:CB:143:LEU:HB3  | 1.81        | 0.62     |
| 35:BV:42:LEU:HD12  | 35:BV:47:VAL:HG21  | 1.82        | 0.62     |
| 1:AA:551:U:O2'     | 11:AL:82:ARG:HD2   | 1.99        | 0.62     |
| 7:AH:11:THR:HA     | 7:AH:14:ARG:NH1    | 2.15        | 0.62     |
| 6:AG:21:LEU:HG     | 6:AG:22:LEU:H      | 1.63        | 0.62     |
| 8:AI:9:GLY:HA3     | 8:AI:81:GLY:N      | 2.14        | 0.62     |
| 1:AA:216:U:H2'     | 1:AA:217:C:C6      | 2.34        | 0.62     |
| 23:BB:634:C:H2'    | 23:BB:635:C:H6     | 1.65        | 0.62     |
| 17:CR:40:PRO:HD2   | 17:CR:43:ILE:HD12  | 1.82        | 0.62     |
| 6:CG:91:ARG:HB3    | 6:CG:92:PRO:HD2    | 1.82        | 0.62     |
| 23:DB:2400:G:O2'   | 23:DB:2401:U:H5'   | 1.98        | 0.62     |
| 23:BB:1509:A:H5'   | 23:BB:1510:G:H5'   | 1.81        | 0.62     |
| 23:BB:414:C:H2'    | 23:BB:415:A:C8     | 2.33        | 0.62     |
| 41:DJ:124:VAL:HG23 | 41:DJ:125:TYR:H    | 1.65        | 0.62     |
| 23:BB:2455:G:H2'   | 23:BB:2456:C:C6    | 2.34        | 0.62     |
| 23:DB:1100:C:H2'   | 23:DB:1101:U:H6    | 1.63        | 0.62     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 53:D6:40:HIS:O    | 53:D6:51:PRO:HA   | 2.00        | 0.62     |
| 35:BV:62:THR:HB   | 35:BV:71:LYS:HG2  | 1.82        | 0.62     |
| 30:DY:6:ILE:O     | 30:DY:34:THR:HA   | 2.00        | 0.62     |
| 13:CN:60:ARG:HG3  | 13:CN:62:ARG:HG3  | 1.81        | 0.62     |
| 18:AS:10:ILE:HG22 | 18:AS:37:SER:HB3  | 1.82        | 0.62     |
| 23:BB:372:G:O2'   | 51:BZ:54:LYS:HE2  | 2.00        | 0.62     |
| 23:DB:2849:U:N3   | 23:DB:2867:G:C8   | 2.66        | 0.62     |
| 23:BB:819:A:H5'   | 23:BB:973:A:N1    | 2.14        | 0.62     |
| 23:BB:1081:U:C5'  | 24:BI:126:ARG:HD2 | 2.28        | 0.62     |
| 25:BC:18:VAL:O    | 25:BC:18:VAL:HG13 | 1.99        | 0.62     |
| 32:D4:2:LYS:HG2   | 32:D4:4:ARG:NE    | 2.14        | 0.62     |
| 23:DB:1657:U:O2'  | 23:DB:1658:C:H5'  | 1.99        | 0.62     |
| 27:DK:118:LEU:C   | 27:DK:120:PRO:HD2 | 2.19        | 0.62     |
| 23:DB:1199:U:H2'  | 23:DB:1200:C:H6   | 1.65        | 0.62     |
| 23:BB:125:A:OP2   | 36:B2:19:ARG:HD2  | 2.00        | 0.62     |
| 7:CH:47:ASP:CG    | 7:CH:48:PHE:H     | 2.02        | 0.62     |
| 3:CD:197:HIS:O    | 3:CD:200:VAL:HG22 | 2.00        | 0.62     |
| 12:AM:6:ILE:O     | 12:AM:8:ILE:HG23  | 1.98        | 0.62     |
| 23:BB:1354:A:H2'  | 23:BB:1355:G:O4'  | 1.99        | 0.62     |
| 23:DB:1001:A:H2'  | 23:DB:1002:G:O4'  | 1.99        | 0.62     |
| 15:AP:59:HIS:O    | 15:AP:63:GLN:HG3  | 1.99        | 0.62     |
| 8:CI:14:SER:HA    | 8:CI:68:GLY:O     | 2.00        | 0.62     |
| 23:DB:1315:C:H2'  | 23:DB:1316:U:C6   | 2.34        | 0.62     |
| 6:AG:91:ARG:HB3   | 6:AG:92:PRO:HD2   | 1.80        | 0.62     |
| 1:AA:398:U:H2'    | 1:AA:399:G:H8     | 1.63        | 0.62     |
| 1:CA:1432:G:H1'   | 1:CA:1468:A:N6    | 2.15        | 0.62     |
| 7:CH:113:ARG:HH21 | 7:CH:114:ALA:HA   | 1.63        | 0.62     |
| 44:DQ:65:ASN:O    | 44:DQ:69:ARG:HB2  | 1.98        | 0.62     |
| 23:DB:2021:C:OP1  | 31:D0:8:THR:HG21  | 1.99        | 0.62     |
| 23:DB:2353:G:N3   | 52:DW:30:VAL:HG13 | 2.15        | 0.62     |
| 23:DB:626:A:H2'   | 37:DL:78:ARG:NH1  | 2.15        | 0.62     |
| 50:BT:54:GLU:HG3  | 50:BT:90:GLY:H    | 1.63        | 0.62     |
| 1:CA:920:U:H2'    | 1:CA:921:U:H6     | 1.61        | 0.62     |
| 23:DB:27:G:H1'    | 23:DB:513:A:H61   | 1.62        | 0.62     |
| 42:BN:97:ILE:HD12 | 42:BN:98:LEU:N    | 2.15        | 0.62     |
| 26:DD:113:SER:HB2 | 26:DD:168:GLU:H   | 1.64        | 0.62     |
| 1:AA:1003:G:N2    | 1:AA:1005:A:H5'   | 2.14        | 0.62     |
| 1:CA:492:C:H2'    | 1:CA:493:A:N3     | 2.15        | 0.62     |
| 39:BX:20:ASN:O    | 39:BX:24:GLU:HB3  | 1.99        | 0.62     |
| 23:DB:743:A:O2'   | 23:DB:744:U:H5'   | 2.00        | 0.62     |
| 23:BB:2720:U:H5'' | 28:BP:52:ARG:NH2  | 2.15        | 0.62     |
| 2:AC:78:LYS:HG3   | 2:AC:81:GLU:CB    | 2.29        | 0.62     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 20:CB:165:ALA:HA  | 20:CB:172:ILE:HD11 | 1.82        | 0.62     |
| 26:DD:79:LEU:HD22 | 26:DD:79:LEU:N     | 2.15        | 0.62     |
| 23:DB:1406:U:H2'  | 23:DB:1407:G:C8    | 2.34        | 0.62     |
| 1:AA:678:U:H2'    | 1:AA:679:C:H6      | 1.64        | 0.62     |
| 23:BB:955:U:H5''  | 38:BM:86:LYS:HD2   | 1.82        | 0.62     |
| 1:CA:1067:A:H4'   | 1:CA:1068:G:O5'    | 1.99        | 0.62     |
| 1:AA:370:C:O2'    | 1:AA:371:A:H5'     | 2.00        | 0.62     |
| 23:DB:1782:U:H3'  | 57:DB:3607:HOH:O   | 1.99        | 0.62     |
| 23:DB:780:G:H1    | 25:DC:228:ASP:CG   | 2.02        | 0.62     |
| 23:DB:1889:A:H2'  | 23:DB:1890:A:C8    | 2.35        | 0.62     |
| 1:CA:285:C:H2'    | 1:CA:286:C:H6      | 1.64        | 0.62     |
| 23:BB:1564:C:H2'  | 23:BB:1565:C:C6    | 2.34        | 0.62     |
| 23:BB:2415:G:H2'  | 23:BB:2416:C:C6    | 2.34        | 0.62     |
| 23:BB:1219:U:H2'  | 23:BB:1220:G:H8    | 1.64        | 0.62     |
| 22:DA:7:G:H5''    | 43:DO:29:HIS:CD2   | 2.35        | 0.62     |
| 5:AF:3:HIS:CG     | 5:AF:92:THR:HG23   | 2.34        | 0.62     |
| 51:DZ:71:LEU:O    | 51:DZ:74:ARG:HG2   | 2.00        | 0.62     |
| 13:AN:65:GLN:HG2  | 13:AN:82:LYS:HE2   | 1.82        | 0.62     |
| 47:BF:8:LYS:HA    | 47:BF:12:VAL:HG21  | 1.82        | 0.62     |
| 42:DN:83:LEU:HA   | 42:DN:86:ARG:CB    | 2.27        | 0.62     |
| 23:BB:2788:C:H2'  | 23:BB:2789:C:C6    | 2.35        | 0.62     |
| 53:D6:107:THR:O   | 53:D6:111:ARG:HG3  | 2.00        | 0.62     |
| 25:DC:32:LEU:O    | 25:DC:63:ILE:HG12  | 1.99        | 0.62     |
| 12:AM:1:ALA:C     | 12:AM:8:ILE:HG22   | 2.20        | 0.62     |
| 23:BB:2247:A:H3'  | 57:BB:3266:HOH:O   | 1.98        | 0.62     |
| 23:DB:2246:G:H2'  | 23:DB:2247:A:H8    | 1.65        | 0.62     |
| 1:AA:1494:G:H5'   | 23:BB:1913:A:C6    | 2.35        | 0.62     |
| 23:DB:2698:U:H2'  | 23:DB:2699:C:C6    | 2.34        | 0.62     |
| 29:BE:34:ALA:HB2  | 29:BE:96:VAL:HG21  | 1.82        | 0.62     |
| 26:BD:125:TRP:CG  | 26:BD:160:LYS:HB3  | 2.35        | 0.62     |
| 3:CD:88:ASN:O     | 3:CD:92:LEU:HD23   | 1.99        | 0.62     |
| 44:BQ:65:ASN:O    | 44:BQ:69:ARG:HB2   | 1.99        | 0.62     |
| 1:AA:577:G:O2'    | 1:AA:578:C:H5'     | 2.00        | 0.62     |
| 23:DB:272:A:H2'   | 23:DB:273:G:C8     | 2.35        | 0.62     |
| 23:DB:184:C:H2'   | 23:DB:185:G:H8     | 1.65        | 0.62     |
| 2:CC:131:ARG:HG2  | 2:CC:131:ARG:HH11  | 1.64        | 0.62     |
| 1:AA:1169:A:H2'   | 1:AA:1170:A:C8     | 2.35        | 0.62     |
| 29:DE:34:ALA:HB2  | 29:DE:96:VAL:HG21  | 1.82        | 0.62     |
| 8:AI:34:LEU:HD21  | 8:AI:48:ARG:HE     | 1.64        | 0.62     |
| 46:BU:3:LYS:HD3   | 46:BU:82:VAL:CG2   | 2.30        | 0.62     |
| 45:DS:17:VAL:C    | 45:DS:19:LEU:H     | 2.03        | 0.62     |
| 47:DF:102:LEU:HA  | 47:DF:106:ALA:HB3  | 1.82        | 0.62     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 47:DF:111:ARG:HH22 | 47:DF:113:PHE:HB2  | 1.62        | 0.62     |
| 33:D1:20:TYR:CD2   | 33:D1:37:LYS:HD3   | 2.35        | 0.62     |
| 23:DB:139:U:O2'    | 50:DT:1:MET:HB2    | 1.99        | 0.62     |
| 22:DA:98:G:N1      | 35:DV:14:LYS:HB2   | 2.14        | 0.62     |
| 6:CG:122:GLU:OE1   | 6:CG:131:GLY:HA3   | 2.00        | 0.62     |
| 23:BB:1196:C:H2'   | 23:BB:1197:G:C8    | 2.34        | 0.62     |
| 38:BM:64:TRP:HB2   | 38:BM:104:GLU:HB2  | 1.81        | 0.62     |
| 46:DU:26:ASN:HD21  | 46:DU:34:ILE:HD12  | 1.63        | 0.62     |
| 3:AD:169:TRP:HB2   | 3:AD:183:ARG:HD2   | 1.82        | 0.62     |
| 11:AL:107:LYS:H    | 11:AL:107:LYS:NZ   | 1.98        | 0.62     |
| 1:CA:707:U:H2'     | 1:CA:708:C:H6      | 1.64        | 0.62     |
| 25:BC:32:LEU:HD22  | 25:BC:63:ILE:HG13  | 1.82        | 0.62     |
| 50:BT:68:LYS:O     | 50:BT:69:ARG:HB3   | 1.98        | 0.62     |
| 23:DB:1947:C:H2'   | 23:DB:1948:G:H8    | 1.64        | 0.62     |
| 23:BB:1866:A:H2'   | 23:BB:1867:G:O4'   | 2.00        | 0.62     |
| 23:BB:2852:G:H2'   | 23:BB:2853:C:C6    | 2.35        | 0.62     |
| 23:DB:2578:G:C5    | 26:DD:145:SER:HB2  | 2.35        | 0.62     |
| 10:CK:51:PHE:HB2   | 10:CK:55:ARG:HB3   | 1.82        | 0.62     |
| 22:BA:7:G:H5''     | 43:BO:29:HIS:CD2   | 2.35        | 0.62     |
| 23:BB:2605:U:H2'   | 23:BB:2606:C:C6    | 2.35        | 0.62     |
| 23:BB:1306:C:H2'   | 23:BB:1307:A:H8    | 1.64        | 0.62     |
| 23:BB:417:C:H2'    | 23:BB:418:C:C6     | 2.34        | 0.62     |
| 8:CI:34:LEU:HD21   | 8:CI:48:ARG:HE     | 1.63        | 0.61     |
| 44:BQ:80:ASN:O     | 44:BQ:83:LYS:HB3   | 2.00        | 0.61     |
| 12:AM:52:ILE:HD12  | 12:AM:55:LEU:HD12  | 1.81        | 0.61     |
| 53:B6:112:LYS:HB2  | 53:B6:116:ARG:HH21 | 1.65        | 0.61     |
| 23:BB:1176:U:H3'   | 23:BB:1177:G:C8    | 2.34        | 0.61     |
| 29:BE:149:ILE:HG23 | 29:BE:188:MET:HA   | 1.80        | 0.61     |
| 23:BB:1199:U:H2'   | 23:BB:1200:C:C6    | 2.35        | 0.61     |
| 37:DL:102:GLY:O    | 37:DL:105:ILE:HG12 | 2.00        | 0.61     |
| 23:DB:2073:C:H5''  | 25:DC:227:VAL:HG12 | 1.81        | 0.61     |
| 7:AH:40:LYS:HD2    | 7:AH:47:ASP:HA     | 1.82        | 0.61     |
| 23:DB:1442:U:H2'   | 23:DB:1443:U:C6    | 2.34        | 0.61     |
| 4:AE:154:ALA:HB1   | 7:AH:65:PHE:CZ     | 2.35        | 0.61     |
| 1:AA:1072:G:H21    | 20:AB:105:THR:HG21 | 1.64        | 0.61     |
| 45:DS:6:LYS:HD3    | 45:DS:104:THR:HG23 | 1.81        | 0.61     |
| 23:DB:321:U:OP2    | 29:DE:130:LYS:HD3  | 1.99        | 0.61     |
| 1:CA:301:G:H2'     | 1:CA:302:G:C8      | 2.33        | 0.61     |
| 1:AA:301:G:H2'     | 1:AA:302:G:C8      | 2.32        | 0.61     |
| 14:AO:78:TYR:CZ    | 14:AO:82:ILE:HD11  | 2.35        | 0.61     |
| 42:BN:90:ARG:HB3   | 42:BN:94:TYR:CE1   | 2.35        | 0.61     |
| 8:CI:9:GLY:HA3     | 8:CI:81:GLY:N      | 2.15        | 0.61     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:1203:U:H4'  | 37:DL:3:LEU:HD12   | 1.81        | 0.61     |
| 16:CQ:80:LYS:H    | 16:CQ:80:LYS:CD    | 2.13        | 0.61     |
| 23:DB:900:A:O2'   | 23:DB:901:C:H5'    | 2.00        | 0.61     |
| 53:D6:14:MET:SD   | 53:D6:164:ILE:HG22 | 2.40        | 0.61     |
| 29:DE:1:MET:HB3   | 29:DE:14:VAL:O     | 2.00        | 0.61     |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:C6     | 2.35        | 0.61     |
| 53:D6:44:GLU:HA   | 53:D6:49:HIS:HA    | 1.81        | 0.61     |
| 1:AA:1307:U:H2'   | 1:AA:1308:U:C6     | 2.35        | 0.61     |
| 23:BB:5:A:H2'     | 23:BB:6:A:C8       | 2.35        | 0.61     |
| 23:DB:2756:U:H1'  | 23:DB:2757:A:H5''  | 1.82        | 0.61     |
| 23:DB:909:A:H2'   | 23:DB:912:C:H5     | 1.65        | 0.61     |
| 1:CA:570:G:H2'    | 1:CA:571:U:C6      | 2.35        | 0.61     |
| 24:BI:85:ILE:HD13 | 24:BI:137:LEU:HD21 | 1.80        | 0.61     |
| 23:BB:1046:A:C3'  | 23:BB:1047:G:H5''  | 2.30        | 0.61     |
| 23:BB:139:U:H3'   | 23:BB:140:C:H4'    | 1.82        | 0.61     |
| 1:CA:783:C:O2'    | 1:CA:784:A:H5'     | 1.99        | 0.61     |
| 1:AA:939:G:H5'    | 6:AG:101:ARG:NH1   | 2.15        | 0.61     |
| 23:BB:2540:C:H2'  | 23:BB:2541:A:C8    | 2.34        | 0.61     |
| 52:BW:81:ILE:O    | 52:BW:81:ILE:HG13  | 2.00        | 0.61     |
| 1:AA:1527:U:H2'   | 1:AA:1528:U:C6     | 2.36        | 0.61     |
| 41:BJ:25:LEU:HD13 | 41:BJ:26:GLY:N     | 2.14        | 0.61     |
| 23:DB:996:A:C4'   | 44:DQ:91:ARG:HH11  | 2.12        | 0.61     |
| 23:DB:2306:C:H3'  | 23:DB:2307:G:H5''  | 1.82        | 0.61     |
| 42:BN:37:THR:OG1  | 42:BN:40:LYS:HE2   | 2.00        | 0.61     |
| 24:DI:112:LYS:O   | 24:DI:116:MET:HG3  | 2.00        | 0.61     |
| 1:CA:1316:G:N2    | 1:CA:1318:A:H3'    | 2.15        | 0.61     |
| 1:CA:1320:C:H41   | 18:CS:36:ARG:HE    | 1.48        | 0.61     |
| 39:BX:6:LEU:O     | 39:BX:7:ARG:HB3    | 2.00        | 0.61     |
| 17:CR:33:THR:HG23 | 17:CR:37:LYS:O     | 1.99        | 0.61     |
| 3:CD:154:VAL:HG23 | 3:CD:155:LYS:H     | 1.65        | 0.61     |
| 23:DB:591:U:H1'   | 34:D3:1:PRO:N      | 2.15        | 0.61     |
| 44:BQ:105:PHE:O   | 44:BQ:109:VAL:HG23 | 2.00        | 0.61     |
| 5:AF:80:PHE:HE1   | 25:BC:135:PRO:HG2  | 1.64        | 0.61     |
| 23:DB:19:A:H2'    | 23:DB:20:C:C6      | 2.34        | 0.61     |
| 19:CT:79:THR:HA   | 19:CT:82:ILE:HG12  | 1.82        | 0.61     |
| 11:CL:107:LYS:H   | 11:CL:107:LYS:NZ   | 1.98        | 0.61     |
| 23:BB:2276:G:OP2  | 38:BM:85:GLY:N     | 2.32        | 0.61     |
| 23:DB:120:U:H4'   | 23:DB:121:G:H5''   | 1.82        | 0.61     |
| 23:DB:2071:A:H2'  | 23:DB:2072:C:C6    | 2.34        | 0.61     |
| 53:B6:2:THR:OG1   | 53:B6:5:GLU:HG3    | 2.00        | 0.61     |
| 23:DB:1152:C:H3'  | 57:DB:3274:HOH:O   | 2.00        | 0.61     |
| 53:D6:113:ASP:HA  | 53:D6:116:ARG:CD   | 2.30        | 0.61     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 22:DA:39:A:H2      | 22:DA:46:A:H61     | 1.48        | 0.61     |
| 23:BB:1947:C:H2'   | 23:BB:1948:G:H8    | 1.65        | 0.61     |
| 35:DV:49:ASN:N     | 35:DV:49:ASN:HD22  | 1.98        | 0.61     |
| 23:BB:2071:A:H2'   | 23:BB:2072:C:C6    | 2.35        | 0.61     |
| 26:BD:121:THR:HB   | 26:BD:127:PHE:CD1  | 2.34        | 0.61     |
| 25:BC:130:PRO:HG2  | 25:BC:133:ASN:HD22 | 1.64        | 0.61     |
| 48:BG:116:LEU:HD23 | 48:BG:121:THR:HA   | 1.83        | 0.61     |
| 47:BF:65:LEU:HD23  | 47:BF:87:LYS:HD2   | 1.82        | 0.61     |
| 10:CK:33:ILE:HG13  | 10:CK:73:VAL:HG21  | 1.83        | 0.61     |
| 50:BT:11:LEU:HD21  | 50:BT:46:ALA:HB1   | 1.81        | 0.61     |
| 12:CM:12:LYS:HD2   | 12:CM:16:ILE:HD13  | 1.81        | 0.61     |
| 1:AA:1080:A:H5''   | 4:AE:51:LYS:HZ3    | 1.64        | 0.61     |
| 47:DF:168:LEU:HD13 | 47:DF:169:LEU:H    | 1.66        | 0.61     |
| 45:DS:24:ILE:HG12  | 45:DS:36:LEU:HD21  | 1.81        | 0.61     |
| 23:BB:1173:U:H2'   | 23:BB:1174:U:C4'   | 2.28        | 0.61     |
| 48:BG:153:PRO:HG3  | 48:BG:162:ARG:HB3  | 1.82        | 0.61     |
| 45:BS:55:ILE:HD12  | 45:BS:107:VAL:HG21 | 1.82        | 0.61     |
| 30:BY:2:LYS:HD3    | 30:BY:2:LYS:H      | 1.64        | 0.61     |
| 1:CA:308:C:H2'     | 1:CA:309:A:H8      | 1.64        | 0.61     |
| 24:BI:18:ASN:N     | 24:BI:19:PRO:HD2   | 2.14        | 0.61     |
| 23:BB:2898:U:H2'   | 23:BB:2899:A:C8    | 2.36        | 0.61     |
| 23:DB:784:G:C6     | 25:DC:227:VAL:HG11 | 2.34        | 0.61     |
| 23:DB:1447:C:H2'   | 23:DB:1448:G:C8    | 2.35        | 0.61     |
| 23:BB:1788:C:O2'   | 23:BB:1789:A:H5'   | 2.00        | 0.61     |
| 45:BS:83:LYS:HD3   | 45:BS:97:LEU:HD11  | 1.82        | 0.61     |
| 23:DB:71:A:H4'     | 23:DB:72:U:H5'     | 1.81        | 0.61     |
| 1:CA:1169:A:H2'    | 1:CA:1170:A:C8     | 2.35        | 0.61     |
| 23:BB:909:A:H2'    | 23:BB:912:C:H5     | 1.64        | 0.61     |
| 23:DB:2455:G:H2'   | 23:DB:2456:C:C6    | 2.34        | 0.61     |
| 20:AB:52:ALA:O     | 20:AB:56:LEU:HB2   | 2.00        | 0.61     |
| 38:DM:82:MET:HE3   | 38:DM:83:GLY:H     | 1.65        | 0.61     |
| 6:CG:77:ARG:HG3    | 6:CG:79:VAL:HG23   | 1.82        | 0.61     |
| 26:BD:79:LEU:N     | 26:BD:79:LEU:HD22  | 2.15        | 0.61     |
| 52:BW:23:LYS:C     | 52:BW:66:VAL:HB    | 2.19        | 0.61     |
| 23:DB:2210:U:N3    | 23:DB:2212:A:N7    | 2.48        | 0.61     |
| 29:BE:105:LEU:HA   | 29:BE:108:ILE:HG22 | 1.82        | 0.61     |
| 46:DU:3:LYS:HD3    | 46:DU:82:VAL:HG21  | 1.82        | 0.61     |
| 29:BE:145:ASP:HB3  | 29:BE:184:ASP:HB2  | 1.82        | 0.61     |
| 38:BM:21:ALA:HB2   | 38:BM:100:LYS:HG2  | 1.82        | 0.61     |
| 50:DT:57:VAL:HG13  | 50:DT:58:VAL:N     | 2.16        | 0.61     |
| 21:CU:24:LYS:HZ3   | 21:CU:25:ALA:H     | 1.47        | 0.61     |
| 35:DV:80:HIS:CD2   | 35:DV:83:LYS:HB2   | 2.35        | 0.61     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:AA:1432:G:H5'    | 28:BP:105:LYS:CG  | 2.29        | 0.61     |
| 23:DB:2615:U:C2    | 31:D0:3:GLN:HA    | 2.36        | 0.61     |
| 41:DJ:110:PRO:HB2  | 41:DJ:111:LYS:HE3 | 1.82        | 0.61     |
| 23:DB:773:U:H4'    | 25:DC:45:ASN:O    | 1.99        | 0.61     |
| 1:CA:321:A:O2'     | 1:CA:322:C:H5'    | 2.01        | 0.61     |
| 23:BB:220:G:H1     | 23:BB:427:U:H2'   | 1.65        | 0.61     |
| 49:DR:71:LYS:HG3   | 49:DR:72:VAL:N    | 2.14        | 0.61     |
| 23:DB:1583:A:H4'   | 23:DB:1585:C:C4   | 2.36        | 0.61     |
| 6:CG:14:ASP:HB3    | 6:CG:19:SER:H     | 1.64        | 0.61     |
| 1:AA:171:A:H2'     | 1:AA:172:A:C8     | 2.36        | 0.61     |
| 23:DB:1376:C:H3'   | 57:DB:3278:HOH:O  | 2.00        | 0.61     |
| 25:BC:61:TYR:HA    | 25:BC:85:ASN:HD21 | 1.64        | 0.61     |
| 1:AA:390:U:H2'     | 1:AA:391:G:C8     | 2.34        | 0.61     |
| 1:CA:390:U:H2'     | 1:CA:391:G:C8     | 2.35        | 0.61     |
| 1:AA:501:C:H1'     | 1:AA:549:C:H1'    | 1.81        | 0.61     |
| 1:AA:505:G:H4'     | 1:AA:534:U:C4     | 2.35        | 0.61     |
| 24:DI:1:ALA:HB1    | 24:DI:2:LYS:HD2   | 1.81        | 0.61     |
| 23:DB:1098:A:C8    | 24:DI:3:LYS:HB3   | 2.34        | 0.61     |
| 25:DC:103:ILE:HG22 | 25:DC:105:ALA:H   | 1.65        | 0.61     |
| 21:CU:38:GLU:C     | 21:CU:40:PRO:HD2  | 2.20        | 0.61     |
| 53:D6:51:PRO:HB2   | 53:D6:53:ASN:ND2  | 2.16        | 0.61     |
| 49:DR:5:PHE:O      | 49:DR:11:GLN:HA   | 2.00        | 0.61     |
| 44:BQ:63:ARG:NH2   | 44:BQ:96:ASP:HA   | 2.16        | 0.61     |
| 46:BU:85:ARG:HH11  | 46:BU:86:PHE:H    | 1.47        | 0.61     |
| 12:CM:38:ILE:HG22  | 12:CM:42:VAL:HG21 | 1.82        | 0.61     |
| 23:BB:2810:A:H2'   | 23:BB:2811:G:O4'  | 2.01        | 0.61     |
| 46:BU:80:ASP:HB3   | 46:BU:96:LYS:N    | 2.15        | 0.61     |
| 13:CN:25:GLU:HB2   | 13:CN:29:ILE:HD11 | 1.81        | 0.61     |
| 1:CA:1313:U:OP2    | 18:CS:5:LYS:HA    | 2.00        | 0.61     |
| 44:BQ:4:LYS:HZ1    | 44:BQ:7:VAL:HG22  | 1.65        | 0.61     |
| 42:DN:33:ILE:HD12  | 42:DN:33:ILE:O    | 2.00        | 0.61     |
| 27:BK:13:ASN:HD21  | 27:BK:98:ARG:H    | 1.48        | 0.61     |
| 4:AE:158:LYS:NZ    | 7:AH:65:PHE:HA    | 2.16        | 0.61     |
| 46:BU:21:ARG:HD3   | 46:BU:72:PHE:CG   | 2.36        | 0.61     |
| 4:CE:82:HIS:HB2    | 4:CE:83:PRO:HD2   | 1.83        | 0.61     |
| 23:BB:2086:U:H2'   | 23:BB:2087:G:C8   | 2.36        | 0.61     |
| 23:BB:1432:G:H2'   | 23:BB:1433:A:C8   | 2.35        | 0.61     |
| 23:BB:2229:U:H2'   | 23:BB:2230:G:C8   | 2.35        | 0.61     |
| 19:CT:35:TYR:O     | 19:CT:38:ILE:HG22 | 2.01        | 0.61     |
| 6:AG:62:GLU:O      | 6:AG:66:GLU:HG3   | 2.01        | 0.61     |
| 23:BB:634:C:H2'    | 23:BB:635:C:C6    | 2.35        | 0.61     |
| 23:DB:833:A:H1'    | 37:DL:52:GLY:N    | 2.15        | 0.61     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 15:CP:74:LEU:O    | 15:CP:78:VAL:HG12  | 2.01        | 0.61     |
| 23:DB:2230:G:H2'  | 23:DB:2231:U:C6    | 2.36        | 0.61     |
| 23:BB:923:G:H1'   | 52:BW:23:LYS:NZ    | 2.16        | 0.61     |
| 52:DW:39:GLN:NE2  | 52:DW:43:LYS:HB2   | 2.16        | 0.61     |
| 48:BG:122:ALA:HA  | 48:BG:132:LEU:HA   | 1.82        | 0.61     |
| 47:DF:32:LYS:HA   | 47:DF:95:MET:HG3   | 1.81        | 0.61     |
| 8:AI:29:ILE:HA    | 8:AI:64:ILE:HB     | 1.82        | 0.61     |
| 22:DA:28:C:OP1    | 43:DO:31:THR:HG21  | 2.00        | 0.61     |
| 1:AA:1302:C:OP2   | 12:AM:16:ILE:HD11  | 2.00        | 0.61     |
| 41:BJ:45:THR:H    | 41:BJ:46:PRO:HD3   | 1.64        | 0.61     |
| 42:BN:83:LEU:HA   | 42:BN:86:ARG:CB    | 2.27        | 0.61     |
| 31:D0:21:LEU:HD12 | 45:DS:19:LEU:O     | 2.00        | 0.61     |
| 1:CA:812:G:H2'    | 1:CA:812:G:N3      | 2.15        | 0.61     |
| 18:CS:18:VAL:CG2  | 18:CS:43:MET:HB3   | 2.30        | 0.61     |
| 45:BS:17:VAL:C    | 45:BS:19:LEU:H     | 2.03        | 0.61     |
| 12:AM:38:ILE:HG22 | 12:AM:42:VAL:HG21  | 1.81        | 0.61     |
| 33:D1:8:ILE:HD11  | 33:D1:52:LYS:HB2   | 1.82        | 0.61     |
| 23:DB:139:U:H3    | 50:DT:49:LYS:HE2   | 1.65        | 0.61     |
| 32:B4:7:VAL:HG23  | 32:B4:35:GLN:CB    | 2.28        | 0.61     |
| 17:CR:34:GLU:HB2  | 21:CU:18:PHE:CZ    | 2.36        | 0.61     |
| 29:BE:188:MET:HE3 | 29:BE:193:VAL:HG13 | 1.82        | 0.61     |
| 44:BQ:107:ALA:HB1 | 49:BR:48:LYS:HE3   | 1.81        | 0.61     |
| 30:BY:18:LYS:O    | 30:BY:22:THR:HG23  | 2.01        | 0.61     |
| 26:DD:37:VAL:CG2  | 26:DD:91:THR:HA    | 2.30        | 0.61     |
| 23:BB:38:A:N3     | 29:BE:43:THR:HB    | 2.16        | 0.61     |
| 1:AA:237:G:H2'    | 1:AA:238:A:H8      | 1.66        | 0.61     |
| 23:DB:1203:U:H1'  | 37:DL:4:ASN:HD21   | 1.65        | 0.61     |
| 1:AA:1021:A:H2'   | 1:AA:1022:A:O4'    | 2.00        | 0.61     |
| 23:DB:2710:C:H2'  | 23:DB:2711:A:C8    | 2.36        | 0.61     |
| 23:BB:664:G:H2'   | 23:BB:665:U:C6     | 2.35        | 0.61     |
| 49:BR:71:LYS:HG3  | 49:BR:72:VAL:N     | 2.16        | 0.61     |
| 1:CA:214:C:H2'    | 1:CA:215:C:C6      | 2.36        | 0.61     |
| 1:CA:216:U:H2'    | 1:CA:217:C:C6      | 2.34        | 0.61     |
| 23:BB:1406:U:H2'  | 23:BB:1407:G:C8    | 2.36        | 0.61     |
| 23:BB:1406:U:H2'  | 23:BB:1407:G:H8    | 1.64        | 0.61     |
| 23:DB:2022:U:O2'  | 23:DB:2617:U:H5'   | 2.01        | 0.61     |
| 23:DB:2229:U:H2'  | 23:DB:2230:G:H8    | 1.65        | 0.61     |
| 23:BB:2292:U:H2'  | 23:BB:2293:G:H8    | 1.66        | 0.61     |
| 26:DD:125:TRP:CG  | 26:DD:160:LYS:HB3  | 2.35        | 0.61     |
| 23:BB:742:A:H2'   | 23:BB:743:A:C8     | 2.36        | 0.61     |
| 23:DB:2567:G:H2'  | 23:DB:2568:U:C6    | 2.36        | 0.61     |
| 48:DG:123:GLU:HG2 | 48:DG:124:CYS:N    | 2.16        | 0.61     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 52:DW:37:VAL:HG13  | 52:DW:55:ASP:O     | 2.00        | 0.61     |
| 48:DG:122:ALA:HA   | 48:DG:132:LEU:HA   | 1.83        | 0.61     |
| 8:AI:46:VAL:HA     | 8:AI:49:GLN:HG3    | 1.83        | 0.61     |
| 47:BF:115:GLY:HA2  | 47:BF:177:ARG:HH11 | 1.66        | 0.61     |
| 23:BB:2199:A:H5'   | 23:BB:2200:C:OP2   | 2.01        | 0.61     |
| 37:BL:42:SER:C     | 37:BL:44:GLY:H     | 2.04        | 0.61     |
| 29:BE:158:PHE:HA   | 29:BE:169:VAL:HG21 | 1.81        | 0.61     |
| 4:CE:28:ARG:NH2    | 4:CE:30:PHE:HA     | 2.15        | 0.61     |
| 1:AA:1313:U:OP2    | 18:AS:5:LYS:HA     | 1.99        | 0.61     |
| 18:AS:39:ILE:HB    | 18:AS:66:VAL:HA    | 1.83        | 0.61     |
| 17:CR:34:GLU:H     | 17:CR:34:GLU:CD    | 2.04        | 0.61     |
| 23:BB:1082:U:N3    | 23:BB:1086:A:C6    | 2.69        | 0.61     |
| 23:BB:28:A:N6      | 23:BB:512:G:H1'    | 2.16        | 0.61     |
| 46:BU:26:ASN:HD21  | 46:BU:34:ILE:HD12  | 1.65        | 0.61     |
| 1:CA:551:U:O2'     | 11:CL:82:ARG:HD2   | 2.01        | 0.61     |
| 42:BN:90:ARG:HB3   | 42:BN:94:TYR:HE1   | 1.65        | 0.61     |
| 1:CA:859:G:H2'     | 1:CA:860:A:H8      | 1.64        | 0.61     |
| 25:DC:245:THR:O    | 25:DC:247:TRP:N    | 2.34        | 0.61     |
| 1:CA:366:A:H1'     | 1:CA:395:C:O2      | 2.00        | 0.61     |
| 1:AA:1515:G:O2'    | 1:AA:1516:G:H5'    | 2.00        | 0.61     |
| 20:CB:160:LEU:HD23 | 20:CB:181:PRO:O    | 2.01        | 0.61     |
| 23:DB:937:C:H2'    | 23:DB:938:G:C8     | 2.36        | 0.61     |
| 23:BB:2092:U:H4'   | 23:BB:2093:G:O5'   | 2.01        | 0.61     |
| 21:AU:11:PHE:O     | 21:AU:13:VAL:N     | 2.34        | 0.61     |
| 1:AA:746:A:H2'     | 1:AA:747:A:C8      | 2.36        | 0.61     |
| 27:DK:13:ASN:HD21  | 27:DK:98:ARG:H     | 1.48        | 0.61     |
| 50:DT:32:LEU:H     | 50:DT:83:ALA:HB3   | 1.66        | 0.61     |
| 2:AC:131:ARG:HG2   | 2:AC:131:ARG:HH11  | 1.64        | 0.61     |
| 5:AF:16:GLU:H      | 5:AF:16:GLU:CD     | 2.02        | 0.61     |
| 6:CG:23:ALA:O      | 6:CG:26:VAL:HG22   | 2.01        | 0.61     |
| 52:BW:18:LYS:HG3   | 52:BW:19:ARG:CZ    | 2.31        | 0.61     |
| 23:DB:2354:C:H4'   | 52:DW:31:LEU:HD22  | 1.81        | 0.61     |
| 26:BD:106:LYS:HB3  | 26:BD:206:ALA:N    | 2.15        | 0.61     |
| 41:BJ:25:LEU:HD22  | 41:BJ:26:GLY:N     | 2.14        | 0.61     |
| 41:BJ:36:LEU:HD11  | 41:BJ:122:LEU:HB2  | 1.82        | 0.61     |
| 47:BF:101:ARG:CZ   | 47:BF:138:PRO:HB2  | 2.30        | 0.61     |
| 1:AA:1060:U:C4'    | 9:AJ:54:SER:HB2    | 2.30        | 0.61     |
| 53:D6:74:ASN:HD22  | 53:D6:74:ASN:N     | 1.93        | 0.61     |
| 21:AU:24:LYS:HZ3   | 21:AU:25:ALA:H     | 1.49        | 0.61     |
| 12:AM:78:ARG:O     | 12:AM:82:LEU:HB2   | 2.00        | 0.61     |
| 53:D6:18:LEU:HD22  | 53:D6:168:PHE:CD2  | 2.36        | 0.61     |
| 45:DS:26:GLY:N     | 45:DS:71:VAL:HG13  | 2.15        | 0.61     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 17:AR:33:THR:HG23 | 17:AR:37:LYS:O     | 2.00        | 0.61     |
| 23:BB:873:C:H2'   | 23:BB:874:G:H8     | 1.63        | 0.61     |
| 45:DS:22:ASP:HA   | 45:DS:25:ARG:NH1   | 2.15        | 0.61     |
| 53:D6:29:ARG:HD3  | 53:D6:110:ARG:NH2  | 2.15        | 0.61     |
| 23:DB:171:U:H2'   | 23:DB:172:A:C8     | 2.36        | 0.61     |
| 1:CA:300:A:H2'    | 1:CA:301:G:O4'     | 2.01        | 0.61     |
| 1:AA:1049:U:H6    | 1:AA:1049:U:H5'    | 1.65        | 0.61     |
| 35:DV:42:LEU:HD12 | 35:DV:47:VAL:HG21  | 1.83        | 0.61     |
| 23:BB:2379:G:H2'  | 23:BB:2380:C:H6    | 1.63        | 0.61     |
| 23:DB:1484:U:H2'  | 23:DB:1485:U:C6    | 2.36        | 0.61     |
| 23:DB:16:C:O2'    | 23:DB:17:G:H5'     | 1.99        | 0.61     |
| 23:DB:307:G:H2'   | 23:DB:309:A:OP2    | 2.00        | 0.61     |
| 1:AA:676:A:H2'    | 1:AA:677:U:C6      | 2.35        | 0.61     |
| 23:BB:523:C:H4'   | 23:BB:540:C:O2     | 2.00        | 0.61     |
| 23:BB:129:C:H2'   | 23:BB:130:C:C6     | 2.36        | 0.61     |
| 20:AB:23:ASN:HD22 | 20:AB:24:PRO:HD2   | 1.65        | 0.61     |
| 23:DB:962:G:N2    | 23:DB:2250:G:H1    | 1.99        | 0.61     |
| 18:CS:32:THR:HG22 | 18:CS:34:SER:H     | 1.65        | 0.61     |
| 23:DB:506:G:H5''  | 23:DB:509:C:O2'    | 2.01        | 0.61     |
| 51:BZ:66:THR:O    | 51:BZ:69:ALA:HB3   | 2.01        | 0.61     |
| 23:BB:184:C:H2'   | 23:BB:185:G:H8     | 1.65        | 0.61     |
| 23:BB:2498:C:O2'  | 23:BB:2499:C:H5'   | 2.00        | 0.61     |
| 23:DB:1993:U:H4'  | 26:DD:133:THR:HG22 | 1.83        | 0.61     |
| 40:BH:80:ILE:HB   | 40:BH:144:VAL:HG13 | 1.83        | 0.61     |
| 20:CB:184:ALA:HB3 | 20:CB:195:VAL:HG21 | 1.82        | 0.61     |
| 29:DE:58:LYS:H    | 29:DE:58:LYS:HZ3   | 1.47        | 0.61     |
| 45:DS:16:LYS:O    | 45:DS:19:LEU:HB3   | 2.01        | 0.61     |
| 23:BB:2109:U:H2'  | 23:BB:2110:G:H5'   | 1.83        | 0.61     |
| 1:AA:1320:C:N3    | 18:AS:35:ARG:HD3   | 2.16        | 0.61     |
| 45:DS:55:ILE:HD12 | 45:DS:107:VAL:HG21 | 1.83        | 0.61     |
| 46:BU:95:PHE:CE1  | 46:BU:102:ILE:HB   | 2.32        | 0.61     |
| 23:DB:1082:U:N3   | 23:DB:1086:A:C6    | 2.69        | 0.61     |
| 25:BC:12:ARG:HA   | 25:BC:15:VAL:HG23  | 1.81        | 0.61     |
| 44:BQ:86:SER:CB   | 49:BR:51:VAL:HA    | 2.31        | 0.61     |
| 27:BK:118:LEU:C   | 27:BK:120:PRO:HD2  | 2.21        | 0.61     |
| 23:DB:1196:C:H2'  | 23:DB:1197:G:C8    | 2.35        | 0.61     |
| 23:BB:2186:G:H2'  | 23:BB:2187:U:C6    | 2.35        | 0.61     |
| 23:DB:2243:U:H2'  | 23:DB:2244:U:H6    | 1.62        | 0.61     |
| 14:AO:25:THR:HB   | 14:AO:70:LEU:HD23  | 1.82        | 0.61     |
| 41:BJ:112:GLY:H   | 41:BJ:113:PRO:HD2  | 1.65        | 0.61     |
| 23:BB:1150:C:H2'  | 23:BB:1151:A:H8    | 1.66        | 0.61     |
| 35:DV:53:LYS:HB3  | 35:DV:55:GLU:OE1   | 2.01        | 0.61     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 30:BY:6:ILE:O      | 30:BY:34:THR:HA    | 2.01        | 0.61     |
| 23:DB:18:U:H2'     | 23:DB:19:A:C8      | 2.36        | 0.61     |
| 20:AB:85:SER:O     | 20:AB:86:CYS:HB2   | 2.01        | 0.61     |
| 23:DB:2875:C:H2'   | 23:DB:2876:G:C8    | 2.36        | 0.61     |
| 22:DA:111:U:H2'    | 22:DA:112:G:H8     | 1.65        | 0.61     |
| 1:AA:676:A:H2'     | 1:AA:677:U:H6      | 1.65        | 0.61     |
| 3:CD:60:VAL:HA     | 3:CD:63:ILE:HD12   | 1.81        | 0.61     |
| 4:AE:96:GLN:HB3    | 4:AE:123:LEU:HD12  | 1.82        | 0.61     |
| 23:DB:1939:U:H5'   | 23:DB:1939:U:H6    | 1.65        | 0.61     |
| 23:BB:1315:C:H2'   | 23:BB:1316:U:C6    | 2.35        | 0.61     |
| 25:DC:143:VAL:HG12 | 25:DC:144:GLU:N    | 2.16        | 0.61     |
| 25:DC:146:LYS:HB3  | 25:DC:147:PRO:HD2  | 1.82        | 0.61     |
| 25:DC:166:ARG:HB2  | 25:DC:171:VAL:HG22 | 1.82        | 0.61     |
| 10:CK:33:ILE:HG12  | 10:CK:69:CYS:SG    | 2.41        | 0.61     |
| 53:B6:59:THR:HG23  | 53:B6:67:VAL:HG23  | 1.82        | 0.61     |
| 38:BM:59:ARG:HE    | 38:BM:60:GLN:H     | 1.49        | 0.61     |
| 23:DB:636:G:O5'    | 37:DL:128:THR:HG22 | 2.00        | 0.61     |
| 41:DJ:25:LEU:HD13  | 41:DJ:26:GLY:N     | 2.15        | 0.61     |
| 22:DA:24:G:N7      | 22:DA:56:G:H2'     | 2.16        | 0.61     |
| 48:BG:17:LYS:HA    | 48:BG:17:LYS:HZ2   | 1.65        | 0.61     |
| 51:BZ:5:CYS:CB     | 51:BZ:10:LYS:H     | 2.12        | 0.61     |
| 13:AN:68:ARG:NH1   | 13:AN:68:ARG:HB3   | 2.11        | 0.61     |
| 3:AD:29:THR:HG22   | 3:AD:30:LYS:H      | 1.66        | 0.61     |
| 47:BF:102:LEU:HD22 | 47:BF:103:ILE:H    | 1.64        | 0.61     |
| 47:BF:24:VAL:O     | 47:BF:27:VAL:HG22  | 2.01        | 0.61     |
| 23:BB:321:U:OP2    | 29:BE:130:LYS:HD3  | 2.00        | 0.61     |
| 1:AA:919:A:O2'     | 1:AA:920:U:H5'     | 2.01        | 0.61     |
| 47:DF:102:LEU:HD13 | 47:DF:103:ILE:HB   | 1.82        | 0.61     |
| 4:CE:89:THR:HG21   | 4:CE:134:ASN:ND2   | 2.15        | 0.61     |
| 25:DC:12:ARG:HA    | 25:DC:15:VAL:HG23  | 1.83        | 0.61     |
| 53:D6:17:SER:O     | 53:D6:20:VAL:HB    | 2.00        | 0.61     |
| 39:DX:6:LEU:O      | 39:DX:7:ARG:HB3    | 2.00        | 0.61     |
| 24:DI:32:VAL:HG22  | 24:DI:60:VAL:HG21  | 1.83        | 0.61     |
| 23:DB:1024:G:C3'   | 23:DB:1025:G:H5''  | 2.27        | 0.61     |
| 25:BC:204:LEU:HD23 | 25:BC:209:ALA:HB1  | 1.82        | 0.61     |
| 23:DB:2722:G:H2'   | 23:DB:2723:C:H6    | 1.66        | 0.61     |
| 23:DB:1796:U:O2'   | 23:DB:1797:G:H5'   | 2.01        | 0.61     |
| 3:CD:187:ARG:NH1   | 3:CD:191:SER:HA    | 2.16        | 0.61     |
| 11:CL:66:ILE:HG21  | 11:CL:71:HIS:HB3   | 1.82        | 0.61     |
| 1:AA:636:U:H2'     | 1:AA:637:C:H6      | 1.65        | 0.61     |
| 23:DB:523:C:H4'    | 23:DB:540:C:O2     | 2.01        | 0.61     |
| 1:CA:1461:G:H2'    | 1:CA:1462:C:C6     | 2.35        | 0.61     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:782:A:N3    | 25:DC:224:MET:HB3  | 2.15        | 0.61     |
| 1:CA:1007:U:H2'   | 1:CA:1008:U:C6     | 2.35        | 0.61     |
| 42:BN:12:ARG:HG3  | 42:BN:13:ASN:H     | 1.66        | 0.61     |
| 25:BC:245:THR:O   | 25:BC:247:TRP:N    | 2.34        | 0.61     |
| 48:DG:54:ARG:HB3  | 48:DG:57:TYR:HD1   | 1.64        | 0.61     |
| 23:DB:899:A:H3'   | 23:DB:900:A:H8     | 1.65        | 0.61     |
| 6:AG:77:ARG:HG3   | 6:AG:79:VAL:HG23   | 1.83        | 0.61     |
| 23:DB:401:A:H2'   | 23:DB:402:A:C8     | 2.36        | 0.61     |
| 6:AG:68:VAL:HG11  | 6:AG:133:ALA:HB1   | 1.82        | 0.61     |
| 23:DB:794:A:H2'   | 23:DB:795:C:C6     | 2.36        | 0.61     |
| 15:CP:59:HIS:O    | 15:CP:63:GLN:HG3   | 2.01        | 0.61     |
| 1:CA:1278:G:H4'   | 1:CA:1279:G:C5'    | 2.31        | 0.61     |
| 23:DB:2292:U:H2'  | 23:DB:2293:G:H8    | 1.66        | 0.61     |
| 20:AB:133:ALA:O   | 20:AB:137:THR:HG23 | 2.00        | 0.61     |
| 23:BB:870:U:O2'   | 23:BB:871:U:H5'    | 2.00        | 0.61     |
| 43:BO:9:ARG:HG3   | 43:BO:10:ARG:N     | 2.16        | 0.61     |
| 1:CA:797:C:O2'    | 1:CA:798:U:H5'     | 1.99        | 0.61     |
| 40:DH:31:VAL:CB   | 40:DH:32:PRO:CD    | 2.77        | 0.60     |
| 23:BB:2748:A:H4'  | 48:BG:3:VAL:HG21   | 1.81        | 0.60     |
| 23:DB:2019:A:H2   | 23:DB:2035:G:H22   | 1.49        | 0.60     |
| 53:D6:92:PRO:HA   | 53:D6:101:ILE:CG1  | 2.28        | 0.60     |
| 38:DM:59:ARG:HE   | 38:DM:60:GLN:H     | 1.48        | 0.60     |
| 38:DM:59:ARG:NH1  | 38:DM:60:GLN:HB3   | 2.07        | 0.60     |
| 8:AI:83:THR:HA    | 8:AI:86:LEU:HD22   | 1.82        | 0.60     |
| 51:DZ:77:LYS:HD2  | 51:DZ:78:TYR:H     | 1.65        | 0.60     |
| 38:DM:21:ALA:HB2  | 38:DM:100:LYS:HG2  | 1.83        | 0.60     |
| 38:BM:35:ALA:HB2  | 38:BM:100:LYS:H    | 1.64        | 0.60     |
| 35:BV:80:HIS:CD2  | 35:BV:83:LYS:HB2   | 2.36        | 0.60     |
| 12:AM:47:LEU:HD13 | 12:AM:51:GLN:O     | 1.99        | 0.60     |
| 23:DB:2267:A:O5'  | 23:DB:2267:A:H8    | 1.83        | 0.60     |
| 23:BB:2267:A:H8   | 23:BB:2267:A:C3'   | 2.10        | 0.60     |
| 23:DB:2722:G:H2'  | 23:DB:2723:C:C6    | 2.36        | 0.60     |
| 23:BB:1283:G:N2   | 23:BB:1285:A:H3'   | 2.16        | 0.60     |
| 1:AA:715:A:H2'    | 1:AA:716:A:C8      | 2.34        | 0.60     |
| 24:DI:123:ALA:HA  | 24:DI:126:ARG:HH12 | 1.65        | 0.60     |
| 20:CB:125:PHE:HA  | 20:CB:127:LYS:HZ1  | 1.66        | 0.60     |
| 23:BB:37:C:O2'    | 29:BE:45:ALA:HA    | 2.01        | 0.60     |
| 1:AA:876:C:H1'    | 7:AH:11:THR:HG21   | 1.82        | 0.60     |
| 43:BO:47:VAL:HG12 | 43:BO:48:LEU:N     | 2.16        | 0.60     |
| 23:DB:1149:G:H2'  | 23:DB:1150:C:H6    | 1.64        | 0.60     |
| 38:DM:68:PHE:CG   | 38:DM:69:PRO:HD2   | 2.36        | 0.60     |
| 23:DB:19:A:H2'    | 23:DB:20:C:H6      | 1.66        | 0.60     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:BB:1387:A:H5'   | 23:BB:1469:A:H1'  | 1.83        | 0.60     |
| 23:BB:2183:A:H2'   | 23:BB:2184:A:C8   | 2.35        | 0.60     |
| 1:AA:1190:G:OP1    | 2:AC:3:LYS:HA     | 2.00        | 0.60     |
| 23:DB:2363:G:O2'   | 23:DB:2364:C:H5'  | 2.01        | 0.60     |
| 1:CA:1190:G:OP1    | 2:CC:3:LYS:HA     | 2.01        | 0.60     |
| 41:DJ:29:ALA:HA    | 41:DJ:32:LEU:HD12 | 1.81        | 0.60     |
| 23:BB:401:A:H2'    | 23:BB:402:A:C8    | 2.36        | 0.60     |
| 23:DB:2671:G:H2'   | 23:DB:2672:U:C6   | 2.36        | 0.60     |
| 23:DB:100:U:OP1    | 23:DB:100:U:H3'   | 2.01        | 0.60     |
| 38:BM:108:VAL:HG13 | 38:BM:112:LEU:HB3 | 1.82        | 0.60     |
| 23:DB:2412:A:H2'   | 23:DB:2413:G:O4'  | 1.99        | 0.60     |
| 25:BC:143:VAL:HG12 | 25:BC:144:GLU:N   | 2.16        | 0.60     |
| 44:BQ:18:LYS:C     | 44:BQ:20:ALA:H    | 2.05        | 0.60     |
| 48:DG:106:LEU:HD12 | 48:DG:151:ARG:HD3 | 1.82        | 0.60     |
| 53:D6:57:THR:O     | 53:D6:69:GLN:N    | 2.34        | 0.60     |
| 23:DB:2366:A:H4'   | 52:DW:61:LYS:HE2  | 1.83        | 0.60     |
| 8:CI:64:ILE:H      | 8:CI:64:ILE:HD12  | 1.65        | 0.60     |
| 41:DJ:40:HIS:CE1   | 41:DJ:41:LYS:HG3  | 2.36        | 0.60     |
| 46:DU:85:ARG:NE    | 46:DU:85:ARG:HA   | 2.15        | 0.60     |
| 34:B3:39:ARG:O     | 34:B3:43:LEU:HG   | 2.01        | 0.60     |
| 35:BV:80:HIS:CG    | 35:BV:83:LYS:HB2  | 2.36        | 0.60     |
| 20:AB:44:LYS:C     | 20:AB:47:PRO:HD2  | 2.22        | 0.60     |
| 23:BB:1170:C:H2'   | 23:BB:1171:G:C8   | 2.36        | 0.60     |
| 1:AA:1432:G:H1'    | 1:AA:1468:A:N6    | 2.15        | 0.60     |
| 1:AA:1469:C:H2'    | 1:AA:1470:U:O4'   | 2.00        | 0.60     |
| 23:BB:30:G:OP1     | 44:BQ:4:LYS:HG2   | 2.01        | 0.60     |
| 23:DB:1440:U:H2'   | 23:DB:1441:G:C8   | 2.35        | 0.60     |
| 36:B2:9:VAL:HG13   | 36:B2:10:LEU:N    | 2.15        | 0.60     |
| 4:AE:82:HIS:HB2    | 4:AE:83:PRO:HD2   | 1.83        | 0.60     |
| 23:DB:63:A:H2'     | 23:DB:63:A:OP2    | 2.01        | 0.60     |
| 23:BB:1656:C:H2'   | 23:BB:1657:U:H6   | 1.65        | 0.60     |
| 1:AA:254:G:OP1     | 16:AQ:68:LYS:O    | 2.18        | 0.60     |
| 23:DB:1248:G:OP1   | 44:DQ:1:ALA:HB3   | 2.01        | 0.60     |
| 23:DB:2153:C:H2'   | 23:DB:2154:A:H8   | 1.67        | 0.60     |
| 40:BH:57:LYS:NZ    | 40:BH:58:LEU:HD13 | 2.16        | 0.60     |
| 3:AD:58:GLN:O      | 3:AD:62:ARG:HG2   | 2.00        | 0.60     |
| 23:DB:1930:G:H2'   | 23:DB:1968:G:C6   | 2.36        | 0.60     |
| 1:AA:539:A:H2'     | 1:AA:540:G:C8     | 2.36        | 0.60     |
| 17:AR:40:PRO:HD2   | 17:AR:43:ILE:HD12 | 1.83        | 0.60     |
| 1:AA:1067:A:H4'    | 1:AA:1068:G:O5'   | 2.01        | 0.60     |
| 23:DB:1061:U:O4'   | 23:DB:1070:A:H1'  | 2.00        | 0.60     |
| 41:DJ:13:ARG:O     | 41:DJ:52:ASP:HA   | 2.01        | 0.60     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:2671:G:H2'   | 23:BB:2672:U:C6    | 2.36        | 0.60     |
| 23:BB:2704:C:H2'   | 23:BB:2705:A:O4'   | 2.02        | 0.60     |
| 23:BB:2341:G:H2'   | 23:BB:2342:C:C6    | 2.35        | 0.60     |
| 25:BC:41:GLY:HA3   | 25:BC:53:ILE:HG21  | 1.82        | 0.60     |
| 26:DD:30:GLU:HG3   | 26:DD:52:THR:CG2   | 2.30        | 0.60     |
| 41:DJ:25:LEU:HD22  | 41:DJ:26:GLY:N     | 2.13        | 0.60     |
| 1:AA:1296:C:C4'    | 1:AA:1302:C:H41    | 2.10        | 0.60     |
| 3:CD:26:ALA:HA     | 3:CD:30:LYS:HE3    | 1.83        | 0.60     |
| 22:BA:30:C:H2'     | 22:BA:31:C:H5'     | 1.84        | 0.60     |
| 1:AA:1260:G:H4'    | 1:AA:1283:U:O2'    | 2.02        | 0.60     |
| 47:DF:107:VAL:HG11 | 47:DF:175:PRO:HG3  | 1.83        | 0.60     |
| 1:CA:1320:C:N3     | 18:CS:35:ARG:HD3   | 2.16        | 0.60     |
| 37:DL:42:SER:C     | 37:DL:44:GLY:H     | 2.05        | 0.60     |
| 1:AA:1319:A:H4'    | 1:AA:1320:C:OP1    | 2.01        | 0.60     |
| 18:AS:62:THR:HG22  | 18:AS:63:ASP:H     | 1.67        | 0.60     |
| 38:DM:126:ILE:N    | 38:DM:126:ILE:HD12 | 2.14        | 0.60     |
| 23:DB:2740:A:H2'   | 23:DB:2741:A:C8    | 2.37        | 0.60     |
| 5:CF:6:ILE:HG23    | 5:CF:62:MET:HB3    | 1.83        | 0.60     |
| 3:CD:116:LEU:HD21  | 3:CD:153:ARG:HD2   | 1.82        | 0.60     |
| 23:BB:2146:C:H1'   | 23:BB:2147:A:H4'   | 1.83        | 0.60     |
| 23:BB:2895:G:H2'   | 23:BB:2896:C:C6    | 2.35        | 0.60     |
| 26:BD:148:GLN:CG   | 26:BD:152:PRO:HG2  | 2.30        | 0.60     |
| 29:DE:130:LYS:C    | 29:DE:132:LYS:H    | 2.05        | 0.60     |
| 27:BK:88:ASN:HB3   | 27:BK:92:GLU:O     | 2.01        | 0.60     |
| 10:CK:17:ASP:HB3   | 10:CK:80:ASN:ND2   | 2.17        | 0.60     |
| 23:DB:2136:G:N1    | 23:DB:2156:G:H1'   | 2.16        | 0.60     |
| 12:AM:28:ARG:NH2   | 12:AM:62:PHE:HB2   | 2.17        | 0.60     |
| 39:BX:13:GLU:HB2   | 39:BX:57:LEU:HD13  | 1.84        | 0.60     |
| 23:BB:2710:C:H2'   | 23:BB:2711:A:C8    | 2.37        | 0.60     |
| 1:CA:1021:A:H2'    | 1:CA:1022:A:O4'    | 2.02        | 0.60     |
| 11:CL:106:VAL:HG23 | 11:CL:116:TYR:HB3  | 1.82        | 0.60     |
| 23:BB:2800:A:H2'   | 23:BB:2801:G:O4'   | 2.01        | 0.60     |
| 20:CB:8:MET:HB2    | 20:CB:11:ALA:CB    | 2.31        | 0.60     |
| 23:DB:1636:U:H2'   | 23:DB:1637:A:C8    | 2.36        | 0.60     |
| 1:CA:482:A:H2'     | 1:CA:483:C:O4'     | 2.00        | 0.60     |
| 1:AA:371:A:O2'     | 1:AA:372:C:H5'     | 2.01        | 0.60     |
| 1:CA:426:U:H4'     | 3:CD:39:GLN:HA     | 1.83        | 0.60     |
| 23:BB:2737:G:H2'   | 23:BB:2738:A:C8    | 2.35        | 0.60     |
| 23:BB:2370:G:H2'   | 23:BB:2371:G:O4'   | 2.01        | 0.60     |
| 23:DB:2801:G:H2'   | 23:DB:2802:G:C8    | 2.35        | 0.60     |
| 23:DB:417:C:H2'    | 23:DB:418:C:C6     | 2.36        | 0.60     |
| 1:CA:1180:A:P      | 8:CI:98:ARG:HH22   | 2.24        | 0.60     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 48:BG:123:GLU:HG2 | 48:BG:124:CYS:N    | 2.15        | 0.60     |
| 1:CA:1035:A:H2'   | 1:CA:1036:A:H8     | 1.67        | 0.60     |
| 16:AQ:30:HIS:CE1  | 16:AQ:32:ILE:HG22  | 2.36        | 0.60     |
| 23:DB:923:G:H1'   | 52:DW:23:LYS:HZ2   | 1.67        | 0.60     |
| 53:B6:60:ALA:HB2  | 53:B6:66:LEU:HG    | 1.83        | 0.60     |
| 8:AI:67:LYS:HB2   | 8:AI:67:LYS:HZ3    | 1.66        | 0.60     |
| 13:CN:79:SER:O    | 13:CN:83:VAL:HG23  | 2.02        | 0.60     |
| 40:DH:77:THR:HA   | 40:DH:143:ILE:O    | 1.99        | 0.60     |
| 33:B1:26:LYS:HB2  | 33:B1:52:LYS:HZ2   | 1.66        | 0.60     |
| 4:CE:22:LYS:HB3   | 4:CE:29:ILE:HB     | 1.84        | 0.60     |
| 1:AA:1320:C:H41   | 18:AS:36:ARG:HE    | 1.47        | 0.60     |
| 46:BU:81:ARG:HH21 | 46:BU:81:ARG:H     | 1.49        | 0.60     |
| 23:DB:1028:A:H2'  | 23:DB:1029:A:C8    | 2.36        | 0.60     |
| 13:CN:48:GLN:O    | 13:CN:51:PRO:HD2   | 2.02        | 0.60     |
| 23:BB:1440:U:H2'  | 23:BB:1441:G:C8    | 2.37        | 0.60     |
| 36:D2:26:ASN:O    | 36:D2:30:VAL:HG23  | 2.00        | 0.60     |
| 6:CG:41:ILE:HG21  | 6:CG:115:MET:HG3   | 1.82        | 0.60     |
| 1:CA:1513:A:H2'   | 1:CA:1514:G:C8     | 2.35        | 0.60     |
| 23:DB:2194:U:H2'  | 23:DB:2195:U:C6    | 2.35        | 0.60     |
| 23:BB:2093:G:O5'  | 40:BH:24:GLY:HA3   | 2.01        | 0.60     |
| 23:BB:2052:A:O4'  | 26:BD:147:GLY:HA3  | 2.01        | 0.60     |
| 23:DB:870:U:O2'   | 23:DB:871:U:H5'    | 2.01        | 0.60     |
| 23:BB:1365:A:OP2  | 51:BZ:3:ARG:HB2    | 2.01        | 0.60     |
| 23:DB:1416:G:HO2' | 23:DB:1417:C:H6    | 1.47        | 0.60     |
| 23:BB:817:C:H2'   | 23:BB:818:G:O4'    | 2.00        | 0.60     |
| 1:CA:746:A:H2'    | 1:CA:747:A:C8      | 2.35        | 0.60     |
| 23:BB:1205:A:N1   | 29:BE:165:HIS:HB2  | 2.16        | 0.60     |
| 23:BB:307:G:H2'   | 23:BB:309:A:OP2    | 2.02        | 0.60     |
| 23:BB:1859:U:H2'  | 23:BB:1860:G:C8    | 2.37        | 0.60     |
| 23:BB:19:A:H2'    | 23:BB:20:C:C6      | 2.37        | 0.60     |
| 20:AB:184:ALA:HB3 | 20:AB:195:VAL:HG21 | 1.83        | 0.60     |
| 23:DB:634:C:H2'   | 23:DB:635:C:C6     | 2.36        | 0.60     |
| 1:CA:1218:C:H2'   | 1:CA:1219:A:C8     | 2.36        | 0.60     |
| 24:DI:128:ILE:HA  | 24:DI:131:THR:HG23 | 1.83        | 0.60     |
| 4:AE:131:ASN:O    | 4:AE:135:VAL:HG23  | 2.02        | 0.60     |
| 50:DT:57:VAL:HG12 | 50:DT:86:THR:OG1   | 2.01        | 0.60     |
| 13:CN:12:ARG:HA   | 13:CN:15:LEU:HD12  | 1.83        | 0.60     |
| 23:BB:1081:U:H4'  | 24:BI:123:ALA:HB1  | 1.83        | 0.60     |
| 44:DQ:105:PHE:O   | 44:DQ:109:VAL:HG23 | 2.01        | 0.60     |
| 23:BB:2630:G:H2'  | 23:BB:2631:G:C8    | 2.36        | 0.60     |
| 28:BP:20:ARG:O    | 28:BP:46:VAL:HG21  | 2.01        | 0.60     |
| 1:AA:1163:A:H2'   | 1:AA:1164:G:C8     | 2.36        | 0.60     |

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| Atom-1            | Atom-2              | Distance(Å) | Clash(Å) |
|-------------------|---------------------|-------------|----------|
| 40:BH:50:ARG:O    | 40:BH:54:LEU:HD21   | 2.01        | 0.60     |
| 23:BB:2284:A:OP2  | 33:B1:5:ARG:HG3     | 2.02        | 0.60     |
| 23:DB:934:U:H2'   | 23:DB:935:C:C6      | 2.37        | 0.60     |
| 19:AT:57:VAL:HG23 | 19:AT:58:ASP:H      | 1.66        | 0.60     |
| 23:DB:2252:G:O2'  | 23:DB:2253:G:H5'    | 2.02        | 0.60     |
| 4:CE:96:GLN:HB3   | 4:CE:123:LEU:HD12   | 1.84        | 0.60     |
| 23:DB:2685:G:O2'  | 23:DB:2686:G:H5'    | 2.00        | 0.60     |
| 23:DB:1564:C:H2'  | 23:DB:1565:C:C6     | 2.36        | 0.60     |
| 23:DB:2751:G:O2'  | 23:DB:2752:C:H5'    | 2.02        | 0.60     |
| 22:DA:30:C:H2'    | 22:DA:31:C:H5'      | 1.84        | 0.60     |
| 44:BQ:96:ASP:C    | 44:BQ:98:ALA:H      | 2.05        | 0.60     |
| 42:BN:55:ALA:HA   | 42:BN:80:PHE:CE1    | 2.36        | 0.60     |
| 47:BF:110:ILE:HA  | 47:BF:111:ARG:NH1   | 2.15        | 0.60     |
| 23:DB:1023:U:H2'  | 23:DB:1024:G:H5'    | 1.82        | 0.60     |
| 48:DG:162:ARG:HG3 | 48:DG:166:GLU:OE2   | 2.02        | 0.60     |
| 1:AA:35:G:H2'     | 1:AA:36:C:C6        | 2.36        | 0.60     |
| 3:AD:197:HIS:O    | 3:AD:200:VAL:HG22   | 2.02        | 0.60     |
| 23:BB:1812:U:H2'  | 23:BB:1813:G:C8     | 2.36        | 0.60     |
| 39:DX:5:GLU:O     | 39:DX:8:GLU:HG2     | 2.01        | 0.60     |
| 23:BB:693:A:H2'   | 23:BB:694:U:H6      | 1.66        | 0.60     |
| 1:AA:707:U:H4'    | 10:AK:21:HIS:CD2    | 2.36        | 0.60     |
| 5:AF:1:MET:SD     | 5:AF:67:PRO:HD3     | 2.42        | 0.60     |
| 23:DB:2070:A:H2'  | 23:DB:2071:A:C8     | 2.37        | 0.60     |
| 23:DB:2605:U:H2'  | 23:DB:2606:C:C6     | 2.37        | 0.60     |
| 23:DB:1920:C:N4   | 55:DB:3112:PAR:H122 | 1.99        | 0.60     |
| 23:BB:2860:A:O5'  | 23:BB:2860:A:H8     | 1.85        | 0.60     |
| 23:BB:479:A:N3    | 23:BB:481:G:H5''    | 2.17        | 0.60     |
| 23:DB:1099:G:O5'  | 24:DI:4:VAL:HG12    | 2.01        | 0.60     |
| 25:DC:64:VAL:HG11 | 25:DC:66:PHE:CZ     | 2.37        | 0.60     |
| 37:DL:143:GLU:HG2 | 37:DL:144:GLU:N     | 2.16        | 0.60     |
| 51:DZ:40:VAL:CG2  | 51:DZ:43:GLU:HB3    | 2.26        | 0.60     |
| 23:DB:2443:C:H2'  | 23:DB:2444:G:C8     | 2.36        | 0.60     |
| 7:CH:76:ARG:HG3   | 7:CH:77:VAL:N       | 2.16        | 0.60     |
| 50:BT:57:VAL:HG13 | 50:BT:58:VAL:N      | 2.17        | 0.60     |
| 29:DE:59:PRO:HB2  | 29:DE:67:ARG:NH2    | 2.14        | 0.60     |
| 47:DF:110:ILE:HA  | 47:DF:111:ARG:NH1   | 2.16        | 0.60     |
| 23:DB:670:A:H5''  | 37:DL:42:SER:HB2    | 1.83        | 0.60     |
| 35:DV:80:HIS:CG   | 35:DV:83:LYS:HB2    | 2.36        | 0.60     |
| 1:CA:1414:U:H2'   | 1:CA:1415:G:H8      | 1.67        | 0.60     |
| 23:DB:1199:U:C5'  | 44:DQ:4:LYS:HD3     | 2.32        | 0.60     |
| 23:DB:2103:C:H3'  | 23:DB:2104:C:C2     | 2.37        | 0.60     |
| 41:DJ:112:GLY:H   | 41:DJ:113:PRO:HD2   | 1.66        | 0.60     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 49:BR:66:HIS:ND1  | 49:BR:94:THR:HG22 | 2.17        | 0.60     |
| 23:BB:1794:A:H2'  | 23:BB:1795:C:H6   | 1.67        | 0.60     |
| 4:CE:12:GLU:HG2   | 4:CE:38:VAL:HG22  | 1.84        | 0.60     |
| 12:CM:87:GLY:HA2  | 12:CM:90:HIS:HD2  | 1.65        | 0.60     |
| 3:AD:201:GLU:OE1  | 4:AE:104:ILE:HG22 | 2.02        | 0.60     |
| 40:BH:44:ILE:HG22 | 40:BH:51:ARG:HH12 | 1.66        | 0.60     |
| 23:DB:1236:G:H1'  | 23:DB:1237:A:H8   | 1.66        | 0.60     |
| 23:DB:96:C:H4'    | 39:DX:41:HIS:CE1  | 2.37        | 0.60     |
| 2:AC:129:PHE:CD2  | 2:AC:156:LEU:HD22 | 2.37        | 0.60     |
| 1:CA:1029:U:H2'   | 1:CA:1031:C:N3    | 2.17        | 0.60     |
| 23:DB:1571:A:H2'  | 23:DB:1572:A:H8   | 1.67        | 0.60     |
| 23:DB:1042:G:H2'  | 23:DB:1043:C:H6   | 1.67        | 0.60     |
| 1:CA:1469:C:H2'   | 1:CA:1470:U:O4'   | 2.02        | 0.60     |
| 23:BB:3:U:O2'     | 23:BB:4:U:H6      | 1.85        | 0.60     |
| 23:DB:1937:A:N7   | 23:DB:1939:U:H2'  | 2.16        | 0.60     |
| 3:CD:115:GLN:HG3  | 3:CD:119:HIS:CE1  | 2.37        | 0.60     |
| 23:DB:1306:C:H2'  | 23:DB:1307:A:H8   | 1.67        | 0.60     |
| 23:BB:2286:G:H4'  | 23:BB:2287:A:O4'  | 2.02        | 0.60     |
| 45:DS:90:LYS:HD2  | 45:DS:92:ARG:NH1  | 2.16        | 0.60     |
| 42:DN:58:ASP:O    | 42:DN:59:SER:HB3  | 2.01        | 0.60     |
| 9:AJ:66:GLU:HB3   | 13:AN:98:ALA:HB2  | 1.84        | 0.60     |
| 43:DO:79:ALA:O    | 43:DO:83:LEU:HB2  | 2.01        | 0.60     |
| 1:CA:1280:A:O4'   | 9:CJ:43:PRO:HG3   | 2.02        | 0.60     |
| 37:BL:23:ILE:HD12 | 37:BL:23:ILE:H    | 1.66        | 0.60     |
| 51:DZ:66:THR:O    | 51:DZ:69:ALA:HB3  | 2.02        | 0.60     |
| 33:D1:18:HIS:NE2  | 33:D1:40:PRO:HD2  | 2.17        | 0.60     |
| 23:DB:5:A:H2'     | 23:DB:6:A:C8      | 2.37        | 0.60     |
| 37:DL:23:ILE:HD12 | 37:DL:23:ILE:H    | 1.67        | 0.60     |
| 23:BB:1236:G:H1'  | 23:BB:1237:A:H8   | 1.66        | 0.60     |
| 21:AU:42:THR:HB   | 21:AU:46:ARG:HE   | 1.67        | 0.60     |
| 8:CI:62:LEU:HD22  | 8:CI:62:LEU:H     | 1.66        | 0.60     |
| 30:DY:43:ILE:O    | 30:DY:47:ILE:HG12 | 2.01        | 0.60     |
| 23:DB:2547:A:H2'  | 23:DB:2548:U:C6   | 2.37        | 0.60     |
| 50:BT:57:VAL:HG12 | 50:BT:86:THR:OG1  | 2.01        | 0.60     |
| 12:CM:52:ILE:HD12 | 12:CM:55:LEU:HD12 | 1.84        | 0.60     |
| 47:DF:7:TYR:O     | 47:DF:11:VAL:HB   | 2.01        | 0.60     |
| 23:DB:140:C:H4'   | 23:DB:141:G:C5    | 2.36        | 0.60     |
| 23:BB:2750:A:H8   | 23:BB:2750:A:OP1  | 1.85        | 0.60     |
| 32:B4:8:LYS:O     | 32:B4:25:VAL:HG21 | 2.02        | 0.60     |
| 13:AN:51:PRO:HB2  | 13:AN:54:SER:CB   | 2.31        | 0.60     |
| 17:CR:34:GLU:HB2  | 21:CU:18:PHE:HZ   | 1.67        | 0.60     |
| 21:CU:24:LYS:CD   | 21:CU:25:ALA:H    | 2.15        | 0.60     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:35:G:H2'      | 1:CA:36:C:C6       | 2.37        | 0.60     |
| 1:AA:1004:A:C8     | 1:AA:1025:U:H1'    | 2.36        | 0.60     |
| 46:BU:10:VAL:O     | 46:BU:21:ARG:HA    | 2.01        | 0.60     |
| 6:CG:62:GLU:O      | 6:CG:66:GLU:HG3    | 2.01        | 0.60     |
| 23:DB:2341:G:H2'   | 23:DB:2342:C:H6    | 1.67        | 0.60     |
| 1:AA:1532:U:H2'    | 1:AA:1533:C:H3'    | 1.83        | 0.60     |
| 23:BB:1001:A:H2'   | 23:BB:1002:G:O4'   | 2.02        | 0.60     |
| 1:AA:1053:G:C3'    | 1:AA:1054:C:H5'    | 2.31        | 0.60     |
| 1:AA:1226:C:H2'    | 12:AM:101:THR:OG1  | 2.01        | 0.60     |
| 23:DB:6:A:H2'      | 23:DB:7:G:H8       | 1.66        | 0.60     |
| 43:BO:108:ASP:HA   | 43:BO:111:ARG:HB3  | 1.83        | 0.60     |
| 23:BB:682:G:O2'    | 23:BB:683:U:H5'    | 2.02        | 0.60     |
| 3:AD:165:GLU:HG3   | 3:AD:166:LYS:H     | 1.67        | 0.60     |
| 22:BA:37:C:H2'     | 22:BA:38:C:O4'     | 2.02        | 0.60     |
| 50:BT:48:GLN:HE21  | 50:BT:48:GLN:HA    | 1.66        | 0.60     |
| 20:AB:112:ARG:HA   | 20:AB:115:ASP:OD2  | 2.01        | 0.60     |
| 23:DB:1291:C:O2'   | 23:DB:1292:G:H5'   | 2.02        | 0.60     |
| 23:BB:222:A:N1     | 23:BB:233:A:H5''   | 2.17        | 0.60     |
| 23:BB:1054:A:H2'   | 23:BB:1055:G:C8    | 2.35        | 0.60     |
| 23:BB:1513:U:O2'   | 23:BB:1514:G:H5'   | 2.02        | 0.60     |
| 25:DC:130:PRO:HG2  | 25:DC:133:ASN:HD22 | 1.65        | 0.60     |
| 10:AK:33:ILE:HG13  | 10:AK:73:VAL:HG21  | 1.82        | 0.60     |
| 48:BG:84:LYS:HG3   | 48:BG:131:VAL:C    | 2.22        | 0.60     |
| 44:DQ:18:LYS:C     | 44:DQ:20:ALA:H     | 2.05        | 0.60     |
| 23:DB:2019:A:H4'   | 44:DQ:33:VAL:HG11  | 1.84        | 0.60     |
| 53:D6:39:LEU:O     | 53:D6:39:LEU:HD12  | 2.01        | 0.60     |
| 53:D6:59:THR:HG22  | 53:D6:67:VAL:CG2   | 2.31        | 0.60     |
| 1:AA:1218:C:H2'    | 1:AA:1219:A:C8     | 2.36        | 0.60     |
| 46:DU:83:GLY:O     | 46:DU:93:ARG:HA    | 2.02        | 0.60     |
| 47:BF:102:LEU:HD13 | 47:BF:103:ILE:HB   | 1.84        | 0.60     |
| 42:DN:77:ALA:O     | 42:DN:81:ASN:HB2   | 2.02        | 0.60     |
| 31:D0:21:LEU:HD13  | 45:DS:23:LEU:HD11  | 1.84        | 0.60     |
| 1:AA:918:A:H2'     | 1:AA:919:A:C8      | 2.37        | 0.60     |
| 1:CA:413:G:H2'     | 1:CA:428:G:N2      | 2.17        | 0.60     |
| 50:DT:38:ALA:O     | 50:DT:39:THR:HB    | 2.01        | 0.60     |
| 23:BB:2267:A:H8    | 23:BB:2267:A:O5'   | 1.84        | 0.60     |
| 23:DB:1278:C:O3'   | 42:DN:34:ILE:HG23  | 2.02        | 0.60     |
| 40:BH:72:ILE:HG23  | 40:BH:140:ALA:CB   | 2.32        | 0.60     |
| 26:BD:8:LYS:HD3    | 26:BD:197:THR:H    | 1.67        | 0.60     |
| 1:CA:272:C:H2'     | 1:CA:273:U:H6      | 1.67        | 0.60     |
| 23:DB:1386:C:H2'   | 23:DB:1387:A:H8    | 1.66        | 0.60     |
| 23:BB:2578:G:C5    | 26:BD:145:SER:HB2  | 2.36        | 0.60     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:501:C:H2'    | 1:AA:502:A:H8      | 1.65        | 0.60     |
| 1:CA:423:G:H2'    | 1:CA:424:G:O4'     | 2.02        | 0.60     |
| 5:AF:81:ASN:OD1   | 5:AF:83:ALA:HB3    | 2.02        | 0.60     |
| 30:DY:29:ARG:H    | 30:DY:33:HIS:CD2   | 2.19        | 0.60     |
| 23:DB:1219:U:H2'  | 23:DB:1220:G:H8    | 1.67        | 0.60     |
| 3:AD:71:PHE:O     | 3:AD:74:TYR:HB2    | 2.02        | 0.60     |
| 1:CA:518:C:H2'    | 1:CA:530:G:C8      | 2.37        | 0.60     |
| 23:DB:1326:U:H2'  | 23:DB:1327:A:H8    | 1.66        | 0.60     |
| 41:BJ:40:HIS:CE1  | 41:BJ:41:LYS:HG3   | 2.36        | 0.60     |
| 40:BH:67:ALA:O    | 40:BH:71:LYS:HB2   | 2.01        | 0.60     |
| 28:DP:97:TYR:O    | 28:DP:100:ARG:HB2  | 2.02        | 0.60     |
| 33:B1:18:HIS:NE2  | 33:B1:40:PRO:HD2   | 2.17        | 0.60     |
| 23:BB:1571:A:H2'  | 23:BB:1572:A:C8    | 2.36        | 0.60     |
| 23:BB:1401:G:H2'  | 23:BB:1402:U:C6    | 2.37        | 0.60     |
| 1:AA:880:C:H2'    | 1:AA:881:G:H8      | 1.65        | 0.60     |
| 23:DB:2:G:O2'     | 23:DB:3:U:H5'      | 2.01        | 0.60     |
| 40:DH:31:VAL:O    | 40:DH:33:GLN:N     | 2.34        | 0.60     |
| 40:BH:89:LYS:HZ1  | 40:BH:123:ARG:HB3  | 1.67        | 0.60     |
| 1:CA:1147:C:O2'   | 8:CI:17:ARG:HD2    | 2.02        | 0.60     |
| 47:DF:78:ILE:N    | 47:DF:78:ILE:HD12  | 2.17        | 0.60     |
| 3:CD:25:ARG:HD3   | 3:CD:25:ARG:C      | 2.22        | 0.60     |
| 47:BF:102:LEU:HA  | 47:BF:106:ALA:HB3  | 1.82        | 0.60     |
| 17:AR:34:GLU:H    | 17:AR:34:GLU:CD    | 2.05        | 0.60     |
| 10:CK:88:PRO:HD3  | 21:CU:28:LEU:HD11  | 1.84        | 0.60     |
| 45:DS:29:VAL:HG23 | 45:DS:70:LYS:HA    | 1.84        | 0.60     |
| 31:B0:41:HIS:HB2  | 42:BN:99:LYS:O     | 2.01        | 0.60     |
| 3:AD:158:LEU:HA   | 3:AD:161:ALA:HB2   | 1.84        | 0.60     |
| 23:BB:1484:U:H2'  | 23:BB:1485:U:C6    | 2.37        | 0.60     |
| 45:DS:83:LYS:HD3  | 45:DS:97:LEU:HD11  | 1.84        | 0.60     |
| 40:BH:47:PHE:HA   | 40:BH:50:ARG:HH21  | 1.65        | 0.60     |
| 1:CA:481:G:HO2'   | 1:CA:482:A:H8      | 1.48        | 0.60     |
| 23:DB:2579:C:O2'  | 26:DD:136:ASN:HA   | 2.01        | 0.60     |
| 53:B6:1:MET:HA    | 53:B6:5:GLU:OE2    | 2.02        | 0.60     |
| 23:BB:2292:U:H2'  | 23:BB:2293:G:C8    | 2.37        | 0.60     |
| 14:CO:55:GLY:O    | 14:CO:59:MET:HG2   | 2.02        | 0.60     |
| 9:AJ:29:ALA:O     | 9:AJ:32:THR:HG22   | 2.01        | 0.60     |
| 3:CD:77:GLU:HA    | 3:CD:80:ARG:HG2    | 1.84        | 0.60     |
| 41:BJ:13:ARG:O    | 41:BJ:52:ASP:HA    | 2.02        | 0.60     |
| 31:D0:9:ARG:O     | 31:D0:12:ARG:HB3   | 2.02        | 0.60     |
| 31:B0:54:ILE:H    | 42:BN:118:ARG:HH12 | 1.48        | 0.60     |
| 3:CD:165:GLU:HG3  | 3:CD:166:LYS:H     | 1.67        | 0.60     |
| 20:AB:94:ARG:N    | 20:AB:94:ARG:HE    | 1.99        | 0.60     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 4:AE:43:GLY:O      | 4:AE:72:ASN:HA    | 2.02        | 0.60     |
| 23:DB:2487:G:H2'   | 23:DB:2488:G:C8   | 2.37        | 0.60     |
| 22:DA:60:C:H2'     | 22:DA:61:G:H8     | 1.66        | 0.60     |
| 23:BB:856:G:H1'    | 52:BW:23:LYS:HB3  | 1.84        | 0.59     |
| 25:BC:170:TYR:HE2  | 25:BC:184:GLU:HG2 | 1.67        | 0.59     |
| 48:DG:8:VAL:HG11   | 48:DG:49:LEU:CB   | 2.31        | 0.59     |
| 37:BL:123:ARG:HH11 | 37:BL:123:ARG:HB3 | 1.65        | 0.59     |
| 23:DB:917:A:H2'    | 23:DB:918:A:O4'   | 2.02        | 0.59     |
| 53:B6:39:LEU:HD12  | 53:B6:40:HIS:N    | 2.17        | 0.59     |
| 47:DF:72:SER:HB2   | 47:DF:80:GLN:HA   | 1.82        | 0.59     |
| 50:BT:38:ALA:O     | 50:BT:39:THR:HB   | 2.02        | 0.59     |
| 38:BM:35:ALA:CB    | 38:BM:100:LYS:H   | 2.15        | 0.59     |
| 23:DB:1789:A:OP2   | 25:DC:220:ARG:HD3 | 2.01        | 0.59     |
| 23:DB:2389:G:C5'   | 23:DB:2390:U:H5'  | 2.32        | 0.59     |
| 48:DG:145:ALA:HA   | 48:DG:148:ARG:HG3 | 1.83        | 0.59     |
| 3:CD:158:LEU:HA    | 3:CD:161:ALA:HB2  | 1.84        | 0.59     |
| 20:AB:102:ASN:OD1  | 20:AB:105:THR:HB  | 2.01        | 0.59     |
| 23:DB:2148:G:H2'   | 23:DB:2148:G:N3   | 2.17        | 0.59     |
| 23:BB:1657:U:O2'   | 23:BB:1658:C:H5'  | 2.02        | 0.59     |
| 4:CE:158:LYS:NZ    | 7:CH:65:PHE:HA    | 2.16        | 0.59     |
| 30:BY:43:ILE:O     | 30:BY:47:ILE:HG12 | 2.02        | 0.59     |
| 23:DB:1354:A:H2'   | 23:DB:1355:G:O4'  | 2.01        | 0.59     |
| 1:AA:215:C:H2'     | 1:AA:216:U:C6     | 2.37        | 0.59     |
| 20:AB:160:LEU:HD23 | 20:AB:181:PRO:O   | 2.02        | 0.59     |
| 23:BB:742:A:H2'    | 23:BB:743:A:H8    | 1.66        | 0.59     |
| 23:DB:863:A:H2'    | 23:DB:864:G:C8    | 2.36        | 0.59     |
| 35:DV:6:ALA:O      | 35:DV:65:VAL:HG12 | 2.02        | 0.59     |
| 1:AA:1463:U:H2'    | 1:AA:1464:U:C6    | 2.37        | 0.59     |
| 1:AA:834:U:H2'     | 1:AA:835:U:C6     | 2.36        | 0.59     |
| 23:DB:1599:U:H2'   | 23:DB:1600:C:C6   | 2.36        | 0.59     |
| 23:BB:1919:A:H2'   | 23:BB:1920:C:H5'  | 1.84        | 0.59     |
| 23:BB:1744:A:H2'   | 23:BB:1745:A:C8   | 2.37        | 0.59     |
| 23:DB:1473:G:O2'   | 23:DB:1474:U:H5'  | 2.02        | 0.59     |
| 23:DB:828:U:H4'    | 23:DB:831:G:N1    | 2.16        | 0.59     |
| 20:CB:128:LEU:HD22 | 20:CB:129:THR:H   | 1.67        | 0.59     |
| 24:DI:1:ALA:C      | 24:DI:2:LYS:HD2   | 2.22        | 0.59     |
| 52:DW:35:ILE:O     | 52:DW:35:ILE:HG12 | 2.00        | 0.59     |
| 47:BF:33:ILE:HD13  | 47:BF:95:MET:HG2  | 1.84        | 0.59     |
| 52:DW:23:LYS:HD2   | 52:DW:24:ARG:N    | 2.17        | 0.59     |
| 40:BH:94:ILE:HB    | 40:BH:121:VAL:HB  | 1.83        | 0.59     |
| 8:CI:83:THR:HA     | 8:CI:86:LEU:HD22  | 1.83        | 0.59     |
| 44:DQ:63:ARG:HH12  | 44:DQ:96:ASP:CB   | 2.09        | 0.59     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 44:DQ:93:ILE:HG23  | 44:DQ:94:LEU:HD22 | 1.84        | 0.59     |
| 23:BB:143:C:H2'    | 23:BB:144:A:C8    | 2.37        | 0.59     |
| 23:DB:634:C:H2'    | 23:DB:635:C:H6    | 1.66        | 0.59     |
| 43:DO:74:VAL:O     | 43:DO:78:VAL:HG23 | 2.02        | 0.59     |
| 24:BI:91:LYS:HB2   | 24:BI:94:LYS:HD2  | 1.83        | 0.59     |
| 1:AA:812:G:H2'     | 1:AA:812:G:N3     | 2.16        | 0.59     |
| 47:DF:102:LEU:HD22 | 47:DF:103:ILE:N   | 2.16        | 0.59     |
| 53:B6:109:GLU:HA   | 53:B6:112:LYS:CE  | 2.32        | 0.59     |
| 26:DD:124:ARG:HA   | 26:DD:165:MET:CE  | 2.32        | 0.59     |
| 42:BN:31:HIS:O     | 42:BN:33:ILE:HG13 | 2.02        | 0.59     |
| 40:BH:73:ASN:HD22  | 40:BH:74:ALA:H    | 1.48        | 0.59     |
| 23:BB:1722:A:H2'   | 23:BB:1723:G:C8   | 2.34        | 0.59     |
| 14:CO:70:LEU:HD11  | 14:CO:77:ARG:HB2  | 1.84        | 0.59     |
| 4:AE:12:GLU:HG2    | 4:AE:38:VAL:HG22  | 1.84        | 0.59     |
| 46:BU:78:LYS:HD3   | 46:BU:79:ALA:H    | 1.66        | 0.59     |
| 23:BB:118:A:N3     | 23:BB:178:G:H1'   | 2.17        | 0.59     |
| 1:CA:860:A:H2'     | 1:CA:861:G:O4'    | 2.01        | 0.59     |
| 1:CA:1356:G:H2'    | 1:CA:1357:A:C8    | 2.37        | 0.59     |
| 1:AA:806:C:H2'     | 1:AA:807:A:H8     | 1.67        | 0.59     |
| 23:BB:1042:G:H2'   | 23:BB:1043:C:C6   | 2.36        | 0.59     |
| 1:AA:482:A:H2'     | 1:AA:483:C:O4'    | 2.02        | 0.59     |
| 23:DB:1316:U:O2'   | 23:DB:1317:G:H5'  | 2.01        | 0.59     |
| 1:AA:390:U:H2'     | 1:AA:391:G:H8     | 1.67        | 0.59     |
| 23:DB:402:A:H2'    | 23:DB:403:U:O4'   | 2.01        | 0.59     |
| 23:DB:2292:U:H2'   | 23:DB:2293:G:C8   | 2.37        | 0.59     |
| 23:BB:402:A:H2'    | 23:BB:403:U:O4'   | 2.02        | 0.59     |
| 1:AA:1062:U:H2'    | 1:AA:1063:C:C6    | 2.37        | 0.59     |
| 3:CD:71:PHE:O      | 3:CD:74:TYR:HB2   | 2.02        | 0.59     |
| 22:BA:94:A:OP1     | 35:BV:19:ARG:HD3  | 2.02        | 0.59     |
| 1:CA:818:G:H3'     | 1:CA:819:A:H5''   | 1.83        | 0.59     |
| 23:DB:1346:G:O2'   | 23:DB:1347:A:H5'  | 2.02        | 0.59     |
| 22:BA:60:C:H2'     | 22:BA:61:G:H8     | 1.67        | 0.59     |
| 23:BB:392:U:O2'    | 23:BB:393:C:H5'   | 2.03        | 0.59     |
| 40:DH:135:HIS:HB3  | 40:DH:138:VAL:HB  | 1.84        | 0.59     |
| 23:DB:753:A:H2'    | 23:DB:754:U:C6    | 2.37        | 0.59     |
| 1:AA:517:G:H22     | 1:AA:533:A:P      | 2.24        | 0.59     |
| 41:DJ:4:PHE:HB3    | 41:DJ:44:TYR:CD1  | 2.37        | 0.59     |
| 41:DJ:6:ALA:HB3    | 41:DJ:45:THR:HG21 | 1.84        | 0.59     |
| 29:DE:58:LYS:C     | 29:DE:60:TRP:N    | 2.56        | 0.59     |
| 23:BB:79:C:HO2'    | 23:BB:346:A:C1'   | 2.12        | 0.59     |
| 47:BF:11:VAL:HG21  | 47:BF:172:PHE:CE1 | 2.37        | 0.59     |
| 23:BB:1440:U:H2'   | 23:BB:1441:G:H8   | 1.67        | 0.59     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:1072:G:N2    | 20:AB:105:THR:HG21 | 2.16        | 0.59     |
| 1:AA:1342:C:H2'   | 1:AA:1343:G:H8     | 1.67        | 0.59     |
| 23:DB:173:A:H2'   | 23:DB:174:U:C6     | 2.37        | 0.59     |
| 23:BB:784:G:C6    | 25:BC:227:VAL:HG11 | 2.37        | 0.59     |
| 1:CA:237:G:H2'    | 1:CA:238:A:H8      | 1.67        | 0.59     |
| 39:DX:17:GLU:HB3  | 39:DX:53:VAL:HG11  | 1.84        | 0.59     |
| 23:BB:1149:G:H2'  | 23:BB:1150:C:H6    | 1.67        | 0.59     |
| 23:BB:71:A:H4'    | 23:BB:72:U:H5'     | 1.84        | 0.59     |
| 1:AA:1521:C:H2'   | 1:AA:1522:U:H6     | 1.66        | 0.59     |
| 1:CA:370:C:O2'    | 1:CA:371:A:H5'     | 2.02        | 0.59     |
| 52:DW:77:LYS:N    | 52:DW:77:LYS:HZ2   | 2.00        | 0.59     |
| 6:AG:24:LYS:HA    | 6:AG:27:ASN:HD22   | 1.67        | 0.59     |
| 22:BA:49:C:H2'    | 22:BA:50:A:H8      | 1.68        | 0.59     |
| 23:DB:826:U:H2'   | 23:DB:828:U:O4'    | 2.02        | 0.59     |
| 48:BG:54:ARG:HB3  | 48:BG:57:TYR:CD1   | 2.37        | 0.59     |
| 23:DB:2704:C:H2'  | 23:DB:2705:A:O4'   | 2.02        | 0.59     |
| 1:CA:1527:U:H2'   | 1:CA:1528:U:C6     | 2.36        | 0.59     |
| 23:DB:315:G:H2'   | 23:DB:316:C:C6     | 2.37        | 0.59     |
| 1:AA:570:G:H2'    | 1:AA:571:U:C6      | 2.37        | 0.59     |
| 26:BD:117:GLY:HA2 | 26:BD:164:GLN:NE2  | 2.17        | 0.59     |
| 22:DA:16:G:O2'    | 22:DA:17:C:H5'     | 2.03        | 0.59     |
| 45:BS:5:ALA:HB3   | 45:BS:54:ALA:HB2   | 1.84        | 0.59     |
| 23:DB:441:U:H2'   | 23:DB:442:G:C8     | 2.37        | 0.59     |
| 42:DN:19:ALA:C    | 42:DN:21:PHE:H     | 2.06        | 0.59     |
| 1:CA:1480:A:H2'   | 1:CA:1481:U:C6     | 2.38        | 0.59     |
| 23:BB:492:A:H2'   | 23:BB:493:G:O4'    | 2.01        | 0.59     |
| 53:B6:178:LYS:O   | 53:B6:181:GLN:HG3  | 2.01        | 0.59     |
| 23:DB:1098:A:P    | 24:DI:3:LYS:HG2    | 2.43        | 0.59     |
| 52:BW:23:LYS:HD2  | 52:BW:24:ARG:N     | 2.17        | 0.59     |
| 44:BQ:30:VAL:HG11 | 44:BQ:33:VAL:HG22  | 1.84        | 0.59     |
| 26:BD:204:LYS:HB2 | 26:BD:205:PRO:HD2  | 1.84        | 0.59     |
| 53:D6:67:VAL:HA   | 53:D6:99:LEU:O     | 2.01        | 0.59     |
| 47:DF:32:LYS:HB2  | 47:DF:90:LEU:O     | 2.03        | 0.59     |
| 8:CI:29:ILE:HA    | 8:CI:64:ILE:HB     | 1.83        | 0.59     |
| 13:CN:63:CYS:HB2  | 13:CN:79:SER:HB3   | 1.85        | 0.59     |
| 34:D3:39:ARG:O    | 34:D3:43:LEU:HG    | 2.03        | 0.59     |
| 51:BZ:40:VAL:CG2  | 51:BZ:43:GLU:HB3   | 2.30        | 0.59     |
| 42:BN:77:ALA:O    | 42:BN:81:ASN:HB2   | 2.02        | 0.59     |
| 13:CN:51:PRO:HB2  | 13:CN:54:SER:CB    | 2.31        | 0.59     |
| 23:DB:1655:A:H5'  | 26:DD:118:PHE:HB2  | 1.83        | 0.59     |
| 46:DU:10:VAL:O    | 46:DU:21:ARG:HA    | 2.02        | 0.59     |
| 29:DE:148:ILE:HA  | 29:DE:187:VAL:HB   | 1.82        | 0.59     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:300:A:H2'     | 1:AA:301:G:O4'     | 2.03        | 0.59     |
| 39:DX:20:ASN:O     | 39:DX:24:GLU:HB3   | 2.02        | 0.59     |
| 12:CM:1:ALA:C      | 12:CM:8:ILE:HG22   | 2.23        | 0.59     |
| 1:CA:1524:C:H2'    | 1:CA:1525:G:H8     | 1.67        | 0.59     |
| 1:CA:1271:A:H5'    | 1:CA:1314:C:H5''   | 1.83        | 0.59     |
| 7:CH:100:ILE:HG13  | 7:CH:128:VAL:O     | 2.02        | 0.59     |
| 1:CA:1008:U:H5''   | 13:CN:23:ARG:HH22  | 1.67        | 0.59     |
| 52:BW:77:LYS:H     | 52:BW:77:LYS:NZ    | 2.01        | 0.59     |
| 1:AA:398:U:H2'     | 1:AA:399:G:C8      | 2.37        | 0.59     |
| 23:DB:2229:U:H2'   | 23:DB:2230:G:C8    | 2.38        | 0.59     |
| 23:DB:794:A:H2'    | 23:DB:795:C:H6     | 1.66        | 0.59     |
| 4:CE:55:VAL:N      | 4:CE:56:PRO:HD2    | 2.18        | 0.59     |
| 1:AA:182:A:O2'     | 1:AA:183:C:H5''    | 2.02        | 0.59     |
| 27:DK:76:VAL:H     | 28:DP:72:VAL:HG23  | 1.68        | 0.59     |
| 3:AD:16:THR:HG22   | 3:AD:17:ASP:N      | 2.17        | 0.59     |
| 1:CA:539:A:H2'     | 1:CA:540:G:C8      | 2.38        | 0.59     |
| 21:CU:11:PHE:O     | 21:CU:13:VAL:N     | 2.34        | 0.59     |
| 41:BJ:64:VAL:O     | 41:BJ:68:LYS:HD2   | 2.01        | 0.59     |
| 26:DD:117:GLY:HA2  | 26:DD:164:GLN:CD   | 2.23        | 0.59     |
| 23:DB:2860:A:H8    | 23:DB:2860:A:O5'   | 1.85        | 0.59     |
| 35:DV:70:ILE:HD13  | 35:DV:70:ILE:N     | 2.16        | 0.59     |
| 23:BB:1505:A:H2'   | 23:BB:1506:U:C6    | 2.38        | 0.59     |
| 23:BB:324:A:H2'    | 23:BB:325:G:O4'    | 2.02        | 0.59     |
| 47:BF:32:LYS:H     | 47:BF:95:MET:HE1   | 1.67        | 0.59     |
| 13:AN:60:ARG:O     | 13:AN:62:ARG:N     | 2.35        | 0.59     |
| 41:DJ:127:GLY:O    | 41:DJ:128:ASN:HB2  | 2.02        | 0.59     |
| 29:BE:108:ILE:O    | 29:BE:108:ILE:HD13 | 2.02        | 0.59     |
| 13:AN:79:SER:O     | 13:AN:83:VAL:HG23  | 2.03        | 0.59     |
| 25:BC:103:ILE:HG22 | 25:BC:105:ALA:H    | 1.66        | 0.59     |
| 10:AK:92:ARG:HE    | 21:AU:20:ARG:HH22  | 1.51        | 0.59     |
| 21:AU:3:ILE:HD11   | 21:AU:23:GLU:HB2   | 1.83        | 0.59     |
| 4:CE:131:ASN:O     | 4:CE:135:VAL:HG23  | 2.02        | 0.59     |
| 23:DB:817:C:H2'    | 23:DB:818:G:O4'    | 2.02        | 0.59     |
| 1:CA:1326:U:H2'    | 1:CA:1327:C:C6     | 2.37        | 0.59     |
| 23:DB:2380:C:H5'   | 43:DO:17:LYS:HZ3   | 1.67        | 0.59     |
| 23:BB:2675:A:N1    | 23:BB:2732:G:O6    | 2.36        | 0.59     |
| 48:BG:162:ARG:HG3  | 48:BG:166:GLU:OE2  | 2.03        | 0.59     |
| 1:AA:308:C:H2'     | 1:AA:309:A:H8      | 1.67        | 0.59     |
| 36:B2:30:VAL:HA    | 36:B2:33:ARG:HH22  | 1.67        | 0.59     |
| 1:CA:253:A:H2'     | 1:CA:254:G:H8      | 1.68        | 0.59     |
| 4:CE:154:ALA:HB1   | 7:CH:65:PHE:CZ     | 2.37        | 0.59     |
| 1:AA:620:C:H2'     | 1:AA:621:A:C8      | 2.37        | 0.59     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DC:244:VAL:HB  | 25:DC:249:VAL:N   | 2.17        | 0.59     |
| 23:BB:2097:A:H2'  | 23:BB:2098:U:H6   | 1.67        | 0.59     |
| 6:AG:129:ASN:HA   | 6:AG:134:VAL:HG21 | 1.84        | 0.59     |
| 25:DC:71:ASP:HA   | 25:DC:117:SER:O   | 2.02        | 0.59     |
| 23:DB:682:G:O2'   | 23:DB:683:U:H5'   | 2.03        | 0.59     |
| 22:BA:98:G:H1     | 35:BV:14:LYS:HB2  | 1.66        | 0.59     |
| 23:DB:2286:G:H4'  | 23:DB:2287:A:O4'  | 2.02        | 0.59     |
| 23:BB:2400:G:O2'  | 23:BB:2401:U:H5'  | 2.01        | 0.59     |
| 42:BN:19:ALA:C    | 42:BN:21:PHE:H    | 2.05        | 0.59     |
| 44:DQ:34:ALA:O    | 44:DQ:37:ALA:HB3  | 2.02        | 0.59     |
| 1:CA:430:A:OP1    | 3:CD:8:LEU:HB2    | 2.03        | 0.59     |
| 47:BF:72:SER:HB2  | 47:BF:80:GLN:HA   | 1.83        | 0.59     |
| 1:AA:764:C:H2'    | 1:AA:765:G:H5'    | 1.84        | 0.59     |
| 47:DF:24:VAL:O    | 47:DF:27:VAL:HG22 | 2.03        | 0.59     |
| 24:BI:27:LEU:CD2  | 24:BI:27:LEU:H    | 2.14        | 0.59     |
| 45:BS:18:ARG:HB3  | 45:BS:76:VAL:CG2  | 2.31        | 0.59     |
| 50:DT:28:ASN:HA   | 50:DT:91:GLN:HE22 | 1.66        | 0.59     |
| 23:DB:161:A:C3'   | 23:DB:162:U:H5''  | 2.32        | 0.59     |
| 23:DB:1032:A:H1'  | 32:D4:23:ILE:HD13 | 1.84        | 0.59     |
| 23:DB:1082:U:C2   | 23:DB:1086:A:C6   | 2.91        | 0.59     |
| 1:AA:1326:U:H2'   | 1:AA:1327:C:C6    | 2.37        | 0.59     |
| 23:DB:1548:A:H2'  | 23:DB:1549:A:H8   | 1.62        | 0.59     |
| 23:DB:1439:A:C6   | 23:DB:1552:A:N7   | 2.71        | 0.59     |
| 23:BB:1548:A:H2'  | 23:BB:1549:A:H8   | 1.67        | 0.59     |
| 12:AM:95:PRO:HD3  | 12:AM:108:ARG:HG2 | 1.85        | 0.59     |
| 43:DO:24:THR:OG1  | 43:DO:90:VAL:HG12 | 2.02        | 0.59     |
| 39:DX:13:GLU:HB2  | 39:DX:57:LEU:HD13 | 1.84        | 0.59     |
| 23:DB:1592:C:H2'  | 23:DB:1593:A:H8   | 1.67        | 0.59     |
| 23:DB:1812:U:H2'  | 23:DB:1813:G:C8   | 2.37        | 0.59     |
| 23:DB:2092:U:H4'  | 23:DB:2093:G:O5'  | 2.03        | 0.59     |
| 23:BB:2070:A:H2'  | 23:BB:2071:A:C8   | 2.38        | 0.59     |
| 23:BB:573:U:O2'   | 23:BB:574:A:H3'   | 2.02        | 0.59     |
| 26:DD:117:GLY:HA2 | 26:DD:164:GLN:NE2 | 2.18        | 0.59     |
| 37:BL:132:ARG:O   | 37:BL:136:GLU:HG3 | 2.03        | 0.59     |
| 1:CA:512:U:O2'    | 1:CA:513:C:H5'    | 2.03        | 0.59     |
| 23:BB:709:U:H2'   | 23:BB:710:U:C6    | 2.38        | 0.59     |
| 43:BO:79:ALA:O    | 43:BO:83:LEU:HB2  | 2.01        | 0.59     |
| 23:BB:1535:A:H3'  | 23:BB:1536:C:H6   | 1.66        | 0.59     |
| 23:BB:2662:A:H2'  | 23:BB:2663:G:O4'  | 2.03        | 0.59     |
| 23:BB:2760:C:O2'  | 23:BB:2761:A:H5'  | 2.02        | 0.59     |
| 23:DB:2746:U:H4'  | 48:DG:137:LYS:HG3 | 1.85        | 0.59     |
| 31:B0:9:ARG:O     | 31:B0:12:ARG:HB3  | 2.01        | 0.59     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:CD:16:THR:HG22   | 3:CD:17:ASP:N      | 2.18        | 0.59     |
| 23:BB:936:A:H2'    | 23:BB:937:C:C6     | 2.37        | 0.59     |
| 23:DB:2356:U:H5''  | 52:DW:16:GLU:HG3   | 1.84        | 0.59     |
| 25:DC:123:ILE:HD12 | 25:DC:191:LEU:CD1  | 2.32        | 0.59     |
| 3:AD:77:GLU:HA     | 3:AD:80:ARG:HG2    | 1.83        | 0.59     |
| 23:DB:479:A:N3     | 23:DB:481:G:H5''   | 2.17        | 0.59     |
| 40:BH:31:VAL:O     | 40:BH:33:GLN:N     | 2.35        | 0.59     |
| 52:BW:37:VAL:HG12  | 52:BW:38:ARG:N     | 2.18        | 0.59     |
| 22:BA:42:C:C5      | 47:BF:65:LEU:HD22  | 2.38        | 0.59     |
| 21:AU:39:LYS:N     | 21:AU:40:PRO:HD2   | 2.18        | 0.59     |
| 48:DG:116:LEU:HD23 | 48:DG:121:THR:HA   | 1.84        | 0.59     |
| 47:DF:34:THR:OG1   | 47:DF:154:THR:HB   | 2.03        | 0.59     |
| 53:B6:70:SER:OG    | 53:B6:75:ALA:HB3   | 2.03        | 0.59     |
| 1:CA:1148:U:O4'    | 8:CL:17:ARG:HD3    | 2.03        | 0.59     |
| 44:DQ:91:ARG:HE    | 49:DR:11:GLN:HB2   | 1.68        | 0.59     |
| 27:BK:47:ILE:CG1   | 27:BK:48:PRO:HD2   | 2.27        | 0.59     |
| 23:BB:1203:U:H3'   | 23:BB:1204:A:C5'   | 2.32        | 0.59     |
| 47:BF:134:GLN:H    | 47:BF:150:GLY:H    | 1.50        | 0.59     |
| 47:BF:7:TYR:O      | 47:BF:11:VAL:HB    | 2.02        | 0.59     |
| 29:BE:146:VAL:HA   | 29:BE:185:LYS:O    | 2.02        | 0.59     |
| 47:DF:134:GLN:C    | 47:DF:136:ILE:H    | 2.06        | 0.59     |
| 21:AU:24:LYS:HD2   | 21:AU:25:ALA:N     | 2.17        | 0.59     |
| 1:CA:1080:A:H5''   | 4:CE:20:VAL:HG11   | 1.84        | 0.59     |
| 29:BE:61:ARG:NH1   | 29:BE:64:GLY:HA3   | 2.17        | 0.59     |
| 50:DT:43:ILE:O     | 50:DT:47:VAL:HG23  | 2.02        | 0.59     |
| 23:DB:2788:C:H2'   | 23:DB:2789:C:C6    | 2.37        | 0.59     |
| 2:AC:8:GLY:HA2     | 2:AC:11:LEU:HG     | 1.84        | 0.59     |
| 48:DG:153:PRO:HG3  | 48:DG:162:ARG:HB3  | 1.85        | 0.59     |
| 1:AA:1250:A:H2'    | 1:AA:1251:A:C8     | 2.37        | 0.59     |
| 23:DB:1656:C:H2'   | 23:DB:1657:U:H6    | 1.67        | 0.59     |
| 27:BK:105:ARG:HB3  | 27:BK:122:VAL:HG12 | 1.85        | 0.59     |
| 1:AA:1342:C:H2'    | 1:AA:1343:G:C8     | 2.37        | 0.59     |
| 43:BO:76:LYS:HG3   | 43:BO:113:ALA:HB1  | 1.83        | 0.59     |
| 23:BB:2680:U:OP2   | 26:BD:114:LYS:HB3  | 2.03        | 0.59     |
| 23:BB:1582:C:H2'   | 23:BB:1583:A:O4'   | 2.02        | 0.59     |
| 29:DE:109:LEU:O    | 29:DE:112:LEU:HB2  | 2.03        | 0.59     |
| 1:AA:737:C:H2'     | 1:AA:738:C:H6      | 1.68        | 0.59     |
| 23:BB:1508:A:H2'   | 23:BB:1509:A:C2    | 2.37        | 0.59     |
| 23:BB:129:C:H2'    | 23:BB:130:C:H6     | 1.67        | 0.59     |
| 20:CB:128:LEU:HD13 | 20:CB:129:THR:N    | 2.18        | 0.59     |
| 23:BB:1425:G:H2'   | 23:BB:1426:G:C8    | 2.38        | 0.59     |
| 50:DT:48:GLN:HA    | 50:DT:48:GLN:HE21  | 1.67        | 0.59     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:659:U:O2'    | 1:AA:660:C:H5'     | 2.02        | 0.59     |
| 23:DB:2261:C:O2'  | 23:DB:2262:U:H5'   | 2.02        | 0.59     |
| 53:B6:123:GLU:O   | 53:B6:127:VAL:HG23 | 2.02        | 0.59     |
| 23:BB:2708:G:H2'  | 23:BB:2709:G:H8    | 1.67        | 0.59     |
| 23:DB:1535:A:H3'  | 23:DB:1536:C:H6    | 1.67        | 0.59     |
| 23:BB:2783:U:H2'  | 23:BB:2784:U:C6    | 2.38        | 0.59     |
| 3:CD:48:SER:O     | 3:CD:52:VAL:HG23   | 2.03        | 0.59     |
| 23:BB:942:G:H2'   | 23:BB:943:A:O4'    | 2.02        | 0.59     |
| 53:B6:142:LYS:HE3 | 53:B6:142:LYS:HA   | 1.84        | 0.59     |
| 44:DQ:80:ASN:O    | 44:DQ:83:LYS:HB3   | 2.03        | 0.59     |
| 13:CN:78:LEU:HD23 | 13:CN:82:LYS:HB3   | 1.85        | 0.59     |
| 23:DB:2675:A:N1   | 23:DB:2732:G:O6    | 2.36        | 0.59     |
| 41:BJ:4:PHE:HB3   | 41:BJ:44:TYR:CD1   | 2.38        | 0.59     |
| 53:D6:45:TYR:OH   | 53:D6:74:ASN:HB2   | 2.02        | 0.59     |
| 23:BB:675:A:H4'   | 29:BE:60:TRP:CZ2   | 2.37        | 0.59     |
| 26:BD:62:LYS:HB2  | 26:BD:63:PRO:HD3   | 1.84        | 0.59     |
| 17:CR:55:ALA:HA   | 17:CR:58:ILE:HD12  | 1.83        | 0.59     |
| 5:CF:68:GLN:O     | 5:CF:71:ILE:HG23   | 2.03        | 0.59     |
| 1:CA:1332:A:H2'   | 1:CA:1333:A:C8     | 2.38        | 0.59     |
| 3:AD:154:VAL:HG23 | 3:AD:155:LYS:H     | 1.66        | 0.59     |
| 23:BB:173:A:H2'   | 23:BB:174:U:C6     | 2.38        | 0.59     |
| 23:DB:2243:U:O2'  | 23:DB:2244:U:H5'   | 2.03        | 0.59     |
| 46:DU:39:ASN:HB3  | 46:DU:62:ALA:HB3   | 1.84        | 0.59     |
| 14:AO:26:GLU:HG3  | 14:AO:77:ARG:NH1   | 2.17        | 0.59     |
| 12:AM:95:PRO:HB2  | 12:AM:99:GLN:OE1   | 2.03        | 0.59     |
| 23:BB:2841:C:H2'  | 23:BB:2842:G:H8    | 1.68        | 0.59     |
| 23:BB:1813:G:N3   | 25:BC:49:THR:HG21  | 2.18        | 0.59     |
| 23:BB:2379:G:H5'  | 43:BO:21:LEU:HD11  | 1.84        | 0.59     |
| 23:BB:1684:G:H2'  | 23:BB:1685:C:C6    | 2.37        | 0.59     |
| 23:DB:2804:U:H2'  | 23:DB:2805:C:C6    | 2.38        | 0.59     |
| 1:AA:586:C:H5''   | 7:AH:81:GLY:HA2    | 1.84        | 0.59     |
| 23:DB:2369:A:O2'  | 23:DB:2370:G:H5'   | 2.03        | 0.59     |
| 23:DB:2041:U:H2'  | 23:DB:2042:A:C8    | 2.38        | 0.59     |
| 1:AA:950:U:H2'    | 1:AA:951:G:C8      | 2.37        | 0.59     |
| 1:CA:476:U:O2'    | 1:CA:477:C:H5'     | 2.03        | 0.59     |
| 1:AA:783:C:O2'    | 1:AA:784:A:H5'     | 2.02        | 0.59     |
| 23:BB:315:G:H2'   | 23:BB:316:C:C6     | 2.38        | 0.59     |
| 23:DB:286:U:H2'   | 23:DB:287:G:H8     | 1.67        | 0.59     |
| 23:DB:2783:U:H2'  | 23:DB:2784:U:C6    | 2.38        | 0.59     |
| 23:BB:2815:C:H2'  | 23:BB:2816:G:H8    | 1.68        | 0.59     |
| 23:DB:492:A:H2'   | 23:DB:493:G:O4'    | 2.03        | 0.59     |
| 26:DD:204:LYS:HB2 | 26:DD:205:PRO:HD2  | 1.84        | 0.59     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 51:BZ:77:LYS:HD2   | 51:BZ:78:TYR:H     | 1.67        | 0.59     |
| 3:AD:25:ARG:C      | 3:AD:25:ARG:HD3    | 2.23        | 0.59     |
| 12:CM:82:LEU:HD22  | 18:CS:73:PHE:HE2   | 1.67        | 0.59     |
| 18:AS:28:LYS:HD2   | 18:AS:28:LYS:H     | 1.68        | 0.59     |
| 23:DB:2472:G:C2'   | 23:DB:2475:C:H42   | 2.14        | 0.59     |
| 23:DB:28:A:N6      | 23:DB:512:G:H1'    | 2.18        | 0.59     |
| 48:BG:152:ARG:HH22 | 48:BG:162:ARG:HA   | 1.66        | 0.59     |
| 40:BH:73:ASN:HB3   | 40:BH:141:LYS:NZ   | 2.17        | 0.59     |
| 35:BV:30:ILE:HG12  | 35:BV:91:PHE:HB2   | 1.85        | 0.59     |
| 23:DB:1080:A:H4'   | 24:DI:126:ARG:HD2  | 1.84        | 0.59     |
| 23:BB:1657:U:O2'   | 26:BD:138:LEU:HD12 | 2.03        | 0.59     |
| 11:AL:79:ILE:HG22  | 11:AL:103:CYS:HB2  | 1.84        | 0.59     |
| 29:BE:148:ILE:HA   | 29:BE:187:VAL:HB   | 1.84        | 0.59     |
| 23:BB:2243:U:O2'   | 23:BB:2244:U:H5'   | 2.03        | 0.59     |
| 2:CC:78:LYS:HG3    | 2:CC:81:GLU:CB     | 2.33        | 0.59     |
| 1:CA:1432:G:H1'    | 1:CA:1468:A:H61    | 1.68        | 0.59     |
| 23:BB:934:U:H2'    | 23:BB:935:C:C6     | 2.38        | 0.59     |
| 18:AS:32:THR:HG22  | 18:AS:34:SER:H     | 1.66        | 0.59     |
| 34:D3:44:ARG:N     | 34:D3:45:PRO:HD2   | 2.17        | 0.59     |
| 23:BB:176:A:O2'    | 23:BB:177:G:H5'    | 2.03        | 0.59     |
| 1:CA:562:U:H1'     | 11:CL:11:ARG:HB3   | 1.84        | 0.59     |
| 23:DB:709:U:H2'    | 23:DB:710:U:C6     | 2.38        | 0.59     |
| 23:BB:2412:A:H2'   | 23:BB:2413:G:O4'   | 2.03        | 0.59     |
| 1:CA:692:U:H2'     | 1:CA:693:G:H3'     | 1.83        | 0.59     |
| 14:AO:55:GLY:O     | 14:AO:59:MET:HG2   | 2.02        | 0.59     |
| 27:BK:76:VAL:H     | 28:BP:72:VAL:HG23  | 1.67        | 0.59     |
| 20:AB:62:ARG:H     | 20:AB:62:ARG:HD2   | 1.67        | 0.59     |
| 1:AA:1332:A:H2'    | 1:AA:1333:A:C8     | 2.38        | 0.59     |
| 52:BW:37:VAL:HG13  | 52:BW:55:ASP:O     | 2.03        | 0.59     |
| 25:BC:146:LYS:HB3  | 25:BC:147:PRO:HD2  | 1.83        | 0.59     |
| 23:DB:1824:G:OP1   | 25:DC:51:ARG:HD3   | 2.03        | 0.59     |
| 23:DB:532:A:N3     | 23:DB:532:A:H2'    | 2.17        | 0.59     |
| 47:BF:32:LYS:HB2   | 47:BF:90:LEU:O     | 2.03        | 0.59     |
| 41:DJ:55:ILE:HG13  | 41:DJ:55:ILE:O     | 2.03        | 0.59     |
| 30:DY:50:VAL:O     | 30:DY:54:VAL:HG22  | 2.02        | 0.59     |
| 42:DN:37:THR:OG1   | 42:DN:40:LYS:HE2   | 2.03        | 0.59     |
| 13:CN:60:ARG:O     | 13:CN:62:ARG:N     | 2.36        | 0.59     |
| 50:BT:28:ASN:HA    | 50:BT:91:GLN:HE22  | 1.68        | 0.59     |
| 23:BB:1242:U:H2'   | 23:BB:1243:C:C6    | 2.38        | 0.59     |
| 42:DN:55:ALA:HA    | 42:DN:80:PHE:CE1   | 2.38        | 0.59     |
| 29:DE:108:ILE:HD13 | 29:DE:108:ILE:O    | 2.02        | 0.59     |
| 18:CS:10:ILE:HG22  | 18:CS:37:SER:HB3   | 1.84        | 0.59     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:2749:A:C3'  | 23:BB:2750:A:H5'' | 2.33        | 0.59     |
| 23:BB:1028:A:H2'  | 23:BB:1029:A:C8   | 2.37        | 0.59     |
| 13:AN:12:ARG:HA   | 13:AN:15:LEU:HD12 | 1.85        | 0.59     |
| 23:DB:2264:C:H41  | 52:DW:11:ASN:HD21 | 1.49        | 0.59     |
| 44:BQ:9:ALA:C     | 44:BQ:11:ALA:H    | 2.05        | 0.59     |
| 20:CB:112:ARG:HA  | 20:CB:115:ASP:OD2 | 2.03        | 0.59     |
| 23:DB:277:G:H4'   | 23:DB:278:A:C5    | 2.38        | 0.59     |
| 14:AO:70:LEU:HD11 | 14:AO:77:ARG:HB2  | 1.85        | 0.59     |
| 12:CM:95:PRO:HB2  | 12:CM:99:GLN:OE1  | 2.03        | 0.59     |
| 28:BP:88:ARG:HG3  | 28:BP:112:ARG:HB3 | 1.85        | 0.59     |
| 23:BB:644:A:O2'   | 23:BB:645:C:H5'   | 2.03        | 0.59     |
| 23:DB:1729:U:H3'  | 23:DB:1730:C:O4'  | 2.03        | 0.59     |
| 33:B1:20:TYR:CD2  | 33:B1:37:LYS:HD3  | 2.37        | 0.59     |
| 23:BB:151:C:H2'   | 23:BB:152:A:H8    | 1.68        | 0.59     |
| 23:DB:644:A:O2'   | 23:DB:645:C:H5'   | 2.03        | 0.59     |
| 39:DX:9:LYS:O     | 39:DX:13:GLU:HG2  | 2.03        | 0.59     |
| 23:DB:1432:G:H2'  | 23:DB:1433:A:C8   | 2.38        | 0.59     |
| 23:DB:2840:C:OP1  | 42:DN:50:PRO:HA   | 2.03        | 0.59     |
| 1:CA:285:C:H2'    | 1:CA:286:C:C6     | 2.38        | 0.59     |
| 1:AA:499:A:H4'    | 1:AA:500:G:H5'    | 1.85        | 0.59     |
| 11:AL:3:VAL:O     | 11:AL:7:VAL:HG23  | 2.03        | 0.59     |
| 15:AP:20:VAL:HG23 | 15:AP:34:GLU:O    | 2.02        | 0.59     |
| 1:AA:451:A:N6     | 1:AA:480:U:H2'    | 2.18        | 0.59     |
| 2:AC:21:TRP:CH2   | 2:AC:31:ASN:HB3   | 2.37        | 0.59     |
| 23:BB:1346:G:O2'  | 23:BB:1347:A:H5'  | 2.03        | 0.59     |
| 1:AA:285:C:H2'    | 1:AA:286:C:H6     | 1.68        | 0.59     |
| 45:BS:40:ASN:O    | 45:BS:41:LYS:HG3  | 2.02        | 0.59     |
| 23:DB:1897:G:O2'  | 23:DB:1898:U:H5'  | 2.03        | 0.59     |
| 23:DB:2825:G:H2'  | 23:DB:2826:A:H5'  | 1.85        | 0.59     |
| 1:AA:1035:A:H2'   | 1:AA:1036:A:H8    | 1.67        | 0.59     |
| 9:AJ:85:ASP:HA    | 9:AJ:88:MET:SD    | 2.42        | 0.59     |
| 1:AA:1039:G:H2'   | 1:AA:1040:U:C6    | 2.38        | 0.59     |
| 22:BA:86:G:H2'    | 22:BA:87:U:O4'    | 2.03        | 0.59     |
| 34:B3:44:ARG:N    | 34:B3:45:PRO:HD2  | 2.17        | 0.59     |
| 23:DB:1113:U:O2'  | 23:DB:1114:C:H5'  | 2.03        | 0.59     |
| 23:BB:2363:G:O2'  | 23:BB:2364:C:H5'  | 2.03        | 0.59     |
| 25:DC:170:TYR:HE2 | 25:DC:184:GLU:HG2 | 1.67        | 0.58     |
| 26:BD:101:PHE:HE2 | 26:BD:205:PRO:HD3 | 1.67        | 0.58     |
| 41:BJ:18:VAL:HG12 | 41:BJ:54:ILE:HD11 | 1.83        | 0.58     |
| 7:AH:94:VAL:HG21  | 7:AH:100:ILE:O    | 2.03        | 0.58     |
| 1:AA:430:A:OP1    | 3:AD:8:LEU:HB2    | 2.02        | 0.58     |
| 6:AG:107:ALA:O    | 6:AG:110:ARG:HB2  | 2.03        | 0.58     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 15:AP:4:ILE:HG12  | 15:AP:21:VAL:HG22 | 1.85        | 0.58     |
| 23:BB:1082:U:C2   | 23:BB:1086:A:C6   | 2.91        | 0.58     |
| 23:BB:2548:U:H1'  | 27:BK:23:LYS:HZ1  | 1.66        | 0.58     |
| 15:CP:4:ILE:HB    | 15:CP:67:ILE:HD12 | 1.84        | 0.58     |
| 38:BM:50:ARG:HA   | 38:BM:53:MET:CE   | 2.32        | 0.58     |
| 23:DB:1722:A:H2'  | 23:DB:1723:G:C8   | 2.33        | 0.58     |
| 23:DB:2899:A:H2'  | 23:DB:2900:A:C8   | 2.38        | 0.58     |
| 23:DB:1794:A:H2'  | 23:DB:1795:C:H6   | 1.67        | 0.58     |
| 43:DO:11:ALA:HB2  | 43:DO:96:GLY:H    | 1.67        | 0.58     |
| 26:DD:148:GLN:CG  | 26:DD:152:PRO:HG2 | 2.31        | 0.58     |
| 23:BB:1442:U:H2'  | 23:BB:1443:U:H6   | 1.68        | 0.58     |
| 1:AA:93:U:O5'     | 1:AA:93:U:H6      | 1.85        | 0.58     |
| 26:BD:124:ARG:HA  | 26:BD:165:MET:CE  | 2.33        | 0.58     |
| 43:DO:76:LYS:HG3  | 43:DO:113:ALA:HB1 | 1.83        | 0.58     |
| 1:AA:1356:G:H2'   | 1:AA:1357:A:C8    | 2.38        | 0.58     |
| 1:CA:264:C:O2'    | 16:CQ:65:PRO:HG2  | 2.02        | 0.58     |
| 23:BB:278:A:H2'   | 23:BB:278:A:N3    | 2.16        | 0.58     |
| 1:AA:441:A:H61    | 1:AA:493:A:N6     | 2.01        | 0.58     |
| 6:CG:104:VAL:O    | 6:CG:108:ARG:HG3  | 2.03        | 0.58     |
| 22:DA:13:G:C2'    | 22:DA:14:U:H5''   | 2.33        | 0.58     |
| 1:CA:735:C:O2'    | 1:CA:736:C:H5'    | 2.02        | 0.58     |
| 23:DB:608:A:H2'   | 23:DB:609:A:C8    | 2.38        | 0.58     |
| 19:AT:38:ILE:HG12 | 19:AT:85:LEU:HD13 | 1.84        | 0.58     |
| 1:AA:501:C:H2'    | 1:AA:502:A:C8     | 2.36        | 0.58     |
| 23:BB:2031:A:C6   | 23:BB:2498:C:H1'  | 2.38        | 0.58     |
| 26:DD:121:THR:HB  | 26:DD:127:PHE:CD1 | 2.37        | 0.58     |
| 23:BB:1709:U:H2'  | 23:BB:1710:G:H8   | 1.68        | 0.58     |
| 23:DB:222:A:N1    | 23:DB:233:A:H5''  | 2.18        | 0.58     |
| 26:DD:67:HIS:O    | 26:DD:70:LYS:HB3  | 2.03        | 0.58     |
| 22:BA:39:A:H2     | 22:BA:46:A:H61    | 1.48        | 0.58     |
| 23:BB:1097:U:H2'  | 23:BB:1098:A:H5'  | 1.85        | 0.58     |
| 49:DR:43:ASN:ND2  | 49:DR:45:GLU:H    | 2.01        | 0.58     |
| 25:BC:2:VAL:HG23  | 25:BC:3:VAL:H     | 1.67        | 0.58     |
| 1:CA:1030:U:O2    | 1:CA:1030:U:H2'   | 2.02        | 0.58     |
| 35:BV:70:ILE:N    | 35:BV:70:ILE:HD13 | 2.17        | 0.58     |
| 7:AH:107:LYS:HE3  | 7:AH:107:LYS:HA   | 1.84        | 0.58     |
| 16:AQ:80:LYS:HD2  | 16:AQ:80:LYS:H    | 1.68        | 0.58     |
| 1:CA:398:U:H2'    | 1:CA:399:G:H8     | 1.66        | 0.58     |
| 23:DB:1098:A:C2'  | 24:DI:4:VAL:N     | 2.65        | 0.58     |
| 48:BG:84:LYS:CG   | 48:BG:85:LYS:H    | 2.16        | 0.58     |
| 22:DA:42:C:C5     | 47:DF:65:LEU:HD22 | 2.38        | 0.58     |
| 41:BJ:26:GLY:O    | 41:BJ:30:THR:HG22 | 2.02        | 0.58     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 44:DQ:90:ASP:O    | 44:DQ:94:LEU:HB2   | 2.02        | 0.58     |
| 9:AJ:9:ARG:CB     | 9:AJ:99:GLN:HB3    | 2.27        | 0.58     |
| 48:DG:17:LYS:NZ   | 48:DG:18:ILE:H     | 2.01        | 0.58     |
| 24:DI:78:LEU:HA   | 24:DI:81:LYS:HE2   | 1.85        | 0.58     |
| 18:AS:30:LEU:HD12 | 18:AS:48:ILE:HG12  | 1.83        | 0.58     |
| 46:DU:46:LYS:HZ1  | 46:DU:47:PRO:HG2   | 1.68        | 0.58     |
| 26:BD:149:ASN:O   | 26:BD:152:PRO:HD2  | 2.03        | 0.58     |
| 23:DB:192:C:H2'   | 23:DB:193:U:H5'    | 1.84        | 0.58     |
| 10:AK:17:ASP:HB3  | 10:AK:80:ASN:ND2   | 2.17        | 0.58     |
| 23:BB:1655:A:H5'  | 26:BD:118:PHE:HB2  | 1.85        | 0.58     |
| 3:AD:90:LEU:HD21  | 3:AD:196:GLU:HB3   | 1.85        | 0.58     |
| 7:CH:51:GLU:HG2   | 7:CH:52:GLY:N      | 2.19        | 0.58     |
| 23:BB:836:G:H2'   | 23:BB:837:C:H6     | 1.67        | 0.58     |
| 23:DB:1667:G:OP1  | 27:DK:6:THR:HA     | 2.02        | 0.58     |
| 1:AA:492:C:H2'    | 1:AA:493:A:N3      | 2.19        | 0.58     |
| 20:CB:63:LYS:HG2  | 20:CB:224:ARG:NH1  | 2.17        | 0.58     |
| 1:CA:636:U:H2'    | 1:CA:637:C:H6      | 1.67        | 0.58     |
| 23:BB:96:C:O2'    | 23:BB:97:C:H5'     | 2.02        | 0.58     |
| 1:AA:1524:C:H2'   | 1:AA:1525:G:H8     | 1.68        | 0.58     |
| 1:AA:1008:U:H5''  | 13:AN:23:ARG:HH22  | 1.67        | 0.58     |
| 19:AT:82:ILE:HA   | 19:AT:85:LEU:HD22  | 1.84        | 0.58     |
| 37:BL:110:VAL:HB  | 37:BL:127:VAL:HG23 | 1.84        | 0.58     |
| 1:CA:1387:G:H2'   | 1:CA:1388:C:C6     | 2.37        | 0.58     |
| 23:BB:6:A:H2'     | 23:BB:7:G:H8       | 1.68        | 0.58     |
| 23:DB:2800:A:H2'  | 23:DB:2801:G:O4'   | 2.03        | 0.58     |
| 23:BB:222:A:N6    | 23:BB:232:G:H1'    | 2.18        | 0.58     |
| 48:BG:54:ARG:HB3  | 48:BG:57:TYR:HD1   | 1.68        | 0.58     |
| 27:DK:70:ARG:HB3  | 27:DK:76:VAL:HG22  | 1.86        | 0.58     |
| 1:AA:451:A:H4'    | 1:AA:452:A:O4'     | 2.02        | 0.58     |
| 1:AA:45:G:H2'     | 1:AA:46:G:H8       | 1.67        | 0.58     |
| 46:BU:25:LYS:HE3  | 46:BU:36:GLU:HG3   | 1.85        | 0.58     |
| 1:CA:659:U:O2'    | 1:CA:660:C:H5'     | 2.03        | 0.58     |
| 50:BT:32:LEU:H    | 50:BT:83:ALA:HB3   | 1.68        | 0.58     |
| 23:BB:2053:G:O2'  | 23:BB:2054:A:H5'   | 2.03        | 0.58     |
| 1:CA:1517:G:H1'   | 23:DB:1919:A:O3'   | 2.03        | 0.58     |
| 20:CB:156:LEU:H   | 20:CB:156:LEU:HD12 | 1.69        | 0.58     |
| 1:AA:1030:U:H2'   | 1:AA:1030:U:O2     | 2.03        | 0.58     |
| 9:CJ:85:ASP:HA    | 9:CJ:88:MET:SD     | 2.43        | 0.58     |
| 23:BB:1798:U:OP1  | 25:BC:257:ARG:HB2  | 2.03        | 0.58     |
| 50:DT:5:GLU:HA    | 50:DT:8:LEU:CB     | 2.20        | 0.58     |
| 23:BB:2385:C:H2'  | 23:BB:2386:A:C8    | 2.38        | 0.58     |
| 23:BB:2313:C:H4'  | 47:BF:87:LYS:HB3   | 1.85        | 0.58     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 41:BJ:29:ALA:HA    | 41:BJ:32:LEU:HD12  | 1.84        | 0.58     |
| 46:DU:3:LYS:HD3    | 46:DU:82:VAL:CG2   | 2.32        | 0.58     |
| 37:BL:3:LEU:O      | 37:BL:5:THR:HG23   | 2.02        | 0.58     |
| 24:DI:108:ILE:HG22 | 24:DI:128:ILE:HD13 | 1.85        | 0.58     |
| 1:CA:1060:U:C4'    | 9:CJ:54:SER:HB2    | 2.30        | 0.58     |
| 47:BF:78:ILE:N     | 47:BF:79:ARG:HH11  | 2.01        | 0.58     |
| 23:BB:322:A:P      | 29:BE:163:ASN:HD22 | 2.27        | 0.58     |
| 40:DH:93:SER:O     | 40:DH:94:ILE:HD12  | 2.03        | 0.58     |
| 47:DF:134:GLN:O    | 47:DF:136:ILE:N    | 2.37        | 0.58     |
| 45:BS:16:LYS:O     | 45:BS:19:LEU:HB3   | 2.02        | 0.58     |
| 1:AA:1316:G:H22    | 1:AA:1318:A:H3'    | 1.68        | 0.58     |
| 27:DK:105:ARG:HB3  | 27:DK:122:VAL:HG12 | 1.85        | 0.58     |
| 23:DB:590:A:H2'    | 23:DB:591:U:H6     | 1.68        | 0.58     |
| 23:DB:2899:A:H2'   | 23:DB:2900:A:H8    | 1.68        | 0.58     |
| 26:DD:8:LYS:HD3    | 26:DD:197:THR:H    | 1.69        | 0.58     |
| 23:BB:62:U:O2'     | 23:BB:63:A:H5'     | 2.03        | 0.58     |
| 23:BB:1485:U:H2'   | 23:BB:1486:U:H6    | 1.69        | 0.58     |
| 23:DB:125:A:C6     | 36:D2:10:LEU:HD23  | 2.38        | 0.58     |
| 23:DB:414:C:H2'    | 23:DB:415:A:H8     | 1.68        | 0.58     |
| 23:BB:296:U:H2'    | 23:BB:297:G:C8     | 2.37        | 0.58     |
| 23:BB:419:U:H2'    | 23:BB:420:C:C6     | 2.37        | 0.58     |
| 1:AA:736:C:H2'     | 1:AA:737:C:H6      | 1.68        | 0.58     |
| 23:BB:328:U:H4'    | 46:BU:65:GLN:HE22  | 1.68        | 0.58     |
| 23:BB:1219:U:H2'   | 23:BB:1220:G:C8    | 2.37        | 0.58     |
| 5:CF:47:LEU:HD21   | 5:CF:57:ALA:HB3    | 1.86        | 0.58     |
| 49:BR:43:ASN:ND2   | 49:BR:45:GLU:H     | 2.01        | 0.58     |
| 29:DE:98:LYS:O     | 29:DE:102:ARG:HG2  | 2.04        | 0.58     |
| 1:AA:1280:A:O4'    | 9:AJ:43:PRO:HG3    | 2.03        | 0.58     |
| 23:BB:2438:U:O2'   | 23:BB:2439:A:H5''  | 2.03        | 0.58     |
| 1:CA:1039:G:H2'    | 1:CA:1040:U:C6     | 2.38        | 0.58     |
| 23:BB:1599:U:H2'   | 23:BB:1600:C:C6    | 2.37        | 0.58     |
| 23:DB:1098:A:H3'   | 24:DI:3:LYS:C      | 2.24        | 0.58     |
| 23:BB:2331:G:O2'   | 52:BW:40:ARG:HB2   | 2.04        | 0.58     |
| 23:DB:1820:U:H4'   | 23:DB:1821:A:OP2   | 2.03        | 0.58     |
| 21:CU:42:THR:HB    | 21:CU:46:ARG:HE    | 1.68        | 0.58     |
| 48:DG:84:LYS:HG3   | 48:DG:131:VAL:C    | 2.24        | 0.58     |
| 47:DF:33:ILE:HD13  | 47:DF:95:MET:HG2   | 1.85        | 0.58     |
| 23:DB:856:G:H1'    | 52:DW:23:LYS:HB3   | 1.84        | 0.58     |
| 1:AA:1147:C:O2'    | 8:AI:17:ARG:HD2    | 2.02        | 0.58     |
| 25:BC:140:VAL:HG12 | 25:BC:141:HIS:H    | 1.67        | 0.58     |
| 26:DD:101:PHE:HE2  | 26:DD:205:PRO:HD3  | 1.68        | 0.58     |
| 26:DD:106:LYS:HB3  | 26:DD:206:ALA:N    | 2.18        | 0.58     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 45:DS:3:THR:HB    | 45:DS:62:ASP:CB   | 2.31        | 0.58     |
| 44:BQ:93:ILE:HG23 | 44:BQ:94:LEU:HD22 | 1.85        | 0.58     |
| 29:BE:130:LYS:C   | 29:BE:132:LYS:H   | 2.05        | 0.58     |
| 46:DU:46:LYS:NZ   | 46:DU:47:PRO:HG2  | 2.18        | 0.58     |
| 35:DV:44:HIS:HE1  | 35:DV:86:LEU:H    | 1.50        | 0.58     |
| 15:CP:6:LEU:CD1   | 15:CP:71:VAL:HB   | 2.34        | 0.58     |
| 1:AA:1432:G:H1'   | 1:AA:1468:A:H61   | 1.68        | 0.58     |
| 45:DS:56:ALA:O    | 45:DS:59:GLU:HB2  | 2.02        | 0.58     |
| 23:DB:2885:G:H2'  | 23:DB:2886:A:O4'  | 2.03        | 0.58     |
| 40:DH:4:ILE:H     | 40:DH:4:ILE:HD12  | 1.67        | 0.58     |
| 9:AJ:15:HIS:HA    | 9:AJ:18:ILE:HG22  | 1.84        | 0.58     |
| 23:DB:321:U:H1'   | 29:DE:162:ARG:NH1 | 2.18        | 0.58     |
| 14:CO:26:GLU:HG3  | 14:CO:77:ARG:NH1  | 2.19        | 0.58     |
| 23:DB:2144:G:N3   | 23:DB:2146:C:H5'  | 2.17        | 0.58     |
| 23:BB:581:C:H2'   | 23:BB:582:A:H8    | 1.65        | 0.58     |
| 23:DB:1387:A:H5'  | 23:DB:1469:A:H1'  | 1.85        | 0.58     |
| 22:BA:111:U:H2'   | 22:BA:112:G:H8    | 1.66        | 0.58     |
| 1:CA:1465:A:H2'   | 1:CA:1466:C:C6    | 2.39        | 0.58     |
| 23:BB:2635:A:H5'  | 26:BD:79:LEU:HD23 | 1.84        | 0.58     |
| 1:CA:390:U:H2'    | 1:CA:391:G:H8     | 1.67        | 0.58     |
| 23:DB:1993:U:H4'  | 26:DD:133:THR:CG2 | 2.32        | 0.58     |
| 23:BB:680:C:H2'   | 23:BB:681:G:H8    | 1.68        | 0.58     |
| 23:DB:1219:U:H2'  | 23:DB:1220:G:C8   | 2.38        | 0.58     |
| 23:BB:1684:G:H2'  | 23:BB:1685:C:H6   | 1.67        | 0.58     |
| 22:DA:89:U:H5'    | 22:DA:90:C:C6     | 2.38        | 0.58     |
| 2:AC:16:PRO:HG2   | 2:AC:53:ARG:NH2   | 2.18        | 0.58     |
| 23:BB:1061:U:H4'  | 23:BB:1070:A:O3'  | 2.04        | 0.58     |
| 23:BB:2776:A:H4'  | 23:BB:2777:G:H5'' | 1.85        | 0.58     |
| 23:DB:813:U:H2'   | 23:DB:814:C:H6    | 1.68        | 0.58     |
| 12:CM:43:LYS:HB2  | 12:CM:46:GLU:HG3  | 1.86        | 0.58     |
| 23:DB:102:U:O2    | 23:DB:102:U:H5''  | 2.03        | 0.58     |
| 23:BB:2261:C:O2'  | 23:BB:2262:U:H5'  | 2.03        | 0.58     |
| 23:DB:1099:G:C5'  | 24:DI:3:LYS:N     | 2.66        | 0.58     |
| 23:BB:917:A:H2'   | 23:BB:918:A:O4'   | 2.03        | 0.58     |
| 48:BG:84:LYS:HB3  | 48:BG:132:LEU:O   | 2.03        | 0.58     |
| 5:CF:36:ILE:HA    | 5:CF:64:VAL:HG13  | 1.84        | 0.58     |
| 40:BH:116:ARG:CZ  | 40:BH:131:SER:HB3 | 2.33        | 0.58     |
| 50:BT:1:MET:C     | 50:BT:2:ILE:HD13  | 2.24        | 0.58     |
| 12:AM:12:LYS:HD2  | 12:AM:16:ILE:HD13 | 1.83        | 0.58     |
| 1:CA:1217:C:OP1   | 13:CN:8:ARG:HD2   | 2.04        | 0.58     |
| 13:CN:9:GLU:OE2   | 13:CN:60:ARG:HG2  | 2.03        | 0.58     |
| 13:AN:78:LEU:HD23 | 13:AN:82:LYS:HB3  | 1.85        | 0.58     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:AD:160:LEU:N     | 3:AD:160:LEU:HD13  | 2.17        | 0.58     |
| 3:AD:26:ALA:HA     | 3:AD:30:LYS:HE3    | 1.84        | 0.58     |
| 47:BF:107:VAL:HG11 | 47:BF:175:PRO:HG3  | 1.86        | 0.58     |
| 37:BL:79:LEU:HB3   | 37:BL:115:GLU:O    | 2.03        | 0.58     |
| 38:BM:34:LYS:HB3   | 38:BM:129:THR:HG22 | 1.85        | 0.58     |
| 1:CA:764:C:H2'     | 1:CA:765:G:H5'     | 1.85        | 0.58     |
| 12:AM:78:ARG:HH22  | 18:AS:68:HIS:CE1   | 2.22        | 0.58     |
| 38:DM:126:ILE:HG22 | 38:DM:127:LYS:N    | 2.19        | 0.58     |
| 35:DV:30:ILE:HD12  | 35:DV:38:LEU:HD23  | 1.84        | 0.58     |
| 35:DV:80:HIS:CD2   | 35:DV:83:LYS:H     | 2.22        | 0.58     |
| 48:BG:145:ALA:HA   | 48:BG:148:ARG:HG3  | 1.85        | 0.58     |
| 40:DH:47:PHE:HB3   | 40:DH:51:ARG:NH2   | 2.19        | 0.58     |
| 23:BB:1439:A:C6    | 23:BB:1552:A:N7    | 2.72        | 0.58     |
| 23:BB:2134:A:H2'   | 23:BB:2135:A:H8    | 1.69        | 0.58     |
| 1:CA:707:U:H4'     | 10:CK:21:HIS:CD2   | 2.38        | 0.58     |
| 44:DQ:101:ASP:HB2  | 49:DR:2:TYR:OH     | 2.03        | 0.58     |
| 23:BB:2023:C:H4'   | 23:BB:2617:U:O3'   | 2.04        | 0.58     |
| 20:AB:63:LYS:HG2   | 20:AB:224:ARG:NH1  | 2.17        | 0.58     |
| 23:DB:1258:U:H2'   | 23:DB:1259:G:C8    | 2.37        | 0.58     |
| 52:BW:46:ALA:HB2   | 52:BW:78:PHE:HD1   | 1.68        | 0.58     |
| 23:DB:2199:A:H3'   | 23:DB:2200:C:H6    | 1.69        | 0.58     |
| 1:AA:373:A:H2'     | 1:AA:374:A:H8      | 1.69        | 0.58     |
| 27:BK:70:ARG:HB3   | 27:BK:76:VAL:HG22  | 1.84        | 0.58     |
| 1:AA:470:C:H2'     | 1:AA:471:U:C6      | 2.38        | 0.58     |
| 41:DJ:72:LYS:HB2   | 41:DJ:89:PHE:H     | 1.69        | 0.58     |
| 4:CE:100:GLU:HA    | 4:CE:121:ASN:ND2   | 2.18        | 0.58     |
| 1:AA:128:G:H2'     | 1:AA:129:A:C8      | 2.39        | 0.58     |
| 23:BB:962:G:N2     | 23:BB:2250:G:H1    | 2.01        | 0.58     |
| 23:DB:649:G:H2'    | 23:DB:650:C:C6     | 2.38        | 0.58     |
| 1:AA:426:U:H4'     | 3:AD:39:GLN:HA     | 1.85        | 0.58     |
| 1:CA:328:C:H4'     | 1:CA:329:A:H5''    | 1.84        | 0.58     |
| 44:BQ:30:VAL:O     | 44:BQ:31:TYR:HB2   | 2.04        | 0.58     |
| 23:DB:570:G:H2'    | 23:DB:2030:A:N7    | 2.17        | 0.58     |
| 23:DB:946:C:H2'    | 23:DB:947:A:H8     | 1.69        | 0.58     |
| 53:D6:68:VAL:O     | 53:D6:98:ALA:HA    | 2.04        | 0.58     |
| 23:DB:923:G:H1'    | 52:DW:23:LYS:NZ    | 2.18        | 0.58     |
| 8:CI:20:ILE:HG23   | 8:CI:60:LEU:CD1    | 2.34        | 0.58     |
| 8:AI:62:LEU:N      | 8:AI:62:LEU:HD22   | 2.19        | 0.58     |
| 47:DF:76:PHE:HD2   | 47:DF:78:ILE:HD13  | 1.68        | 0.58     |
| 29:BE:150:THR:HG21 | 29:BE:153:LEU:HA   | 1.86        | 0.58     |
| 40:DH:119:ASN:OD1  | 40:DH:121:VAL:HG13 | 2.03        | 0.58     |
| 40:DH:85:GLY:H     | 40:DH:89:LYS:C     | 2.06        | 0.58     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:1319:A:H4'   | 1:CA:1320:C:OP1   | 2.03        | 0.58     |
| 1:AA:1250:A:H4'   | 8:AI:69:GLY:H     | 1.68        | 0.58     |
| 23:DB:2379:G:C5'  | 43:DO:21:LEU:HD11 | 2.32        | 0.58     |
| 31:D0:48:TYR:CG   | 31:D0:49:ARG:N    | 2.71        | 0.58     |
| 1:CA:1004:A:C8    | 1:CA:1025:U:H1'   | 2.38        | 0.58     |
| 23:DB:98:G:C2'    | 23:DB:99:U:H5''   | 2.34        | 0.58     |
| 12:AM:2:ARG:HG3   | 12:AM:6:ILE:N     | 2.19        | 0.58     |
| 23:BB:64:A:H2'    | 23:BB:65:U:H6     | 1.66        | 0.58     |
| 36:D2:10:LEU:HD11 | 36:D2:14:ARG:CZ   | 2.34        | 0.58     |
| 39:BX:49:ASP:O    | 39:BX:53:VAL:HG23 | 2.04        | 0.58     |
| 1:CA:1009:U:H5'   | 1:CA:1010:U:OP2   | 2.02        | 0.58     |
| 19:AT:35:TYR:O    | 19:AT:38:ILE:HG22 | 2.02        | 0.58     |
| 6:CG:24:LYS:HA    | 6:CG:27:ASN:HD22  | 1.67        | 0.58     |
| 29:DE:103:GLY:O   | 29:DE:106:LYS:HB2 | 2.03        | 0.58     |
| 1:AA:1458:G:H5''  | 19:AT:25:SER:HB2  | 1.85        | 0.58     |
| 23:BB:2553:G:H2'  | 23:BB:2554:U:C4'  | 2.33        | 0.58     |
| 23:BB:521:U:H2'   | 23:BB:522:A:C8    | 2.38        | 0.58     |
| 23:BB:2569:G:O2'  | 23:BB:2570:G:H5'  | 2.04        | 0.58     |
| 53:B6:19:GLU:HA   | 53:B6:22:GLU:HB2  | 1.84        | 0.58     |
| 23:BB:1341:G:H3'  | 23:BB:1397:U:O2   | 2.03        | 0.58     |
| 1:AA:1507:A:H2'   | 1:AA:1508:A:C8    | 2.37        | 0.58     |
| 12:AM:64:VAL:HA   | 12:AM:68:LEU:CD1  | 2.34        | 0.58     |
| 23:DB:2678:C:H2'  | 23:DB:2679:A:C8   | 2.38        | 0.58     |
| 23:BB:690:G:H2'   | 23:BB:691:C:O4'   | 2.03        | 0.58     |
| 23:BB:1881:C:H2'  | 23:BB:1882:U:O4'  | 2.03        | 0.58     |
| 23:BB:18:U:H2'    | 23:BB:19:A:C8     | 2.37        | 0.58     |
| 44:DQ:30:VAL:O    | 44:DQ:31:TYR:HB2  | 2.03        | 0.58     |
| 1:CA:1250:A:H4'   | 8:CI:69:GLY:H     | 1.68        | 0.58     |
| 53:B6:10:THR:HG22 | 53:B6:14:MET:CE   | 2.34        | 0.58     |
| 1:AA:522:C:H41    | 11:AL:49:ARG:NH2  | 2.01        | 0.58     |
| 6:AG:122:GLU:OE1  | 6:AG:131:GLY:HA3  | 2.04        | 0.58     |
| 1:CA:522:C:H41    | 11:CL:49:ARG:NH2  | 2.00        | 0.58     |
| 23:DB:850:U:H2'   | 23:DB:851:C:C6    | 2.39        | 0.58     |
| 27:BK:118:LEU:O   | 27:BK:120:PRO:HD2 | 2.02        | 0.58     |
| 29:BE:109:LEU:O   | 29:BE:112:LEU:HB2 | 2.03        | 0.58     |
| 1:AA:844:G:H2'    | 1:AA:845:A:C8     | 2.39        | 0.58     |
| 20:CB:79:VAL:HG12 | 20:CB:90:PHE:HB2  | 1.86        | 0.58     |
| 40:DH:113:SER:H   | 40:DH:132:PHE:HE1 | 1.51        | 0.58     |
| 1:CA:1048:G:H4'   | 13:CN:2:LYS:HZ2   | 1.68        | 0.58     |
| 39:DX:8:GLU:HB2   | 39:DX:13:GLU:OE1  | 2.03        | 0.58     |
| 23:DB:1374:G:H2'  | 23:DB:1375:U:C6   | 2.39        | 0.58     |
| 23:DB:296:U:H2'   | 23:DB:297:G:C8    | 2.38        | 0.58     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 19:AT:79:THR:HA    | 19:AT:82:ILE:HG12  | 1.85        | 0.58     |
| 23:DB:544:C:H2'    | 23:DB:545:U:C4     | 2.38        | 0.58     |
| 1:AA:1461:G:H2'    | 1:AA:1462:C:C6     | 2.38        | 0.58     |
| 25:BC:61:TYR:HA    | 25:BC:85:ASN:ND2   | 2.19        | 0.58     |
| 1:CA:591:U:OP1     | 7:CH:30:LYS:HE2    | 2.03        | 0.58     |
| 23:DB:324:A:H2'    | 23:DB:325:G:O4'    | 2.03        | 0.58     |
| 23:DB:1857:G:N2    | 23:DB:1884:G:H2'   | 2.19        | 0.58     |
| 23:BB:904:G:H2'    | 23:BB:905:A:H8     | 1.67        | 0.58     |
| 19:AT:49:ALA:O     | 19:AT:52:GLU:HG2   | 2.04        | 0.58     |
| 24:BI:5:GLN:HG2    | 24:BI:6:ALA:N      | 2.18        | 0.58     |
| 3:CD:146:GLU:HA    | 3:CD:149:LYS:HG2   | 1.85        | 0.58     |
| 40:DH:41:LYS:O     | 40:DH:44:ILE:HG12  | 2.03        | 0.58     |
| 28:DP:103:THR:HG22 | 28:DP:104:GLY:H    | 1.68        | 0.58     |
| 23:BB:826:U:H2'    | 23:BB:828:U:O4'    | 2.04        | 0.58     |
| 2:CC:21:TRP:CH2    | 2:CC:31:ASN:HB3    | 2.39        | 0.58     |
| 23:DB:654:A:H2'    | 23:DB:655:A:H5''   | 1.86        | 0.58     |
| 23:DB:1899:A:O2'   | 23:DB:1900:A:H5''  | 2.02        | 0.58     |
| 1:AA:90:C:H2'      | 1:AA:91:U:C5       | 2.39        | 0.58     |
| 4:AE:55:VAL:N      | 4:AE:56:PRO:HD2    | 2.18        | 0.58     |
| 7:CH:107:LYS:HA    | 7:CH:107:LYS:HE3   | 1.86        | 0.58     |
| 23:DB:690:G:H2'    | 23:DB:691:C:O4'    | 2.03        | 0.58     |
| 4:CE:43:GLY:O      | 4:CE:72:ASN:HA     | 2.04        | 0.58     |
| 29:DE:31:VAL:HG21  | 29:DE:104:ALA:HB2  | 1.85        | 0.58     |
| 47:BF:62:GLN:NE2   | 47:BF:90:LEU:HD13  | 2.06        | 0.58     |
| 6:AG:146:ALA:HA    | 10:AK:55:ARG:HH12  | 1.68        | 0.58     |
| 40:BH:68:ARG:HB3   | 40:BH:134:VAL:HG11 | 1.86        | 0.58     |
| 26:BD:30:GLU:HG3   | 26:BD:52:THR:CG2   | 2.33        | 0.58     |
| 53:B6:83:ILE:O     | 53:B6:88:LEU:HB2   | 2.03        | 0.58     |
| 8:CI:46:VAL:HA     | 8:CI:49:GLN:HG3    | 1.85        | 0.58     |
| 8:CI:79:ARG:HA     | 8:CI:82:ILE:HD12   | 1.86        | 0.58     |
| 41:DJ:44:TYR:CE2   | 44:DQ:59:LEU:HD11  | 2.38        | 0.58     |
| 25:BC:128:THR:HG23 | 25:BC:190:THR:HG22 | 1.86        | 0.58     |
| 12:AM:106:ARG:HD3  | 12:AM:110:GLY:O    | 2.03        | 0.58     |
| 25:BC:64:VAL:HG11  | 25:BC:66:PHE:CZ    | 2.39        | 0.58     |
| 43:BO:74:VAL:O     | 43:BO:78:VAL:HG23  | 2.04        | 0.58     |
| 1:AA:413:G:H2'     | 1:AA:428:G:N2      | 2.19        | 0.58     |
| 47:DF:11:VAL:HG12  | 47:DF:12:VAL:N     | 2.15        | 0.58     |
| 47:DF:134:GLN:H    | 47:DF:150:GLY:H    | 1.52        | 0.58     |
| 18:AS:35:ARG:HB3   | 18:AS:50:VAL:CG1   | 2.34        | 0.58     |
| 10:AK:91:GLY:O     | 10:AK:95:THR:HG22  | 2.03        | 0.58     |
| 23:DB:138:U:H2'    | 23:DB:140:C:N1     | 2.18        | 0.58     |
| 32:B4:24:ARG:HG2   | 32:B4:36:ARG:CG    | 2.33        | 0.58     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 32:D4:24:ARG:HG2   | 32:D4:36:ARG:CG    | 2.34        | 0.58     |
| 29:DE:146:VAL:HA   | 29:DE:185:LYS:O    | 2.04        | 0.58     |
| 44:DQ:107:ALA:HB1  | 49:DR:48:LYS:HE3   | 1.85        | 0.58     |
| 3:AD:116:LEU:O     | 3:AD:121:ALA:HB3   | 2.03        | 0.58     |
| 23:BB:1789:A:P     | 25:BC:220:ARG:HD3  | 2.44        | 0.58     |
| 23:BB:2722:G:H2'   | 23:BB:2723:C:C6    | 2.39        | 0.58     |
| 1:CA:193:C:H2'     | 1:CA:194:C:C5      | 2.39        | 0.58     |
| 41:BJ:96:ARG:N     | 41:BJ:97:PRO:HD3   | 2.19        | 0.58     |
| 27:DK:88:ASN:HB3   | 27:DK:92:GLU:O     | 2.04        | 0.58     |
| 23:BB:2230:G:H2'   | 23:BB:2231:U:H6    | 1.69        | 0.58     |
| 23:DB:1351:C:O2'   | 23:DB:1571:A:H1'   | 2.03        | 0.58     |
| 1:CA:777:A:H2'     | 1:CA:778:G:H8      | 1.69        | 0.58     |
| 1:CA:1512:U:H2'    | 1:CA:1513:A:H8     | 1.67        | 0.58     |
| 23:BB:2369:A:O2'   | 23:BB:2370:G:H5'   | 2.04        | 0.58     |
| 23:DB:441:U:H2'    | 23:DB:442:G:H8     | 1.68        | 0.58     |
| 23:BB:937:C:H2'    | 23:BB:938:G:H8     | 1.69        | 0.58     |
| 23:BB:1429:G:H2'   | 23:BB:1430:G:H8    | 1.69        | 0.58     |
| 19:AT:27:MET:O     | 19:AT:31:ILE:HG13  | 2.04        | 0.58     |
| 25:DC:221:GLY:C    | 25:DC:223:ALA:H    | 2.07        | 0.58     |
| 23:BB:2835:A:N6    | 23:BB:2878:U:H2'   | 2.19        | 0.58     |
| 23:DB:2662:A:H2'   | 23:DB:2663:G:O4'   | 2.03        | 0.58     |
| 1:AA:512:U:O2'     | 1:AA:513:C:H5'     | 2.04        | 0.58     |
| 26:BD:67:HIS:O     | 26:BD:70:LYS:HB3   | 2.03        | 0.58     |
| 7:AH:26:MET:HB2    | 7:AH:27:PRO:HD2    | 1.86        | 0.58     |
| 25:BC:170:TYR:CD2  | 25:BC:184:GLU:HA   | 2.38        | 0.58     |
| 6:AG:149:ALA:HB2   | 10:AK:55:ARG:NE    | 2.02        | 0.58     |
| 47:DF:65:LEU:N     | 47:DF:88:VAL:HG22  | 2.17        | 0.58     |
| 47:DF:32:LYS:H     | 47:DF:95:MET:HE1   | 1.67        | 0.58     |
| 8:AI:70:GLY:O      | 8:AI:74:GLN:HB2    | 2.04        | 0.58     |
| 26:DD:106:LYS:HB3  | 26:DD:206:ALA:HB3  | 1.86        | 0.58     |
| 26:DD:107:VAL:HA   | 26:DD:204:LYS:O    | 2.04        | 0.58     |
| 41:DJ:26:GLY:O     | 41:DJ:30:THR:HG22  | 2.03        | 0.58     |
| 41:DJ:19:ASP:OD2   | 41:DJ:58:ASN:HB2   | 2.04        | 0.58     |
| 25:DC:75:ALA:CB    | 25:DC:95:TYR:HA    | 2.32        | 0.58     |
| 47:BF:168:LEU:HD13 | 47:BF:169:LEU:H    | 1.69        | 0.58     |
| 1:AA:764:C:N4      | 1:AA:812:G:H1      | 2.02        | 0.58     |
| 1:CA:918:A:H2'     | 1:CA:919:A:C8      | 2.39        | 0.58     |
| 18:CS:27:LYS:NZ    | 18:CS:27:LYS:HB3   | 2.18        | 0.58     |
| 25:DC:16:VAL:H     | 25:DC:203:VAL:HG12 | 1.68        | 0.58     |
| 23:DB:2810:A:H2'   | 23:DB:2811:G:O4'   | 2.03        | 0.58     |
| 38:DM:64:TRP:HB2   | 38:DM:104:GLU:HB2  | 1.85        | 0.58     |
| 42:BN:33:ILE:O     | 42:BN:33:ILE:HD12  | 2.04        | 0.58     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 2:CC:8:GLY:HA2    | 2:CC:11:LEU:HG     | 1.85        | 0.58     |
| 5:AF:38:ARG:HH21  | 5:AF:63:ASN:HD21   | 1.48        | 0.58     |
| 3:CD:90:LEU:HD21  | 3:CD:196:GLU:HB3   | 1.85        | 0.58     |
| 23:BB:2753:A:H2'  | 23:BB:2754:U:C6    | 2.39        | 0.58     |
| 42:BN:49:GLU:OE2  | 42:BN:95:THR:HG22  | 2.03        | 0.58     |
| 23:DB:220:G:H1    | 23:DB:427:U:H2'    | 1.69        | 0.58     |
| 6:AG:19:SER:OG    | 6:AG:22:LEU:HB2    | 2.04        | 0.58     |
| 42:DN:12:ARG:HG3  | 42:DN:13:ASN:H     | 1.68        | 0.58     |
| 1:CA:1308:U:OP2   | 12:CM:97:ARG:HD3   | 2.03        | 0.58     |
| 23:BB:1709:U:H2'  | 23:BB:1710:G:C8    | 2.39        | 0.58     |
| 41:DJ:96:ARG:N    | 41:DJ:97:PRO:HD3   | 2.19        | 0.58     |
| 48:DG:87:GLN:HG2  | 48:DG:164:ALA:HA   | 1.84        | 0.58     |
| 1:AA:1151:A:HO2'  | 1:AA:1152:A:H8     | 1.51        | 0.58     |
| 29:BE:122:GLU:O   | 29:BE:123:LYS:HB2  | 2.04        | 0.58     |
| 15:AP:74:LEU:O    | 15:AP:78:VAL:HG12  | 2.04        | 0.58     |
| 23:DB:1419:A:H2'  | 23:DB:1421:G:N7    | 2.19        | 0.58     |
| 23:BB:39:G:O2'    | 23:BB:40:U:H5'     | 2.04        | 0.58     |
| 23:BB:2041:U:H2'  | 23:BB:2042:A:C8    | 2.38        | 0.58     |
| 1:AA:692:U:H2'    | 1:AA:693:G:H3'     | 1.84        | 0.58     |
| 23:DB:1092:C:H2'  | 23:DB:1093:G:H5'   | 1.86        | 0.58     |
| 23:BB:1117:C:H2'  | 23:BB:1118:C:H6    | 1.69        | 0.58     |
| 1:CA:204:G:H1'    | 1:CA:466:A:N7      | 2.19        | 0.58     |
| 3:AD:115:GLN:HG3  | 3:AD:119:HIS:CE1   | 2.38        | 0.58     |
| 27:DK:109:SER:HB2 | 27:DK:111:LYS:HE2  | 1.85        | 0.58     |
| 25:DC:170:TYR:CD2 | 25:DC:184:GLU:HA   | 2.38        | 0.58     |
| 10:AK:33:ILE:HG12 | 10:AK:69:CYS:SG    | 2.44        | 0.58     |
| 40:BH:116:ARG:CB  | 40:BH:133:GLN:HB2  | 2.27        | 0.58     |
| 40:BH:99:ILE:CD1  | 40:BH:144:VAL:HG21 | 2.34        | 0.58     |
| 41:BJ:55:ILE:O    | 41:BJ:55:ILE:HG13  | 2.04        | 0.58     |
| 46:DU:85:ARG:HH11 | 46:DU:86:PHE:H     | 1.50        | 0.58     |
| 47:DF:109:ARG:CB  | 47:DF:135:ILE:HD12 | 2.34        | 0.58     |
| 29:BE:58:LYS:HE2  | 29:BE:60:TRP:HD1   | 1.68        | 0.58     |
| 26:DD:62:LYS:HB2  | 26:DD:63:PRO:HD3   | 1.86        | 0.58     |
| 45:DS:27:LYS:HD2  | 45:DS:27:LYS:H     | 1.68        | 0.58     |
| 24:DI:121:ILE:CD1 | 24:DI:121:ILE:H    | 2.14        | 0.58     |
| 25:BC:209:ALA:O   | 25:BC:213:ARG:HB2  | 2.04        | 0.58     |
| 1:CA:719:C:O2     | 17:CR:37:LYS:HA    | 2.03        | 0.58     |
| 26:DD:113:SER:HB3 | 26:DD:167:ASN:CA   | 2.34        | 0.58     |
| 34:B3:22:LYS:HD2  | 34:B3:46:LYS:HB2   | 1.85        | 0.58     |
| 36:D2:21:ARG:HH21 | 36:D2:43:THR:CG2   | 2.17        | 0.58     |
| 20:AB:95:TRP:CZ2  | 20:AB:100:LEU:HD13 | 2.39        | 0.58     |
| 23:DB:581:C:H2'   | 23:DB:582:A:H8     | 1.67        | 0.58     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 7:CH:40:LYS:HD2   | 7:CH:47:ASP:HA    | 1.85        | 0.58     |
| 3:AD:196:GLU:O    | 3:AD:199:ILE:HG12 | 2.03        | 0.58     |
| 41:BJ:110:PRO:HB2 | 41:BJ:111:LYS:HE3 | 1.86        | 0.58     |
| 36:D2:33:ARG:HH21 | 36:D2:33:ARG:HB2  | 1.68        | 0.58     |
| 52:DW:44:PHE:HB3  | 52:DW:78:PHE:CD1  | 2.39        | 0.58     |
| 23:DB:1930:G:H2'  | 23:DB:1968:G:O6   | 2.03        | 0.58     |
| 22:BA:95:U:H2'    | 22:BA:96:G:C8     | 2.39        | 0.58     |
| 23:BB:2095:A:H2'  | 23:BB:2096:C:C6   | 2.39        | 0.58     |
| 9:CJ:40:ILE:HD12  | 9:CJ:73:LEU:HD12  | 1.86        | 0.58     |
| 5:CF:81:ASN:OD1   | 5:CF:83:ALA:HB3   | 2.03        | 0.58     |
| 22:DA:35:C:H2'    | 22:DA:36:C:C5'    | 2.34        | 0.58     |
| 19:CT:49:ALA:O    | 19:CT:52:GLU:HG2  | 2.04        | 0.58     |
| 26:BD:15:PHE:H    | 26:BD:15:PHE:HD1  | 1.51        | 0.58     |
| 34:B3:7:ARG:HH11  | 34:B3:7:ARG:HG3   | 1.68        | 0.58     |
| 25:DC:2:VAL:HG23  | 25:DC:3:VAL:H     | 1.67        | 0.58     |
| 1:CA:505:G:H4'    | 1:CA:534:U:C4     | 2.39        | 0.58     |
| 21:CU:39:LYS:N    | 21:CU:40:PRO:HD2  | 2.18        | 0.57     |
| 8:CI:56:MET:CG    | 8:CI:57:VAL:H     | 2.17        | 0.57     |
| 8:CI:61:ASP:C     | 8:CI:62:LEU:HD13  | 2.24        | 0.57     |
| 23:BB:996:A:C4'   | 44:BQ:91:ARG:HH11 | 2.15        | 0.57     |
| 23:BB:2849:U:N3   | 23:BB:2867:G:C8   | 2.72        | 0.57     |
| 23:BB:981:A:H2'   | 23:BB:982:C:H5''  | 1.85        | 0.57     |
| 31:B0:42:ILE:HG12 | 42:BN:99:LYS:O    | 2.04        | 0.57     |
| 23:BB:1082:U:O4   | 23:BB:1086:A:C2   | 2.57        | 0.57     |
| 17:CR:38:ILE:H    | 17:CR:38:ILE:HD13 | 1.69        | 0.57     |
| 37:BL:6:LEU:H     | 37:BL:6:LEU:CD2   | 2.17        | 0.57     |
| 3:AD:122:ILE:O    | 3:AD:128:VAL:HG23 | 2.04        | 0.57     |
| 23:BB:2899:A:H2'  | 23:BB:2900:A:C8   | 2.39        | 0.57     |
| 23:BB:362:A:H3'   | 23:BB:363:G:H8    | 1.68        | 0.57     |
| 44:DQ:9:ALA:C     | 44:DQ:11:ALA:H    | 2.06        | 0.57     |
| 1:CA:844:G:H2'    | 1:CA:845:A:C8     | 2.39        | 0.57     |
| 34:D3:22:LYS:HD2  | 34:D3:46:LYS:HB2  | 1.86        | 0.57     |
| 21:AU:10:PRO:HB2  | 2:CC:71:ARG:CD    | 2.34        | 0.57     |
| 1:CA:926:G:H3'    | 1:CA:1505:G:H21   | 1.69        | 0.57     |
| 23:DB:2590:A:H2'  | 23:DB:2591:C:C6   | 2.39        | 0.57     |
| 23:BB:946:C:H2'   | 23:BB:947:A:H8    | 1.68        | 0.57     |
| 20:CB:94:ARG:N    | 20:CB:94:ARG:HE   | 2.01        | 0.57     |
| 19:CT:82:ILE:HA   | 19:CT:85:LEU:HD22 | 1.86        | 0.57     |
| 45:BS:31:GLN:C    | 45:BS:33:LEU:H    | 2.07        | 0.57     |
| 23:BB:1258:U:H2'  | 23:BB:1259:G:C8   | 2.39        | 0.57     |
| 1:CA:1463:U:H2'   | 1:CA:1464:U:C6    | 2.39        | 0.57     |
| 23:BB:743:A:O2'   | 23:BB:744:U:H5'   | 2.04        | 0.57     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:662:U:H2'     | 1:AA:663:A:C8      | 2.39        | 0.57     |
| 1:CA:1481:U:O2'    | 1:CA:1482:G:H5'    | 2.03        | 0.57     |
| 1:CA:611:C:H2'     | 1:CA:612:C:H6      | 1.69        | 0.57     |
| 43:DO:108:ASP:HA   | 43:DO:111:ARG:HB3  | 1.85        | 0.57     |
| 23:BB:1291:C:O2'   | 23:BB:1292:G:H5'   | 2.04        | 0.57     |
| 23:DB:1720:U:O2'   | 23:DB:1721:G:H5'   | 2.04        | 0.57     |
| 35:BV:49:ASN:HD22  | 35:BV:49:ASN:N     | 2.02        | 0.57     |
| 23:DB:1647:U:H3'   | 23:DB:1647:U:P     | 2.44        | 0.57     |
| 23:BB:794:A:H2'    | 23:BB:795:C:C6     | 2.39        | 0.57     |
| 47:BF:34:THR:OG1   | 47:BF:154:THR:HB   | 2.04        | 0.57     |
| 26:BD:106:LYS:HB3  | 26:BD:206:ALA:HB3  | 1.85        | 0.57     |
| 23:DB:854:C:O2'    | 23:DB:855:G:H5'    | 2.03        | 0.57     |
| 30:DY:8:GLN:CG     | 30:DY:31:ILE:HA    | 2.27        | 0.57     |
| 47:BF:134:GLN:C    | 47:BF:136:ILE:H    | 2.08        | 0.57     |
| 1:AA:1278:G:H4'    | 1:AA:1279:G:C5'    | 2.34        | 0.57     |
| 47:BF:102:LEU:HD22 | 47:BF:103:ILE:N    | 2.17        | 0.57     |
| 45:BS:18:ARG:HB3   | 45:BS:76:VAL:HG22  | 1.85        | 0.57     |
| 13:AN:48:GLN:O     | 13:AN:51:PRO:HD2   | 2.04        | 0.57     |
| 15:AP:6:LEU:CD1    | 15:AP:71:VAL:HB    | 2.34        | 0.57     |
| 3:CD:187:ARG:O     | 3:CD:191:SER:HB3   | 2.04        | 0.57     |
| 1:AA:1389:C:H2'    | 1:AA:1390:U:C6     | 2.39        | 0.57     |
| 23:BB:850:U:O2'    | 30:BY:22:THR:HG22  | 2.04        | 0.57     |
| 14:CO:24:SER:HB3   | 14:CO:27:VAL:CG2   | 2.33        | 0.57     |
| 23:BB:580:U:H2'    | 23:BB:581:C:H6     | 1.66        | 0.57     |
| 12:CM:95:PRO:HD3   | 12:CM:108:ARG:HG2  | 1.85        | 0.57     |
| 38:BM:40:ARG:HB2   | 38:BM:93:VAL:CG2   | 2.34        | 0.57     |
| 39:BX:5:GLU:O      | 39:BX:8:GLU:HG2    | 2.04        | 0.57     |
| 23:DB:1682:G:H2'   | 23:DB:1683:U:C6    | 2.38        | 0.57     |
| 21:CU:11:PHE:O     | 21:CU:13:VAL:HG12  | 2.03        | 0.57     |
| 1:AA:1150:A:H1'    | 1:AA:1280:A:N6     | 2.18        | 0.57     |
| 23:BB:828:U:H4'    | 23:BB:831:G:N1     | 2.18        | 0.57     |
| 38:BM:82:MET:HE3   | 38:BM:83:GLY:H     | 1.69        | 0.57     |
| 1:CA:586:C:H5''    | 7:CH:81:GLY:HA2    | 1.86        | 0.57     |
| 44:BQ:40:LYS:HA    | 44:BQ:43:GLN:OE1   | 2.04        | 0.57     |
| 38:BM:67:VAL:HG11  | 38:BM:102:LEU:HD13 | 1.86        | 0.57     |
| 17:CR:36:GLY:HA3   | 17:CR:70:THR:HA    | 1.85        | 0.57     |
| 23:DB:2812:G:H2'   | 23:DB:2813:A:C8    | 2.39        | 0.57     |
| 23:DB:1513:U:O2'   | 23:DB:1514:G:H5'   | 2.03        | 0.57     |
| 23:DB:2737:G:H2'   | 23:DB:2738:A:C8    | 2.39        | 0.57     |
| 23:BB:654:A:H2'    | 23:BB:655:A:H5''   | 1.86        | 0.57     |
| 21:AU:8:ASN:O      | 21:AU:9:GLU:HB3    | 2.04        | 0.57     |
| 3:AD:48:SER:O      | 3:AD:52:VAL:HG23   | 2.04        | 0.57     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:443:A:OP1   | 29:DE:40:ARG:HD2   | 2.04        | 0.57     |
| 23:DB:904:G:H2'   | 23:DB:905:A:H8     | 1.68        | 0.57     |
| 24:BI:96:LYS:N    | 24:BI:96:LYS:HD2   | 2.20        | 0.57     |
| 1:AA:518:C:H2'    | 1:AA:530:G:C8      | 2.39        | 0.57     |
| 23:DB:1047:G:H1'  | 23:DB:1110:G:N2    | 2.18        | 0.57     |
| 23:DB:942:G:H2'   | 23:DB:943:A:O4'    | 2.03        | 0.57     |
| 23:BB:1820:U:H4'  | 23:BB:1821:A:OP2   | 2.04        | 0.57     |
| 47:BF:65:LEU:O    | 47:BF:86:CYS:HA    | 2.04        | 0.57     |
| 35:DV:63:ILE:HD13 | 35:DV:72:VAL:HG22  | 1.86        | 0.57     |
| 47:BF:43:ILE:HB   | 47:BF:82:TYR:OH    | 2.04        | 0.57     |
| 45:DS:18:ARG:HB3  | 45:DS:76:VAL:CG2   | 2.34        | 0.57     |
| 45:DS:18:ARG:HB3  | 45:DS:76:VAL:HG22  | 1.86        | 0.57     |
| 1:CA:1226:C:C4    | 12:CM:102:LYS:HB3  | 2.39        | 0.57     |
| 1:CA:950:U:H2'    | 1:CA:951:G:C8      | 2.39        | 0.57     |
| 18:CS:39:ILE:HG12 | 18:CS:70:LEU:HD12  | 1.86        | 0.57     |
| 1:AA:978:A:H5'    | 1:AA:1362:A:H62    | 1.69        | 0.57     |
| 23:BB:2487:G:H2'  | 23:BB:2488:G:C8    | 2.39        | 0.57     |
| 10:CK:92:ARG:HE   | 21:CU:20:ARG:HH22  | 1.51        | 0.57     |
| 48:BG:148:ARG:HA  | 48:BG:161:VAL:CB   | 2.34        | 0.57     |
| 38:DM:40:ARG:HB2  | 38:DM:93:VAL:CG2   | 2.33        | 0.57     |
| 1:AA:843:U:OP2    | 1:AA:843:U:H4'     | 2.04        | 0.57     |
| 23:BB:1729:U:H3'  | 23:BB:1730:C:O4'   | 2.05        | 0.57     |
| 9:CJ:15:HIS:HA    | 9:CJ:18:ILE:HG22   | 1.86        | 0.57     |
| 23:BB:2723:C:H5'' | 42:BN:1:MET:HE2    | 1.87        | 0.57     |
| 1:CA:1071:C:H2'   | 1:CA:1072:G:C8     | 2.38        | 0.57     |
| 23:DB:1728:C:H2'  | 23:DB:1730:C:O2    | 2.05        | 0.57     |
| 1:AA:859:G:H2'    | 1:AA:860:A:H8      | 1.68        | 0.57     |
| 23:DB:2630:G:H2'  | 23:DB:2631:G:C8    | 2.39        | 0.57     |
| 1:AA:57:G:H2'     | 1:AA:58:C:H6       | 1.69        | 0.57     |
| 1:AA:213:G:H5''   | 1:AA:214:C:H5      | 1.69        | 0.57     |
| 23:BB:1816:C:H3'  | 25:BC:61:TYR:CE2   | 2.39        | 0.57     |
| 21:AU:11:PHE:O    | 21:AU:11:PHE:HD1   | 1.87        | 0.57     |
| 23:BB:2340:A:H2'  | 23:BB:2341:G:H8    | 1.70        | 0.57     |
| 22:DA:86:G:H2'    | 22:DA:87:U:O4'     | 2.04        | 0.57     |
| 23:DB:2813:A:H2'  | 23:DB:2814:A:C8    | 2.40        | 0.57     |
| 53:D6:25:LEU:HD21 | 53:D6:118:VAL:HG13 | 1.86        | 0.57     |
| 1:CA:1260:G:H4'   | 1:CA:1283:U:O2'    | 2.05        | 0.57     |
| 23:BB:1636:U:H2'  | 23:BB:1637:A:H8    | 1.68        | 0.57     |
| 23:BB:269:C:H2'   | 23:BB:270:A:H8     | 1.69        | 0.57     |
| 23:DB:1744:A:H2'  | 23:DB:1745:A:C8    | 2.40        | 0.57     |
| 24:BI:75:ALA:HB2  | 24:BI:112:LYS:HE2  | 1.85        | 0.57     |
| 23:BB:1930:G:H2'  | 23:BB:1968:G:O6    | 2.05        | 0.57     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:BB:1958:C:O2'   | 23:BB:1959:G:H5'  | 2.04        | 0.57     |
| 2:CC:190:THR:HG22  | 2:CC:191:THR:N    | 2.19        | 0.57     |
| 52:DW:39:GLN:HG2   | 52:DW:40:ARG:H    | 1.68        | 0.57     |
| 23:BB:532:A:N3     | 23:BB:532:A:H2'   | 2.18        | 0.57     |
| 5:CF:3:HIS:CD2     | 5:CF:65:GLU:HG3   | 2.39        | 0.57     |
| 41:BJ:19:ASP:OD2   | 41:BJ:58:ASN:HB2  | 2.05        | 0.57     |
| 25:BC:71:ASP:HA    | 25:BC:117:SER:O   | 2.04        | 0.57     |
| 1:CA:1060:U:C5     | 2:CC:1:GLY:HA3    | 2.38        | 0.57     |
| 47:BF:41:GLU:O     | 47:BF:43:ILE:HG22 | 2.05        | 0.57     |
| 1:CA:1206:G:H2'    | 1:CA:1207:G:O4'   | 2.05        | 0.57     |
| 37:DL:6:LEU:H      | 37:DL:6:LEU:CD2   | 2.15        | 0.57     |
| 9:CJ:57:VAL:HG13   | 9:CJ:58:ASN:N     | 2.18        | 0.57     |
| 31:B0:38:LEU:HD23  | 31:B0:39:ARG:H    | 1.69        | 0.57     |
| 4:AE:148:SER:HB2   | 4:AE:150:GLU:OE1  | 2.04        | 0.57     |
| 36:B2:26:ASN:O     | 36:B2:30:VAL:HG23 | 2.04        | 0.57     |
| 1:CA:441:A:H61     | 1:CA:493:A:N6     | 2.02        | 0.57     |
| 41:BJ:72:LYS:HB2   | 41:BJ:89:PHE:H    | 1.68        | 0.57     |
| 1:AA:1095:U:H2'    | 1:AA:1096:C:C6    | 2.40        | 0.57     |
| 40:BH:44:ILE:C     | 40:BH:46:PHE:H    | 2.07        | 0.57     |
| 35:BV:28:ALA:HA    | 35:BV:88:HIS:CE1  | 2.39        | 0.57     |
| 5:AF:80:PHE:CE1    | 25:BC:135:PRO:HG2 | 2.38        | 0.57     |
| 34:D3:62:PRO:HG2   | 37:DL:48:ARG:NH2  | 2.19        | 0.57     |
| 1:AA:404:G:O2'     | 1:AA:405:U:H5'    | 2.04        | 0.57     |
| 1:AA:1123:U:H4'    | 9:AJ:39:PRO:HD2   | 1.86        | 0.57     |
| 39:DX:39:GLN:O     | 39:DX:42:LEU:HB2  | 2.05        | 0.57     |
| 23:DB:1259:G:H2'   | 23:DB:1260:A:C8   | 2.39        | 0.57     |
| 1:CA:215:C:H2'     | 1:CA:216:U:C6     | 2.39        | 0.57     |
| 23:DB:833:A:C1'    | 37:DL:52:GLY:H    | 2.18        | 0.57     |
| 1:AA:399:G:H2'     | 1:AA:400:C:C6     | 2.40        | 0.57     |
| 26:DD:136:ASN:HD21 | 26:DD:140:HIS:N   | 2.03        | 0.57     |
| 23:BB:2537:U:H2'   | 23:BB:2538:C:C6   | 2.39        | 0.57     |
| 23:DB:2512:C:H2'   | 23:DB:2513:A:O4'  | 2.04        | 0.57     |
| 23:BB:1419:A:H2'   | 23:BB:1421:G:N7   | 2.19        | 0.57     |
| 1:CA:407:U:O2'     | 3:CD:112:GLU:HG3  | 2.04        | 0.57     |
| 25:DC:61:TYR:HA    | 25:DC:85:ASN:HD21 | 1.69        | 0.57     |
| 1:CA:1450:U:H2'    | 1:CA:1452:C:C5    | 2.39        | 0.57     |
| 23:DB:1709:U:H2'   | 23:DB:1710:G:H8   | 1.70        | 0.57     |
| 23:DB:1164:C:H2'   | 23:DB:1165:A:H8   | 1.69        | 0.57     |
| 23:BB:833:A:H1'    | 37:BL:52:GLY:N    | 2.19        | 0.57     |
| 23:DB:1716:U:H2'   | 23:DB:1717:A:H8   | 1.70        | 0.57     |
| 26:DD:15:PHE:HD1   | 26:DD:15:PHE:H    | 1.52        | 0.57     |
| 14:AO:35:GLN:O     | 14:AO:39:LEU:HD13 | 2.05        | 0.57     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 48:BG:87:GLN:HG2   | 48:BG:164:ALA:HA   | 1.86        | 0.57     |
| 20:CB:62:ARG:H     | 20:CB:62:ARG:HD2   | 1.70        | 0.57     |
| 23:DB:1015:U:H2'   | 23:DB:1016:G:C8    | 2.39        | 0.57     |
| 23:DB:576:U:H2'    | 23:DB:577:G:C8     | 2.39        | 0.57     |
| 1:CA:414:A:H2'     | 1:CA:415:A:O4'     | 2.04        | 0.57     |
| 40:BH:130:VAL:HG21 | 40:BH:144:VAL:HG23 | 1.87        | 0.57     |
| 44:DQ:86:SER:HB2   | 49:DR:50:GLY:O     | 2.04        | 0.57     |
| 7:AH:87:ARG:H      | 7:AH:90:GLU:HB3    | 1.70        | 0.57     |
| 3:CD:28:ASP:HB2    | 3:CD:33:ILE:HG21   | 1.85        | 0.57     |
| 40:DH:127:GLU:HB2  | 40:DH:143:ILE:CG2  | 2.33        | 0.57     |
| 47:BF:78:ILE:HD12  | 47:BF:78:ILE:N     | 2.19        | 0.57     |
| 38:BM:34:LYS:HE2   | 38:BM:99:GLY:HA2   | 1.87        | 0.57     |
| 47:DF:168:LEU:HD13 | 47:DF:169:LEU:N    | 2.19        | 0.57     |
| 50:DT:38:ALA:HB1   | 50:DT:43:ILE:HD11  | 1.85        | 0.57     |
| 6:CG:110:ARG:HB2   | 6:CG:118:ARG:HB3   | 1.87        | 0.57     |
| 23:DB:2267:A:C3'   | 23:DB:2267:A:H8    | 2.10        | 0.57     |
| 35:DV:48:MET:O     | 35:DV:51:GLN:HG3   | 2.03        | 0.57     |
| 23:DB:2106:U:O2    | 23:DB:2106:U:H2'   | 2.03        | 0.57     |
| 49:DR:40:MET:HG3   | 49:DR:48:LYS:HA    | 1.87        | 0.57     |
| 1:CA:313:A:H2'     | 1:CA:314:C:C6      | 2.39        | 0.57     |
| 23:BB:1725:U:O2'   | 23:BB:1726:C:H5'   | 2.04        | 0.57     |
| 1:CA:268:U:H2'     | 1:CA:269:C:C6      | 2.39        | 0.57     |
| 1:AA:272:C:H2'     | 1:AA:273:U:H6      | 1.68        | 0.57     |
| 23:BB:155:A:H2'    | 23:BB:156:A:C8     | 2.40        | 0.57     |
| 23:BB:2557:G:H2'   | 23:BB:2558:C:H6    | 1.66        | 0.57     |
| 6:CG:63:VAL:HA     | 6:CG:66:GLU:CD     | 2.25        | 0.57     |
| 23:DB:2841:C:H2'   | 23:DB:2842:G:H8    | 1.69        | 0.57     |
| 43:DO:47:VAL:HG12  | 43:DO:48:LEU:N     | 2.18        | 0.57     |
| 1:CA:1513:A:H2'    | 1:CA:1514:G:H8     | 1.70        | 0.57     |
| 23:BB:1259:G:H2'   | 23:BB:1260:A:C8    | 2.40        | 0.57     |
| 23:DB:2370:G:H2'   | 23:DB:2371:G:O4'   | 2.03        | 0.57     |
| 24:BI:109:ALA:HB1  | 24:BI:124:MET:HG3  | 1.86        | 0.57     |
| 1:AA:1450:U:H2'    | 1:AA:1452:C:C5     | 2.39        | 0.57     |
| 2:AC:14:VAL:O      | 2:AC:15:LYS:HD2    | 2.04        | 0.57     |
| 41:DJ:105:VAL:O    | 41:DJ:109:LEU:HG   | 2.04        | 0.57     |
| 23:DB:1927:A:O2'   | 23:DB:1928:A:H5'   | 2.03        | 0.57     |
| 23:DB:2633:G:H2'   | 23:DB:2634:A:O4'   | 2.05        | 0.57     |
| 1:AA:204:G:H1'     | 1:AA:466:A:N7      | 2.20        | 0.57     |
| 23:DB:2648:G:H2'   | 23:DB:2649:C:O4'   | 2.04        | 0.57     |
| 23:BB:2322:A:N6    | 23:BB:2333:A:H62   | 2.02        | 0.57     |
| 23:BB:111:A:O2'    | 23:BB:112:U:H5'    | 2.04        | 0.57     |
| 23:DB:1760:C:H2'   | 23:DB:1761:C:O4'   | 2.04        | 0.57     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 45:DS:5:ALA:HB3    | 45:DS:54:ALA:HB2   | 1.85        | 0.57     |
| 52:BW:23:LYS:NZ    | 52:BW:24:ARG:HG3   | 2.20        | 0.57     |
| 52:BW:33:GLY:O     | 52:BW:34:SER:HB2   | 2.04        | 0.57     |
| 23:DB:2327:A:H2'   | 23:DB:2328:A:C8    | 2.39        | 0.57     |
| 47:BF:65:LEU:N     | 47:BF:88:VAL:HG22  | 2.16        | 0.57     |
| 26:BD:107:VAL:HA   | 26:BD:204:LYS:O    | 2.04        | 0.57     |
| 53:D6:80:GLU:OE1   | 53:D6:99:LEU:HD22  | 2.05        | 0.57     |
| 26:DD:109:VAL:HG11 | 26:DD:193:VAL:HG11 | 1.85        | 0.57     |
| 44:BQ:57:ARG:HH11  | 44:BQ:57:ARG:HG2   | 1.68        | 0.57     |
| 47:DF:149:ARG:HA   | 47:DF:149:ARG:NH1  | 2.19        | 0.57     |
| 29:BE:58:LYS:C     | 29:BE:60:TRP:N     | 2.57        | 0.57     |
| 23:BB:2389:G:C5'   | 23:BB:2390:U:H5'   | 2.33        | 0.57     |
| 1:CA:699:C:C2'     | 1:CA:700:G:H5''    | 2.33        | 0.57     |
| 23:DB:2264:C:H41   | 52:DW:11:ASN:ND2   | 2.02        | 0.57     |
| 24:DI:125:THR:O    | 24:DI:129:GLU:HG3  | 2.05        | 0.57     |
| 23:DB:1688:U:O2    | 23:DB:1700:A:H5'   | 2.05        | 0.57     |
| 46:BU:34:ILE:HG12  | 46:BU:63:ALA:CB    | 2.34        | 0.57     |
| 23:BB:1794:A:H2'   | 23:BB:1795:C:C6    | 2.39        | 0.57     |
| 23:BB:1805:A:N3    | 25:BC:49:THR:CG2   | 2.68        | 0.57     |
| 23:DB:540:C:H2'    | 23:DB:541:A:C8     | 2.39        | 0.57     |
| 30:BY:50:VAL:O     | 30:BY:54:VAL:HG22  | 2.04        | 0.57     |
| 50:DT:54:GLU:HG3   | 50:DT:90:GLY:N     | 2.20        | 0.57     |
| 1:AA:1123:U:O2'    | 1:AA:1124:G:H5'    | 2.05        | 0.57     |
| 39:DX:39:GLN:HB2   | 39:DX:42:LEU:HD22  | 1.86        | 0.57     |
| 40:BH:42:LYS:O     | 40:BH:47:PHE:HB2   | 2.04        | 0.57     |
| 23:DB:2635:A:H4'   | 26:DD:79:LEU:HB2   | 1.87        | 0.57     |
| 1:AA:1008:U:H5''   | 13:AN:23:ARG:NH2   | 2.20        | 0.57     |
| 23:DB:543:G:C6     | 23:DB:544:C:H1'    | 2.39        | 0.57     |
| 1:CA:373:A:H2'     | 1:CA:374:A:H8      | 1.68        | 0.57     |
| 1:CA:451:A:N6      | 1:CA:480:U:H2'     | 2.19        | 0.57     |
| 23:BB:417:C:H2'    | 23:BB:418:C:H6     | 1.68        | 0.57     |
| 23:DB:1061:U:H4'   | 23:DB:1070:A:O3'   | 2.03        | 0.57     |
| 23:BB:1351:C:O2'   | 23:BB:1571:A:H1'   | 2.05        | 0.57     |
| 25:DC:69:ASN:O     | 25:DC:70:LYS:C     | 2.42        | 0.57     |
| 1:CA:1151:A:HO2'   | 1:CA:1152:A:H8     | 1.53        | 0.57     |
| 28:BP:97:TYR:O     | 28:BP:100:ARG:HB2  | 2.04        | 0.57     |
| 22:BA:91:C:H2'     | 22:BA:92:C:H6      | 1.70        | 0.57     |
| 48:BG:174:LYS:NZ   | 48:BG:176:LYS:HG2  | 2.20        | 0.57     |
| 6:AG:23:ALA:O      | 6:AG:26:VAL:HG22   | 2.03        | 0.57     |
| 1:AA:414:A:H2'     | 1:AA:415:A:O4'     | 2.05        | 0.57     |
| 11:AL:122:LYS:HG3  | 11:AL:123:ALA:H    | 1.70        | 0.57     |
| 23:DB:2324:U:H3'   | 23:DB:2325:G:H5''  | 1.85        | 0.57     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:16:C:O2'     | 23:BB:17:G:H5'     | 2.04        | 0.57     |
| 23:DB:2035:G:H4'   | 23:DB:2036:C:OP2   | 2.03        | 0.57     |
| 52:DW:59:PHE:O     | 52:DW:60:ALA:CB    | 2.52        | 0.57     |
| 8:CI:82:ILE:O      | 8:CI:86:LEU:HD13   | 2.04        | 0.57     |
| 44:DQ:96:ASP:C     | 44:DQ:98:ALA:H     | 2.07        | 0.57     |
| 8:AI:20:ILE:HG23   | 8:AI:60:LEU:CD1    | 2.34        | 0.57     |
| 1:AA:1217:C:OP1    | 13:AN:8:ARG:HD2    | 2.03        | 0.57     |
| 37:DL:110:VAL:HB   | 37:DL:127:VAL:HG23 | 1.85        | 0.57     |
| 1:CA:429:U:H1'     | 1:CA:430:A:H5''    | 1.87        | 0.57     |
| 46:BU:83:GLY:O     | 46:BU:93:ARG:HA    | 2.04        | 0.57     |
| 46:DU:81:ARG:HH21  | 46:DU:81:ARG:H     | 1.51        | 0.57     |
| 40:DH:82:SER:OG    | 40:DH:94:ILE:HD11  | 2.05        | 0.57     |
| 23:DB:1021:A:H62   | 23:DB:1141:U:H3    | 1.52        | 0.57     |
| 7:AH:35:ILE:O      | 7:AH:39:LEU:HG     | 2.05        | 0.57     |
| 18:AS:27:LYS:NZ    | 18:AS:27:LYS:HB3   | 2.19        | 0.57     |
| 26:DD:116:LYS:HB2  | 26:DD:165:MET:HB3  | 1.87        | 0.57     |
| 23:DB:2898:U:H2'   | 23:DB:2899:A:H8    | 1.69        | 0.57     |
| 43:BO:11:ALA:HB2   | 43:BO:96:GLY:H     | 1.68        | 0.57     |
| 23:DB:1443:U:H2'   | 23:DB:1444:G:C8    | 2.39        | 0.57     |
| 20:CB:85:SER:O     | 20:CB:86:CYS:HB2   | 2.04        | 0.57     |
| 53:B6:102:ASN:HD22 | 53:B6:102:ASN:H    | 1.51        | 0.57     |
| 1:AA:93:U:H3'      | 1:AA:94:G:H5''     | 1.86        | 0.57     |
| 1:CA:1342:C:H2'    | 1:CA:1343:G:C8     | 2.39        | 0.57     |
| 29:BE:46:GLN:HB2   | 29:BE:87:ALA:O     | 2.05        | 0.57     |
| 1:AA:735:C:O2'     | 1:AA:736:C:H5'     | 2.05        | 0.57     |
| 19:CT:38:ILE:HG12  | 19:CT:85:LEU:HD13  | 1.86        | 0.57     |
| 23:BB:1667:G:OP1   | 27:BK:6:THR:HA     | 2.04        | 0.57     |
| 23:DB:2537:U:H2'   | 23:DB:2538:C:C6    | 2.39        | 0.57     |
| 1:AA:707:U:H2'     | 1:AA:708:C:H6      | 1.70        | 0.57     |
| 52:BW:44:PHE:O     | 52:BW:78:PHE:HA    | 2.05        | 0.57     |
| 23:DB:2182:U:H2'   | 23:DB:2183:A:H8    | 1.69        | 0.57     |
| 23:BB:2290:G:H2'   | 23:BB:2291:U:C6    | 2.39        | 0.57     |
| 21:CU:11:PHE:O     | 21:CU:11:PHE:HD1   | 1.87        | 0.57     |
| 23:DB:950:G:H2'    | 23:DB:951:C:C6     | 2.40        | 0.57     |
| 23:DB:234:U:H2'    | 23:DB:235:U:H6     | 1.69        | 0.57     |
| 37:DL:131:ALA:C    | 37:DL:133:ALA:H    | 2.08        | 0.57     |
| 26:BD:108:ASP:OD2  | 26:BD:173:GLN:HA   | 2.03        | 0.57     |
| 23:DB:2636:C:H4'   | 26:DD:81:GLU:OE2   | 2.03        | 0.57     |
| 1:CA:182:A:O2'     | 1:CA:183:C:H5''    | 2.04        | 0.57     |
| 24:DI:37:PHE:CZ    | 24:DI:58:ILE:HD11  | 2.39        | 0.57     |
| 19:CT:27:MET:O     | 19:CT:31:ILE:HG13  | 2.05        | 0.57     |
| 1:CA:128:G:H2'     | 1:CA:129:A:C8      | 2.40        | 0.57     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 46:DU:25:LYS:HE3   | 46:DU:36:GLU:HG3   | 1.86        | 0.57     |
| 23:DB:392:U:O2'    | 23:DB:393:C:H5'    | 2.05        | 0.57     |
| 40:BH:27:ARG:H     | 40:BH:31:VAL:HG21  | 1.69        | 0.57     |
| 27:DK:35:VAL:HG12  | 27:DK:69:VAL:CG2   | 2.35        | 0.57     |
| 53:D6:59:THR:O     | 53:D6:61:PRO:HD3   | 2.05        | 0.57     |
| 8:AI:23:GLY:N      | 8:AI:60:LEU:HA     | 2.20        | 0.57     |
| 25:BC:69:ASN:O     | 25:BC:70:LYS:C     | 2.42        | 0.57     |
| 25:BC:94:LEU:HB2   | 25:BC:100:ARG:CD   | 2.35        | 0.57     |
| 37:DL:79:LEU:HB3   | 37:DL:115:GLU:O    | 2.05        | 0.57     |
| 22:BA:28:C:OP1     | 43:BO:31:THR:HG21  | 2.05        | 0.57     |
| 3:AD:28:ASP:HB2    | 3:AD:33:ILE:HG21   | 1.85        | 0.57     |
| 24:DI:71:LYS:HB3   | 24:DI:115:ASP:OD2  | 2.04        | 0.57     |
| 37:BL:57:LEU:C     | 37:BL:59:ARG:H     | 2.07        | 0.57     |
| 10:AK:111:ASP:HB2  | 21:AU:19:LYS:CE    | 2.33        | 0.57     |
| 18:CS:15:LEU:O     | 18:CS:18:VAL:HG12  | 2.05        | 0.57     |
| 37:BL:17:LYS:HD2   | 37:BL:19:LEU:HD11  | 1.86        | 0.57     |
| 37:DL:57:LEU:C     | 37:DL:59:ARG:H     | 2.08        | 0.57     |
| 31:B0:48:TYR:CG    | 31:B0:49:ARG:N     | 2.72        | 0.57     |
| 29:BE:151:GLY:CA   | 29:BE:195:GLN:HE22 | 2.18        | 0.57     |
| 35:DV:30:ILE:HG12  | 35:DV:91:PHE:HB2   | 1.85        | 0.57     |
| 27:DK:71:ARG:HB3   | 27:DK:72:PRO:HD2   | 1.86        | 0.57     |
| 23:BB:591:U:H1'    | 34:B3:1:PRO:N      | 2.19        | 0.57     |
| 24:DI:45:THR:CA    | 24:DI:48:ILE:HG22  | 2.33        | 0.57     |
| 29:DE:150:THR:HG21 | 29:DE:153:LEU:HA   | 1.85        | 0.57     |
| 46:DU:11:ILE:CG2   | 46:DU:70:ALA:HB3   | 2.34        | 0.57     |
| 31:D0:33:SER:C     | 31:D0:35:GLU:H     | 2.08        | 0.57     |
| 3:CD:196:GLU:O     | 3:CD:199:ILE:HG12  | 2.05        | 0.57     |
| 36:B2:33:ARG:HH21  | 36:B2:33:ARG:HB2   | 1.70        | 0.57     |
| 8:CI:123:ARG:HB3   | 8:CI:123:ARG:NH1   | 2.20        | 0.57     |
| 12:CM:90:HIS:HA    | 12:CM:108:ARG:HH22 | 1.69        | 0.57     |
| 23:BB:2615:U:C2    | 31:B0:3:GLN:HA     | 2.39        | 0.57     |
| 46:BU:11:ILE:CG2   | 46:BU:70:ALA:HB3   | 2.34        | 0.57     |
| 23:BB:1487:U:H2'   | 23:BB:1488:C:C6    | 2.40        | 0.57     |
| 24:BI:105:LEU:HD11 | 24:BI:139:VAL:CG1  | 2.34        | 0.57     |
| 29:DE:46:GLN:HB2   | 29:DE:87:ALA:O     | 2.04        | 0.57     |
| 20:AB:83:ALA:HB3   | 20:AB:90:PHE:HB3   | 1.87        | 0.57     |
| 1:AA:1009:U:H5'    | 1:AA:1010:U:OP2    | 2.04        | 0.57     |
| 39:BX:9:LYS:O      | 39:BX:13:GLU:HG2   | 2.04        | 0.57     |
| 23:BB:2188:U:H2'   | 23:BB:2189:U:C6    | 2.40        | 0.57     |
| 1:CA:1468:A:O2'    | 1:CA:1469:C:H5'    | 2.05        | 0.57     |
| 23:DB:417:C:H2'    | 23:DB:418:C:H6     | 1.68        | 0.57     |
| 42:DN:61:ALA:C     | 42:DN:63:ARG:H     | 2.08        | 0.57     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2487:G:H2'   | 23:DB:2488:G:H8    | 1.70        | 0.57     |
| 23:DB:222:A:N6     | 23:DB:232:G:H1'    | 2.20        | 0.57     |
| 23:BB:833:A:H1'    | 37:BL:52:GLY:H     | 1.69        | 0.57     |
| 24:DI:99:LYS:HD3   | 24:DI:99:LYS:H     | 1.69        | 0.57     |
| 51:BZ:41:GLU:O     | 51:BZ:44:LYS:HD2   | 2.05        | 0.57     |
| 1:CA:903:G:O2'     | 1:CA:904:U:H5'     | 2.05        | 0.57     |
| 25:BC:270:ARG:HB3  | 25:BC:270:ARG:NH1  | 2.20        | 0.57     |
| 23:BB:485:C:O2'    | 23:BB:486:C:H5'    | 2.03        | 0.57     |
| 23:BB:1760:C:H2'   | 23:BB:1761:C:O4'   | 2.05        | 0.57     |
| 1:AA:545:C:H5''    | 3:AD:68:GLU:HG2    | 1.85        | 0.57     |
| 23:BB:1647:U:H3'   | 23:BB:1647:U:P     | 2.44        | 0.57     |
| 23:DB:127:A:N7     | 36:D2:46:LYS:HE2   | 2.20        | 0.57     |
| 40:DH:32:PRO:O     | 40:DH:33:GLN:HB2   | 2.04        | 0.57     |
| 48:BG:68:ARG:HH12  | 48:BG:72:ASN:ND2   | 2.02        | 0.57     |
| 26:BD:32:ASN:HA    | 26:BD:51:THR:O     | 2.05        | 0.57     |
| 53:B6:59:THR:HG23  | 53:B6:67:VAL:CG2   | 2.35        | 0.57     |
| 47:DF:115:GLY:HA2  | 47:DF:177:ARG:HH11 | 1.67        | 0.57     |
| 23:BB:1021:A:H62   | 23:BB:1141:U:H3    | 1.52        | 0.57     |
| 8:AI:79:ARG:O      | 8:AI:83:THR:HG22   | 2.04        | 0.57     |
| 38:DM:34:LYS:HE2   | 38:DM:99:GLY:HA2   | 1.85        | 0.57     |
| 44:BQ:91:ARG:CZ    | 49:BR:11:GLN:H     | 2.18        | 0.57     |
| 23:BB:988:A:P      | 30:BY:11:SER:HB3   | 2.45        | 0.57     |
| 47:DF:141:ASP:CB   | 47:DF:144:LYS:HB2  | 2.35        | 0.57     |
| 23:BB:1119:U:OP1   | 35:BV:83:LYS:HE3   | 2.04        | 0.57     |
| 1:AA:1319:A:H3'    | 18:AS:2:ARG:HA     | 1.86        | 0.57     |
| 23:BB:2867:G:N3    | 23:BB:2867:G:C2'   | 2.68        | 0.57     |
| 50:DT:50:LEU:HD22  | 50:DT:50:LEU:H     | 1.70        | 0.57     |
| 7:CH:35:ILE:O      | 7:CH:39:LEU:HG     | 2.04        | 0.57     |
| 23:BB:587:C:O2'    | 37:BL:19:LEU:HD13  | 2.05        | 0.57     |
| 11:CL:86:VAL:HB    | 11:CL:89:LEU:HB2   | 1.86        | 0.57     |
| 23:BB:2264:C:H41   | 52:BW:11:ASN:HD21  | 1.52        | 0.57     |
| 29:BE:188:MET:HG2  | 29:BE:193:VAL:HG22 | 1.87        | 0.57     |
| 1:AA:1370:G:O2'    | 1:AA:1371:G:H5'    | 2.05        | 0.57     |
| 23:DB:2379:G:H5'   | 43:DO:21:LEU:CD1   | 2.33        | 0.57     |
| 35:DV:80:HIS:HB3   | 35:DV:83:LYS:O     | 2.05        | 0.57     |
| 23:BB:1080:A:H2'   | 23:BB:1081:U:H6    | 1.70        | 0.57     |
| 45:BS:56:ALA:O     | 45:BS:59:GLU:HB2   | 2.04        | 0.57     |
| 29:DE:145:ASP:HB3  | 29:DE:184:ASP:HB2  | 1.87        | 0.57     |
| 29:DE:115:GLN:HE22 | 37:DL:2:ARG:HD3    | 1.68        | 0.57     |
| 38:BM:126:ILE:HG22 | 38:BM:127:LYS:N    | 2.18        | 0.57     |
| 23:DB:1338:G:H4'   | 50:DT:18:GLU:CG    | 2.34        | 0.57     |
| 4:AE:155:LYS:O     | 4:AE:158:LYS:HE3   | 2.04        | 0.57     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:268:U:H2'    | 1:AA:269:C:C6      | 2.38        | 0.57     |
| 23:BB:1789:A:OP2  | 25:BC:220:ARG:HD3  | 2.04        | 0.57     |
| 23:DB:1725:U:O2'  | 23:DB:1726:C:H5'   | 2.05        | 0.57     |
| 22:BA:13:G:C2'    | 22:BA:14:U:H5''    | 2.33        | 0.57     |
| 23:DB:2028:U:H2'  | 23:DB:2029:G:C8    | 2.39        | 0.57     |
| 6:CG:129:ASN:HA   | 6:CG:134:VAL:HG21  | 1.87        | 0.57     |
| 1:AA:1513:A:H2'   | 1:AA:1514:G:H8     | 1.67        | 0.57     |
| 1:AA:214:C:H2'    | 1:AA:215:C:C6      | 2.39        | 0.57     |
| 14:AO:8:THR:O     | 14:AO:12:VAL:HG23  | 2.04        | 0.57     |
| 52:BW:44:PHE:HB3  | 52:BW:78:PHE:CD1   | 2.40        | 0.57     |
| 1:AA:1308:U:OP2   | 12:AM:97:ARG:HD3   | 2.05        | 0.57     |
| 3:CD:39:GLN:HG3   | 3:CD:40:HIS:N      | 2.19        | 0.57     |
| 43:BO:79:ALA:HA   | 43:BO:115:LEU:HD23 | 1.87        | 0.57     |
| 1:CA:692:U:H2'    | 1:CA:694:A:OP2     | 2.05        | 0.57     |
| 23:BB:1636:U:H2'  | 23:BB:1637:A:C8    | 2.39        | 0.57     |
| 23:BB:1930:G:H2'  | 23:BB:1968:G:C6    | 2.38        | 0.57     |
| 23:DB:1709:U:H2'  | 23:DB:1710:G:C8    | 2.40        | 0.57     |
| 2:AC:13:ILE:O     | 2:AC:14:VAL:HG22   | 2.05        | 0.57     |
| 23:BB:2333:A:H5'  | 23:BB:2335:A:H1'   | 1.87        | 0.57     |
| 28:DP:30:TRP:HD1  | 28:DP:39:LEU:HG    | 1.70        | 0.57     |
| 23:BB:2660:A:H2'  | 23:BB:2661:G:C8    | 2.40        | 0.57     |
| 2:CC:16:PRO:HG2   | 2:CC:53:ARG:NH2    | 2.20        | 0.57     |
| 23:DB:956:G:OP2   | 38:DM:86:LYS:HE2   | 2.05        | 0.57     |
| 23:BB:1534:U:H6   | 23:BB:1534:U:O5'   | 1.88        | 0.57     |
| 23:BB:2804:U:H2'  | 23:BB:2805:C:C6    | 2.39        | 0.57     |
| 23:BB:2035:G:H4'  | 23:BB:2036:C:OP2   | 2.04        | 0.57     |
| 20:AB:202:ASN:C   | 20:AB:202:ASN:HD22 | 2.07        | 0.57     |
| 53:D6:30:THR:C    | 53:D6:32:ARG:H     | 2.07        | 0.57     |
| 52:DW:23:LYS:O    | 52:DW:66:VAL:HB    | 2.04        | 0.57     |
| 8:CI:70:GLY:O     | 8:CI:74:GLN:HB2    | 2.04        | 0.57     |
| 26:DD:104:VAL:HA  | 26:DD:106:LYS:HZ3  | 1.70        | 0.57     |
| 23:DB:633:A:O5'   | 23:DB:633:A:H8     | 1.87        | 0.57     |
| 43:DO:51:ALA:O    | 43:DO:74:VAL:HG13  | 2.05        | 0.57     |
| 7:AH:100:ILE:HG13 | 7:AH:128:VAL:O     | 2.05        | 0.57     |
| 46:DU:73:ASN:C    | 46:DU:75:ALA:H     | 2.08        | 0.57     |
| 40:DH:80:ILE:HD11 | 40:DH:146:VAL:HA   | 1.87        | 0.57     |
| 47:DF:131:VAL:C   | 47:DF:133:GLU:H    | 2.07        | 0.57     |
| 35:BV:80:HIS:HB3  | 35:BV:83:LYS:O     | 2.05        | 0.57     |
| 1:CA:1226:C:H2'   | 12:CM:101:THR:OG1  | 2.04        | 0.57     |
| 1:CA:1360:A:H2'   | 1:CA:1361:G:O4'    | 2.05        | 0.57     |
| 50:DT:40:LYS:HG2  | 50:DT:60:THR:HG23  | 1.87        | 0.57     |
| 32:D4:7:VAL:HG23  | 32:D4:35:GLN:CB    | 2.32        | 0.57     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:546:U:H5'    | 23:BB:548:G:O6     | 2.05        | 0.57     |
| 1:CA:719:C:O2'     | 17:CR:37:LYS:HB2   | 2.05        | 0.57     |
| 23:DB:2723:C:H5''  | 42:DN:1:MET:HE2    | 1.87        | 0.57     |
| 23:DB:1283:G:N2    | 23:DB:1285:A:H3'   | 2.20        | 0.57     |
| 23:BB:513:A:O5'    | 23:BB:513:A:H8     | 1.88        | 0.57     |
| 44:DQ:10:ARG:HB2   | 44:DQ:10:ARG:CZ    | 2.33        | 0.57     |
| 23:BB:1443:U:H2'   | 23:BB:1444:G:C8    | 2.40        | 0.57     |
| 20:AB:103:TRP:O    | 20:AB:107:ARG:HG2  | 2.05        | 0.57     |
| 1:CA:1301:U:H2'    | 1:CA:1301:U:O2     | 2.04        | 0.57     |
| 23:DB:151:C:H2'    | 23:DB:152:A:H8     | 1.68        | 0.57     |
| 23:BB:2216:G:H2'   | 23:BB:2217:G:C8    | 2.39        | 0.57     |
| 1:CA:394:G:H2'     | 1:CA:395:C:C6      | 2.39        | 0.57     |
| 23:BB:2099:U:H2'   | 23:BB:2100:G:H8    | 1.70        | 0.57     |
| 23:DB:936:A:H2'    | 23:DB:937:C:C6     | 2.39        | 0.57     |
| 26:BD:117:GLY:HA2  | 26:BD:164:GLN:CD   | 2.25        | 0.57     |
| 23:BB:2496:C:OP1   | 38:BM:82:MET:HB2   | 2.05        | 0.57     |
| 23:DB:1164:C:H2'   | 23:DB:1165:A:C8    | 2.40        | 0.57     |
| 23:DB:993:G:H1'    | 49:DR:91:GLN:NE2   | 2.19        | 0.57     |
| 23:BB:1716:U:H2'   | 23:BB:1717:A:H8    | 1.70        | 0.57     |
| 13:AN:14:ALA:O     | 13:AN:18:LYS:HG3   | 2.05        | 0.57     |
| 23:BB:1475:G:H4'   | 23:BB:1476:U:O5'   | 2.05        | 0.57     |
| 29:BE:31:VAL:HG21  | 29:BE:104:ALA:HB2  | 1.86        | 0.57     |
| 23:BB:1120:G:O2'   | 23:BB:1121:C:H5'   | 2.04        | 0.57     |
| 23:DB:485:C:O2'    | 23:DB:486:C:H5'    | 2.04        | 0.57     |
| 15:CP:20:VAL:HG23  | 15:CP:34:GLU:O     | 2.05        | 0.57     |
| 23:DB:1859:U:H2'   | 23:DB:1860:G:C8    | 2.40        | 0.57     |
| 23:BB:2633:G:H2'   | 23:BB:2634:A:O4'   | 2.05        | 0.57     |
| 52:BW:39:GLN:HG2   | 52:BW:40:ARG:H     | 1.69        | 0.56     |
| 52:BW:23:LYS:O     | 52:BW:66:VAL:HB    | 2.04        | 0.56     |
| 25:DC:143:VAL:HG12 | 25:DC:144:GLU:H    | 1.68        | 0.56     |
| 44:BQ:29:ARG:HH11  | 44:BQ:29:ARG:HG2   | 1.69        | 0.56     |
| 22:BA:43:C:H1'     | 47:BF:91:ARG:NH2   | 2.20        | 0.56     |
| 40:BH:133:GLN:HA   | 40:BH:139:PHE:CB   | 2.35        | 0.56     |
| 40:BH:134:VAL:HG22 | 40:BH:135:HIS:N    | 2.17        | 0.56     |
| 53:D6:56:ALA:HB1   | 53:D6:70:SER:HB2   | 1.87        | 0.56     |
| 53:D6:70:SER:HB3   | 53:D6:76:LEU:CD2   | 2.35        | 0.56     |
| 52:DW:48:ALA:HB3   | 52:DW:81:ILE:O     | 2.05        | 0.56     |
| 20:CB:202:ASN:C    | 20:CB:202:ASN:HD22 | 2.08        | 0.56     |
| 7:CH:87:ARG:H      | 7:CH:90:GLU:HB3    | 1.70        | 0.56     |
| 53:B6:126:ARG:HD3  | 53:B6:169:ILE:HD12 | 1.87        | 0.56     |
| 43:DO:88:LYS:HG2   | 43:DO:89:ASP:N     | 2.20        | 0.56     |
| 35:BV:80:HIS:CD2   | 35:BV:83:LYS:H     | 2.23        | 0.56     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:138:U:H4'    | 23:DB:139:U:H2'    | 1.86        | 0.56     |
| 50:DT:55:VAL:HG13  | 50:DT:85:VAL:HG12  | 1.87        | 0.56     |
| 45:DS:52:GLU:HA    | 45:DS:55:ILE:CG2   | 2.33        | 0.56     |
| 6:CG:107:ALA:O     | 6:CG:110:ARG:HB2   | 2.05        | 0.56     |
| 27:DK:20:MET:C     | 27:DK:41:ILE:HD12  | 2.25        | 0.56     |
| 29:DE:151:GLY:CA   | 29:DE:195:GLN:HE22 | 2.18        | 0.56     |
| 42:BN:32:GLU:O     | 42:BN:114:GLU:HA   | 2.05        | 0.56     |
| 35:BV:30:ILE:HD12  | 35:BV:38:LEU:HD23  | 1.87        | 0.56     |
| 1:AA:1390:U:H2'    | 1:AA:1391:U:C6     | 2.40        | 0.56     |
| 9:CJ:14:ASP:OD1    | 9:CJ:17:LEU:HB2    | 2.05        | 0.56     |
| 23:BB:192:C:H2'    | 23:BB:193:U:H5'    | 1.86        | 0.56     |
| 23:DB:419:U:H2'    | 23:DB:420:C:C6     | 2.39        | 0.56     |
| 36:D2:30:VAL:HA    | 36:D2:33:ARG:HH22  | 1.68        | 0.56     |
| 26:DD:33:ARG:NE    | 26:DD:74:GLU:HB3   | 2.20        | 0.56     |
| 2:AC:156:LEU:HD11  | 2:AC:165:GLU:HB2   | 1.87        | 0.56     |
| 23:BB:2847:U:H5''  | 28:BP:94:ALA:CB    | 2.34        | 0.56     |
| 1:AA:68:G:H2'      | 1:AA:69:G:O4'      | 2.05        | 0.56     |
| 23:BB:2457:U:C2'   | 23:BB:2458:G:H5'   | 2.35        | 0.56     |
| 52:DW:77:LYS:HZ2   | 52:DW:77:LYS:H     | 1.51        | 0.56     |
| 23:BB:2880:C:C1'   | 42:BN:91:ALA:HB3   | 2.34        | 0.56     |
| 23:DB:2577:A:H5''  | 23:DB:2578:G:H5'   | 1.87        | 0.56     |
| 23:BB:1046:A:H3'   | 23:BB:1047:G:H5''  | 1.87        | 0.56     |
| 41:DJ:103:ILE:HA   | 41:DJ:106:LYS:HB3  | 1.87        | 0.56     |
| 23:BB:2648:G:H2'   | 23:BB:2649:C:O4'   | 2.04        | 0.56     |
| 49:BR:36:ALA:HA    | 49:BR:58:VAL:HA    | 1.87        | 0.56     |
| 28:BP:103:THR:HG22 | 28:BP:104:GLY:H    | 1.70        | 0.56     |
| 23:DB:2708:G:H2'   | 23:DB:2709:G:H8    | 1.69        | 0.56     |
| 22:DA:109:A:H2'    | 22:DA:110:C:C6     | 2.40        | 0.56     |
| 7:CH:37:ASN:O      | 7:CH:41:GLU:HG2    | 2.05        | 0.56     |
| 9:AJ:80:THR:HB     | 9:AJ:83:THR:OG1    | 2.03        | 0.56     |
| 27:BK:109:SER:HB2  | 27:BK:111:LYS:HE2  | 1.87        | 0.56     |
| 23:DB:460:A:H2'    | 23:DB:461:C:O4'    | 2.05        | 0.56     |
| 1:CA:1488:G:H2'    | 1:CA:1489:G:H8     | 1.70        | 0.56     |
| 30:DY:21:ALA:O     | 30:DY:24:LEU:HB3   | 2.04        | 0.56     |
| 23:DB:1098:A:C3'   | 24:DI:4:VAL:N      | 2.68        | 0.56     |
| 25:DC:90:ILE:CD1   | 25:DC:102:TYR:HB3  | 2.36        | 0.56     |
| 22:BA:42:C:O4'     | 47:BF:65:LEU:HB2   | 2.05        | 0.56     |
| 53:B6:79:ILE:HA    | 53:B6:82:ALA:HB3   | 1.87        | 0.56     |
| 23:DB:2359:C:H2'   | 23:DB:2360:G:C8    | 2.40        | 0.56     |
| 13:AN:79:SER:OG    | 13:AN:82:LYS:HG2   | 2.05        | 0.56     |
| 23:BB:2393:U:H5'   | 37:BL:60:ARG:O     | 2.06        | 0.56     |
| 9:AJ:57:VAL:HG13   | 9:AJ:58:ASN:N      | 2.20        | 0.56     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 16:AQ:60:ILE:HA   | 16:AQ:75:VAL:HG13 | 1.85        | 0.56     |
| 23:DB:2867:G:N3   | 23:DB:2867:G:C2'  | 2.68        | 0.56     |
| 23:DB:1082:U:O4   | 23:DB:1086:A:C2   | 2.57        | 0.56     |
| 1:CA:1392:G:O2'   | 1:CA:1393:U:H5'   | 2.05        | 0.56     |
| 23:DB:2078:C:H2'  | 23:DB:2079:U:H6   | 1.68        | 0.56     |
| 23:BB:2297:A:N6   | 23:BB:2319:G:H1'  | 2.19        | 0.56     |
| 39:DX:49:ASP:O    | 39:DX:53:VAL:HG23 | 2.05        | 0.56     |
| 23:DB:1203:U:H3'  | 23:DB:1204:A:C5'  | 2.34        | 0.56     |
| 25:DC:245:THR:C   | 25:DC:247:TRP:H   | 2.09        | 0.56     |
| 53:B6:143:LEU:O   | 53:B6:147:LEU:HG  | 2.04        | 0.56     |
| 1:CA:501:C:H1'    | 1:CA:549:C:H1'    | 1.85        | 0.56     |
| 1:CA:369:G:O2'    | 1:CA:370:C:H5'    | 2.05        | 0.56     |
| 23:BB:1166:G:H2'  | 23:BB:1167:C:H6   | 1.70        | 0.56     |
| 23:BB:633:A:O5'   | 23:BB:633:A:H8    | 1.88        | 0.56     |
| 23:DB:2216:G:H2'  | 23:DB:2217:G:C8   | 2.40        | 0.56     |
| 26:BD:125:TRP:CD2 | 26:BD:160:LYS:HB3 | 2.40        | 0.56     |
| 1:AA:562:U:H1'    | 11:AL:11:ARG:HB3  | 1.85        | 0.56     |
| 6:AG:70:PRO:O     | 6:AG:95:ARG:HG3   | 2.06        | 0.56     |
| 23:DB:2438:U:O2'  | 23:DB:2439:A:H5'' | 2.05        | 0.56     |
| 7:AH:113:ARG:HH21 | 7:AH:114:ALA:HA   | 1.70        | 0.56     |
| 1:CA:1095:U:H2'   | 1:CA:1096:C:C6    | 2.40        | 0.56     |
| 44:DQ:40:LYS:HA   | 44:DQ:43:GLN:OE1  | 2.04        | 0.56     |
| 22:BA:109:A:H2'   | 22:BA:110:C:C6    | 2.40        | 0.56     |
| 40:BH:32:PRO:O    | 40:BH:33:GLN:HB2  | 2.03        | 0.56     |
| 52:BW:59:PHE:O    | 52:BW:60:ALA:CB   | 2.52        | 0.56     |
| 41:BJ:36:LEU:HD12 | 41:BJ:118:MET:O   | 2.04        | 0.56     |
| 44:DQ:91:ARG:CZ   | 49:DR:11:GLN:H    | 2.18        | 0.56     |
| 8:AI:46:VAL:O     | 8:AI:79:ARG:HG3   | 2.05        | 0.56     |
| 1:AA:1348:U:C4'   | 8:AI:121:ARG:HG3  | 2.27        | 0.56     |
| 26:DD:7:LYS:HB2   | 26:DD:77:ARG:NH1  | 2.18        | 0.56     |
| 26:DD:4:LEU:HD23  | 26:DD:101:PHE:CE1 | 2.40        | 0.56     |
| 47:DF:41:GLU:O    | 47:DF:43:ILE:HG22 | 2.05        | 0.56     |
| 22:DA:27:C:N4     | 22:DA:28:C:N4     | 2.54        | 0.56     |
| 7:AH:94:VAL:HG12  | 7:AH:99:GLY:HA3   | 1.87        | 0.56     |
| 50:BT:40:LYS:HG2  | 50:BT:60:THR:HG23 | 1.87        | 0.56     |
| 1:CA:1296:C:H4'   | 1:CA:1302:C:N4    | 2.13        | 0.56     |
| 25:DC:76:VAL:CG1  | 25:DC:114:GLN:HG2 | 2.32        | 0.56     |
| 25:DC:94:LEU:HB2  | 25:DC:100:ARG:CD  | 2.35        | 0.56     |
| 22:DA:2:G:O2'     | 22:DA:3:C:H5'     | 2.05        | 0.56     |
| 42:BN:38:LEU:O    | 42:BN:42:LYS:HG3  | 2.06        | 0.56     |
| 12:CM:44:ILE:HA   | 12:CM:47:LEU:CD1  | 2.36        | 0.56     |
| 43:DO:88:LYS:HG2  | 43:DO:89:ASP:H    | 1.70        | 0.56     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 47:DF:11:VAL:HG21 | 47:DF:172:PHE:CE1  | 2.40        | 0.56     |
| 47:DF:137:PHE:HB2 | 47:DF:138:PRO:CD   | 2.33        | 0.56     |
| 35:BV:44:HIS:HE1  | 35:BV:86:LEU:H     | 1.51        | 0.56     |
| 1:CA:1080:A:H2'   | 1:CA:1081:A:H5'    | 1.87        | 0.56     |
| 1:CA:922:G:H2'    | 1:CA:923:A:C8      | 2.40        | 0.56     |
| 10:AK:22:ILE:HD13 | 10:AK:95:THR:CG2   | 2.35        | 0.56     |
| 43:DO:26:LEU:HB2  | 43:DO:39:VAL:HG22  | 1.88        | 0.56     |
| 6:AG:114:SER:O    | 6:AG:118:ARG:HG3   | 2.05        | 0.56     |
| 52:BW:10:ARG:O    | 52:BW:11:ASN:HB2   | 2.06        | 0.56     |
| 21:CU:19:LYS:HD3  | 21:CU:20:ARG:HH21  | 1.69        | 0.56     |
| 23:DB:979:A:H3'   | 23:DB:980:A:C5'    | 2.35        | 0.56     |
| 23:DB:1655:A:H2'  | 23:DB:1656:C:O4'   | 2.05        | 0.56     |
| 23:DB:2722:G:O2'  | 23:DB:2723:C:H5'   | 2.06        | 0.56     |
| 29:DE:189:THR:O   | 29:DE:193:VAL:HG23 | 2.04        | 0.56     |
| 31:D0:41:HIS:HB2  | 42:DN:99:LYS:O     | 2.05        | 0.56     |
| 40:DH:14:SER:HB2  | 40:DH:17:ASP:CB    | 2.35        | 0.56     |
| 1:CA:909:A:H2'    | 1:CA:910:C:O4'     | 2.06        | 0.56     |
| 44:BQ:104:ALA:O   | 44:BQ:105:PHE:HB3  | 2.05        | 0.56     |
| 49:BR:39:LEU:O    | 49:BR:40:MET:HB2   | 2.04        | 0.56     |
| 36:B2:21:ARG:HH21 | 36:B2:43:THR:CG2   | 2.17        | 0.56     |
| 1:AA:1071:C:H2'   | 1:AA:1072:G:C8     | 2.39        | 0.56     |
| 2:CC:129:PHE:CD2  | 2:CC:156:LEU:HD22  | 2.40        | 0.56     |
| 23:BB:2135:A:C2   | 23:BB:2136:G:H1'   | 2.40        | 0.56     |
| 12:AM:95:PRO:N    | 12:AM:108:ARG:HG2  | 2.20        | 0.56     |
| 23:BB:1785:A:O2'  | 23:BB:1786:A:H5'   | 2.05        | 0.56     |
| 27:DK:87:LEU:HD12 | 27:DK:92:GLU:HA    | 1.87        | 0.56     |
| 23:DB:125:A:C2    | 36:D2:10:LEU:HA    | 2.40        | 0.56     |
| 23:DB:155:A:H2'   | 23:DB:156:A:C8     | 2.40        | 0.56     |
| 23:DB:836:G:H2'   | 23:DB:837:C:H6     | 1.68        | 0.56     |
| 1:AA:193:C:H2'    | 1:AA:194:C:C5      | 2.40        | 0.56     |
| 23:BB:1824:G:OP1  | 25:BC:51:ARG:HD3   | 2.05        | 0.56     |
| 23:DB:1487:U:H2'  | 23:DB:1488:C:C6    | 2.40        | 0.56     |
| 23:DB:1488:C:O2'  | 23:DB:1489:C:H5'   | 2.05        | 0.56     |
| 23:DB:1429:G:H2'  | 23:DB:1430:G:H8    | 1.71        | 0.56     |
| 20:AB:79:VAL:HG12 | 20:AB:90:PHE:HB2   | 1.87        | 0.56     |
| 42:DN:47:VAL:C    | 42:DN:50:PRO:HD2   | 2.25        | 0.56     |
| 39:BX:39:GLN:O    | 39:BX:42:LEU:HB2   | 2.04        | 0.56     |
| 39:BX:39:GLN:HB2  | 39:BX:42:LEU:HD22  | 1.86        | 0.56     |
| 1:AA:394:G:H2'    | 1:AA:395:C:C6      | 2.40        | 0.56     |
| 14:CO:8:THR:O     | 14:CO:12:VAL:HG23  | 2.04        | 0.56     |
| 11:CL:64:SER:OG   | 11:CL:96:THR:HG23  | 2.04        | 0.56     |
| 1:CA:1008:U:H5''  | 13:CN:23:ARG:NH2   | 2.21        | 0.56     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:547:A:H2'    | 23:DB:547:A:N3     | 2.19        | 0.56     |
| 6:AG:4:ARG:HE      | 6:AG:6:ILE:HG23    | 1.69        | 0.56     |
| 20:AB:128:LEU:HD13 | 20:AB:129:THR:H    | 1.69        | 0.56     |
| 23:BB:1374:G:H2'   | 23:BB:1375:U:C6    | 2.40        | 0.56     |
| 23:DB:1923:U:H2'   | 23:DB:1924:C:C6    | 2.40        | 0.56     |
| 25:BC:244:VAL:HB   | 25:BC:249:VAL:N    | 2.20        | 0.56     |
| 23:BB:1403:A:O2'   | 23:BB:1404:C:H5'   | 2.04        | 0.56     |
| 11:CL:7:VAL:HG22   | 16:CQ:33:TYR:HD1   | 1.70        | 0.56     |
| 26:BD:122:VAL:HA   | 26:BD:127:PHE:H    | 1.70        | 0.56     |
| 23:BB:570:G:H2'    | 23:BB:2030:A:N7    | 2.19        | 0.56     |
| 1:CA:796:C:OP1     | 10:CK:127:ARG:HB3  | 2.05        | 0.56     |
| 23:BB:1573:G:H2'   | 23:BB:1574:C:H5'   | 1.88        | 0.56     |
| 1:AA:950:U:H2'     | 1:AA:951:G:H8      | 1.69        | 0.56     |
| 3:AD:39:GLN:HG3    | 3:AD:40:HIS:N      | 2.20        | 0.56     |
| 34:B3:7:ARG:HG3    | 34:B3:7:ARG:NH1    | 2.19        | 0.56     |
| 1:AA:825:A:H2'     | 1:AA:826:C:H6      | 1.70        | 0.56     |
| 1:CA:628:G:O2'     | 1:CA:629:A:H5'     | 2.05        | 0.56     |
| 23:DB:2276:G:OP2   | 38:DM:85:GLY:N     | 2.38        | 0.56     |
| 1:CA:55:A:OP2      | 1:CA:352:C:N4      | 2.37        | 0.56     |
| 1:CA:939:G:H5'     | 6:CG:101:ARG:NH1   | 2.20        | 0.56     |
| 1:CA:54:C:H2'      | 1:CA:352:C:H41     | 1.69        | 0.56     |
| 1:CA:154:U:H2'     | 1:CA:155:A:C8      | 2.39        | 0.56     |
| 23:BB:1164:C:H2'   | 23:BB:1165:A:H8    | 1.70        | 0.56     |
| 5:CF:43:GLY:HA2    | 5:CF:58:HIS:NE2    | 2.21        | 0.56     |
| 21:CU:26:GLY:O     | 21:CU:30:GLU:HB2   | 2.06        | 0.56     |
| 13:CN:14:ALA:O     | 13:CN:18:LYS:HG3   | 2.05        | 0.56     |
| 49:BR:91:GLN:HG3   | 49:BR:92:TRP:H     | 1.70        | 0.56     |
| 23:DB:2691:C:H2'   | 23:DB:2692:G:H8    | 1.70        | 0.56     |
| 29:BE:103:GLY:O    | 29:BE:106:LYS:HB2  | 2.05        | 0.56     |
| 23:BB:1857:G:N2    | 23:BB:1884:G:H2'   | 2.19        | 0.56     |
| 1:AA:1206:G:H2'    | 1:AA:1207:G:O4'    | 2.06        | 0.56     |
| 48:DG:84:LYS:HB3   | 48:DG:132:LEU:O    | 2.05        | 0.56     |
| 26:BD:7:LYS:HB2    | 26:BD:77:ARG:NH1   | 2.17        | 0.56     |
| 8:CI:79:ARG:NH2    | 8:CI:102:PHE:HA    | 2.21        | 0.56     |
| 8:CI:46:VAL:O      | 8:CI:79:ARG:HG3    | 2.05        | 0.56     |
| 8:AI:20:ILE:HG23   | 8:AI:60:LEU:HD11   | 1.87        | 0.56     |
| 8:AI:55:ASP:HB2    | 8:AI:59:LYS:HG3    | 1.87        | 0.56     |
| 26:DD:25:THR:HG21  | 26:DD:193:VAL:HG22 | 1.88        | 0.56     |
| 41:DJ:58:ASN:HA    | 41:DJ:127:GLY:HA3  | 1.86        | 0.56     |
| 50:BT:55:VAL:HG13  | 50:BT:85:VAL:HG12  | 1.88        | 0.56     |
| 33:B1:34:GLU:HA    | 33:B1:48:TYR:O     | 2.06        | 0.56     |
| 47:DF:135:ILE:HD11 | 47:DF:137:PHE:CD1  | 2.40        | 0.56     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:764:C:N4      | 1:CA:812:G:H1     | 2.03        | 0.56     |
| 18:CS:35:ARG:HB3   | 18:CS:50:VAL:CG1  | 2.35        | 0.56     |
| 53:D6:19:GLU:HA    | 53:D6:22:GLU:HG3  | 1.88        | 0.56     |
| 21:CU:19:LYS:HB2   | 21:CU:20:ARG:HE   | 1.69        | 0.56     |
| 23:DB:981:A:H2'    | 23:DB:982:C:H5''  | 1.86        | 0.56     |
| 22:DA:78:A:H2'     | 22:DA:79:G:O4'    | 2.05        | 0.56     |
| 1:CA:719:C:H2'     | 17:CR:38:ILE:CD1  | 2.35        | 0.56     |
| 23:BB:28:A:H61     | 23:BB:512:G:H1'   | 1.69        | 0.56     |
| 1:CA:715:A:H2'     | 1:CA:716:A:C8     | 2.37        | 0.56     |
| 3:CD:201:GLU:OE1   | 4:CE:104:ILE:HG22 | 2.06        | 0.56     |
| 35:DV:28:ALA:HA    | 35:DV:88:HIS:CE1  | 2.40        | 0.56     |
| 1:CA:1123:U:H4'    | 9:CJ:39:PRO:HD2   | 1.87        | 0.56     |
| 1:CA:635:A:H2'     | 1:CA:636:U:H6     | 1.70        | 0.56     |
| 26:BD:136:ASN:HD21 | 26:BD:140:HIS:N   | 2.03        | 0.56     |
| 1:CA:502:A:H2'     | 1:CA:503:C:H6     | 1.71        | 0.56     |
| 50:BT:69:ARG:HB2   | 50:BT:69:ARG:HH11 | 1.70        | 0.56     |
| 26:BD:159:LYS:O    | 26:BD:161:MET:HG2 | 2.05        | 0.56     |
| 10:CK:61:ALA:O     | 10:CK:64:VAL:HG12 | 2.05        | 0.56     |
| 11:AL:7:VAL:HG22   | 16:AQ:33:TYR:HD1  | 1.71        | 0.56     |
| 1:CA:398:U:H2'     | 1:CA:399:G:C8     | 2.40        | 0.56     |
| 41:DJ:93:ILE:O     | 41:DJ:97:PRO:HG3  | 2.05        | 0.56     |
| 1:CA:612:C:H2'     | 1:CA:613:C:C6     | 2.41        | 0.56     |
| 6:CG:35:LYS:O      | 6:CG:39:GLU:HG3   | 2.05        | 0.56     |
| 22:DA:95:U:H2'     | 22:DA:96:G:C8     | 2.39        | 0.56     |
| 23:DB:1881:C:H2'   | 23:DB:1882:U:O4'  | 2.06        | 0.56     |
| 23:DB:1885:A:H3'   | 23:DB:1886:U:C6   | 2.40        | 0.56     |
| 2:CC:13:ILE:H      | 2:CC:13:ILE:HD13  | 1.70        | 0.56     |
| 23:BB:2021:C:OP1   | 31:B0:8:THR:HG21  | 2.05        | 0.56     |
| 33:D1:10:LEU:O     | 33:D1:19:PHE:HB2  | 2.05        | 0.56     |
| 23:BB:549:G:H3'    | 23:BB:549:G:OP2   | 2.06        | 0.56     |
| 1:CA:779:C:H5''    | 10:CK:123:PRO:HB3 | 1.88        | 0.56     |
| 25:BC:221:GLY:C    | 25:BC:223:ALA:H   | 2.09        | 0.56     |
| 44:BQ:24:TYR:O     | 44:BQ:27:ARG:HB2  | 2.06        | 0.56     |
| 53:D6:51:PRO:HB2   | 53:D6:53:ASN:HD21 | 1.70        | 0.56     |
| 23:DB:855:G:N3     | 52:DW:23:LYS:HE3  | 2.21        | 0.56     |
| 53:B6:58:VAL:HG12  | 53:B6:59:THR:N    | 2.20        | 0.56     |
| 25:BC:75:ALA:CB    | 25:BC:95:TYR:HA   | 2.33        | 0.56     |
| 23:DB:673:C:C2'    | 23:DB:674:G:H5'   | 2.36        | 0.56     |
| 29:DE:61:ARG:NH1   | 29:DE:64:GLY:HA3  | 2.21        | 0.56     |
| 42:DN:38:LEU:O     | 42:DN:42:LYS:HG3  | 2.05        | 0.56     |
| 44:BQ:94:LEU:HD21  | 49:BR:11:GLN:HB2  | 1.87        | 0.56     |
| 3:CD:160:LEU:N     | 3:CD:160:LEU:HD13 | 2.18        | 0.56     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 47:BF:168:LEU:HD13 | 47:BF:169:LEU:N    | 2.21        | 0.56     |
| 29:BE:134:LEU:HD21 | 29:BE:161:ALA:HB2  | 1.87        | 0.56     |
| 17:AR:34:GLU:HB2   | 21:AU:18:PHE:CZ    | 2.40        | 0.56     |
| 12:AM:44:ILE:HD12  | 12:AM:45:SER:H     | 1.70        | 0.56     |
| 50:DT:1:MET:C      | 50:DT:2:ILE:HD13   | 2.26        | 0.56     |
| 38:DM:50:ARG:HA    | 38:DM:53:MET:CE    | 2.33        | 0.56     |
| 10:CK:111:ASP:HB2  | 21:CU:19:LYS:CE    | 2.34        | 0.56     |
| 29:BE:189:THR:O    | 29:BE:193:VAL:HG23 | 2.05        | 0.56     |
| 1:CA:1313:U:OP1    | 18:CS:6:LYS:HD3    | 2.06        | 0.56     |
| 45:BS:26:GLY:N     | 45:BS:71:VAL:HG13  | 2.20        | 0.56     |
| 45:BS:27:LYS:H     | 45:BS:27:LYS:HD2   | 1.71        | 0.56     |
| 28:DP:112:ARG:HH11 | 28:DP:112:ARG:HB2  | 1.71        | 0.56     |
| 29:BE:47:LYS:HB3   | 29:BE:51:GLU:HB2   | 1.87        | 0.56     |
| 2:AC:61:LYS:O      | 2:AC:96:VAL:HB     | 2.04        | 0.56     |
| 23:DB:17:G:H2'     | 23:DB:18:U:C6      | 2.41        | 0.56     |
| 11:CL:54:VAL:HG21  | 11:CL:79:ILE:HD11  | 1.87        | 0.56     |
| 52:DW:44:PHE:O     | 52:DW:78:PHE:HA    | 2.05        | 0.56     |
| 25:BC:245:THR:C    | 25:BC:247:TRP:H    | 2.09        | 0.56     |
| 23:BB:309:A:H4'    | 46:BU:15:GLY:HA3   | 1.88        | 0.56     |
| 25:DC:123:ILE:O    | 25:DC:123:ILE:HG13 | 2.04        | 0.56     |
| 1:AA:638:U:H2'     | 1:AA:639:G:O4'     | 2.06        | 0.56     |
| 1:AA:154:U:H2'     | 1:AA:155:A:C8      | 2.40        | 0.56     |
| 23:DB:408:G:O2'    | 23:DB:409:G:H5'    | 2.05        | 0.56     |
| 23:BB:596:U:H2'    | 23:BB:597:G:C8     | 2.41        | 0.56     |
| 23:BB:596:U:H2'    | 23:BB:597:G:H8     | 1.70        | 0.56     |
| 21:AU:26:GLY:O     | 21:AU:30:GLU:HB2   | 2.06        | 0.56     |
| 21:AU:27:VAL:O     | 21:AU:31:VAL:HG23  | 2.05        | 0.56     |
| 1:CA:731:G:O2'     | 1:CA:732:C:H5'     | 2.05        | 0.56     |
| 1:AA:591:U:H2'     | 1:AA:592:G:H8      | 1.70        | 0.56     |
| 23:DB:659:G:H4'    | 29:DE:95:LYS:HB3   | 1.87        | 0.56     |
| 23:BB:2888:C:H2'   | 23:BB:2889:C:C6    | 2.40        | 0.56     |
| 20:AB:156:LEU:HD12 | 20:AB:156:LEU:H    | 1.71        | 0.56     |
| 1:AA:1175:G:O2'    | 1:AA:1176:A:H5'    | 2.05        | 0.56     |
| 23:BB:2902:C:C2    | 23:BB:2903:U:H5    | 2.24        | 0.56     |
| 23:BB:2352:A:H2'   | 23:BB:2353:G:O4'   | 2.06        | 0.56     |
| 23:DB:2386:A:H2'   | 23:DB:2387:U:C6    | 2.40        | 0.56     |
| 52:DW:18:LYS:HG3   | 52:DW:19:ARG:CZ    | 2.35        | 0.56     |
| 48:BG:10:VAL:HG12  | 48:BG:10:VAL:O     | 2.04        | 0.56     |
| 23:DB:1826:G:H2'   | 23:DB:1827:U:H6    | 1.70        | 0.56     |
| 6:AG:145:GLU:C     | 6:AG:147:ASN:H     | 2.08        | 0.56     |
| 16:CQ:60:ILE:HA    | 16:CQ:75:VAL:HG13  | 1.87        | 0.56     |
| 53:D6:32:ARG:O     | 53:D6:103:ILE:HG12 | 2.06        | 0.56     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 53:D6:80:GLU:HG3  | 53:D6:92:PRO:HB3   | 1.86        | 0.56     |
| 41:BJ:58:ASN:HA   | 41:BJ:127:GLY:HA3  | 1.86        | 0.56     |
| 41:BJ:127:GLY:O   | 41:BJ:128:ASN:HB2  | 2.04        | 0.56     |
| 7:AH:86:LYS:HB3   | 7:AH:90:GLU:HB3    | 1.88        | 0.56     |
| 44:BQ:91:ARG:HB2  | 44:BQ:94:LEU:HD23  | 1.88        | 0.56     |
| 47:BF:137:PHE:HB2 | 47:BF:138:PRO:CD   | 2.34        | 0.56     |
| 1:AA:1060:U:C5    | 2:AC:1:GLY:HA3     | 2.40        | 0.56     |
| 23:BB:161:A:C3'   | 23:BB:162:U:H5''   | 2.33        | 0.56     |
| 30:DY:2:LYS:CD    | 30:DY:2:LYS:H      | 2.18        | 0.56     |
| 23:BB:2144:G:O2'  | 23:BB:2146:C:H5'   | 2.06        | 0.56     |
| 2:CC:156:LEU:HD11 | 2:CC:165:GLU:HB2   | 1.87        | 0.56     |
| 14:AO:77:ARG:O    | 14:AO:81:LEU:HB2   | 2.06        | 0.56     |
| 4:CE:45:VAL:O     | 4:CE:71:ILE:HG22   | 2.06        | 0.56     |
| 50:BT:80:TRP:CZ3  | 50:BT:82:LYS:HG2   | 2.41        | 0.56     |
| 23:DB:1242:U:H2'  | 23:DB:1243:C:C6    | 2.40        | 0.56     |
| 1:CA:737:C:H2'    | 1:CA:738:C:H6      | 1.71        | 0.56     |
| 42:DN:49:GLU:OE2  | 42:DN:95:THR:HG22  | 2.05        | 0.56     |
| 50:DT:69:ARG:HB2  | 50:DT:69:ARG:HH11  | 1.71        | 0.56     |
| 23:BB:782:A:N3    | 25:BC:224:MET:HB3  | 2.20        | 0.56     |
| 22:BA:41:G:H21    | 23:BB:2340:A:H5'   | 1.70        | 0.56     |
| 23:BB:1859:U:H2'  | 23:BB:1860:G:H8    | 1.70        | 0.56     |
| 44:DQ:43:GLN:NE2  | 49:DR:77:PHE:HB3   | 2.21        | 0.56     |
| 1:AA:591:U:OP1    | 7:AH:30:LYS:HE2    | 2.06        | 0.56     |
| 22:BA:10:G:H2'    | 22:BA:11:C:O4'     | 2.06        | 0.56     |
| 1:AA:696:A:H2'    | 1:AA:697:U:C6      | 2.40        | 0.56     |
| 12:CM:92:ARG:HE   | 12:CM:92:ARG:HA    | 1.71        | 0.56     |
| 23:BB:2080:A:OP1  | 51:BZ:20:HIS:HB3   | 2.05        | 0.56     |
| 4:AE:100:GLU:HA   | 4:AE:121:ASN:ND2   | 2.21        | 0.56     |
| 7:AH:37:ASN:O     | 7:AH:41:GLU:HG2    | 2.04        | 0.56     |
| 23:DB:2834:G:H2'  | 23:DB:2879:A:H61   | 1.71        | 0.56     |
| 23:DB:2888:C:H2'  | 23:DB:2889:C:C6    | 2.41        | 0.56     |
| 1:AA:909:A:H2'    | 1:AA:910:C:O4'     | 2.05        | 0.56     |
| 23:DB:2269:G:H4'  | 52:DW:19:ARG:NH1   | 2.20        | 0.56     |
| 23:BB:19:A:H2'    | 23:BB:20:C:H6      | 1.70        | 0.56     |
| 48:DG:10:VAL:HG23 | 48:DG:48:THR:HA    | 1.88        | 0.56     |
| 40:BH:68:ARG:CZ   | 40:BH:134:VAL:HG21 | 2.36        | 0.56     |
| 26:BD:25:THR:HG21 | 26:BD:193:VAL:HG22 | 1.88        | 0.56     |
| 53:D6:32:ARG:HH22 | 53:D6:88:LEU:C     | 2.08        | 0.56     |
| 8:CI:22:PRO:HA    | 8:CI:60:LEU:CB     | 2.36        | 0.56     |
| 8:CI:67:LYS:NZ    | 8:CI:67:LYS:HB2    | 2.20        | 0.56     |
| 41:DJ:45:THR:HG21 | 41:DJ:50:THR:HG21  | 1.88        | 0.56     |
| 41:DJ:56:VAL:HG12 | 41:DJ:57:LEU:N     | 2.21        | 0.56     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 48:BG:34:ARG:HD3  | 48:BG:34:ARG:N     | 2.21        | 0.56     |
| 24:BI:76:ALA:O    | 24:BI:80:LYS:HG3   | 2.06        | 0.56     |
| 23:BB:673:C:C2'   | 23:BB:674:G:H5'    | 2.36        | 0.56     |
| 23:DB:2868:A:H2'  | 23:DB:2869:G:C8    | 2.41        | 0.56     |
| 48:DG:148:ARG:HA  | 48:DG:161:VAL:CB   | 2.32        | 0.56     |
| 15:CP:72:ALA:HA   | 15:CP:75:ILE:HD12  | 1.87        | 0.56     |
| 29:DE:131:THR:HB  | 29:DE:164:LEU:HG   | 1.87        | 0.56     |
| 26:DD:118:PHE:HE2 | 42:DN:1:MET:SD     | 2.28        | 0.56     |
| 23:BB:27:G:HO2'   | 23:BB:28:A:H8      | 1.52        | 0.56     |
| 31:D0:39:ARG:HG3  | 31:D0:39:ARG:HH11  | 1.71        | 0.56     |
| 40:BH:73:ASN:ND2  | 40:BH:74:ALA:H     | 2.02        | 0.56     |
| 44:DQ:104:ALA:O   | 44:DQ:105:PHE:HB3  | 2.06        | 0.56     |
| 44:BQ:10:ARG:CZ   | 44:BQ:10:ARG:HB2   | 2.36        | 0.56     |
| 20:CB:83:ALA:HB3  | 20:CB:90:PHE:HB3   | 1.88        | 0.56     |
| 20:AB:102:ASN:O   | 20:AB:106:VAL:HG23 | 2.06        | 0.56     |
| 3:AD:96:ARG:O     | 3:AD:100:VAL:HG23  | 2.05        | 0.56     |
| 13:CN:2:LYS:O     | 13:CN:6:LYS:HB2    | 2.06        | 0.56     |
| 11:AL:54:VAL:HG21 | 11:AL:79:ILE:HD11  | 1.88        | 0.56     |
| 23:BB:649:G:H2'   | 23:BB:650:C:C6     | 2.40        | 0.56     |
| 23:DB:152:A:H2'   | 23:DB:153:U:H6     | 1.71        | 0.56     |
| 23:BB:945:A:H3'   | 23:BB:946:C:H5''   | 1.88        | 0.56     |
| 23:BB:1826:G:H2'  | 23:BB:1827:U:H6    | 1.70        | 0.56     |
| 25:DC:242:HIS:O   | 25:DC:244:VAL:HG13 | 2.06        | 0.56     |
| 29:DE:21:ARG:HG3  | 29:DE:22:ASP:N     | 2.20        | 0.56     |
| 24:BI:10:LEU:HD12 | 24:BI:10:LEU:O     | 2.05        | 0.56     |
| 3:CD:2:ARG:HG3    | 3:CD:114:ARG:NH1   | 2.20        | 0.56     |
| 23:BB:753:A:H2'   | 23:BB:754:U:H6     | 1.69        | 0.56     |
| 11:CL:3:VAL:O     | 11:CL:7:VAL:HG23   | 2.06        | 0.56     |
| 1:CA:284:C:H2'    | 1:CA:285:C:H6      | 1.70        | 0.56     |
| 1:CA:1150:A:H1'   | 1:CA:1280:A:N6     | 2.21        | 0.56     |
| 51:DZ:70:GLU:O    | 51:DZ:72:ARG:N     | 2.38        | 0.56     |
| 1:CA:692:U:C2     | 1:CA:694:A:H5''    | 2.41        | 0.56     |
| 22:BA:89:U:H5'    | 22:BA:90:C:C6      | 2.40        | 0.56     |
| 1:CA:399:G:H2'    | 1:CA:400:C:C6      | 2.41        | 0.56     |
| 23:BB:1117:C:H2'  | 23:BB:1118:C:C6    | 2.40        | 0.56     |
| 29:BE:98:LYS:O    | 29:BE:102:ARG:HG2  | 2.06        | 0.56     |
| 29:BE:72:SER:C    | 29:BE:74:LYS:H     | 2.08        | 0.56     |
| 23:DB:2553:G:H2'  | 23:DB:2554:U:C4'   | 2.35        | 0.56     |
| 23:BB:2685:G:O2'  | 23:BB:2686:G:H5'   | 2.05        | 0.56     |
| 23:BB:576:U:H2'   | 23:BB:577:G:C8     | 2.41        | 0.56     |
| 23:DB:2491:U:H5'' | 23:DB:2570:G:H5''  | 1.87        | 0.56     |
| 53:D6:129:ILE:O   | 53:D6:132:ILE:HB   | 2.06        | 0.56     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:1186:G:H21   | 13:AN:100:TRP:C   | 2.09        | 0.56     |
| 23:BB:2825:G:H2'  | 23:BB:2826:A:H5'  | 1.88        | 0.56     |
| 23:BB:950:G:H2'   | 23:BB:951:C:C6    | 2.41        | 0.56     |
| 1:AA:423:G:H2'    | 1:AA:424:G:O4'    | 2.05        | 0.56     |
| 23:DB:1098:A:H3'  | 24:DI:3:LYS:CB    | 2.35        | 0.56     |
| 23:DB:2031:A:C6   | 23:DB:2498:C:H1'  | 2.40        | 0.56     |
| 44:DQ:24:TYR:O    | 44:DQ:27:ARG:HB2  | 2.06        | 0.56     |
| 10:AK:61:ALA:O    | 10:AK:64:VAL:HG12 | 2.06        | 0.56     |
| 48:DG:68:ARG:HH12 | 48:DG:72:ASN:ND2  | 2.03        | 0.56     |
| 48:DG:6:ALA:HB3   | 48:DG:68:ARG:NE   | 2.21        | 0.56     |
| 48:DG:9:VAL:H     | 48:DG:48:THR:HB   | 1.70        | 0.56     |
| 40:BH:135:HIS:HB2 | 40:BH:138:VAL:HB  | 1.88        | 0.56     |
| 52:DW:23:LYS:NZ   | 52:DW:24:ARG:HG3  | 2.21        | 0.56     |
| 8:AI:56:MET:CG    | 8:AI:57:VAL:H     | 2.19        | 0.56     |
| 51:DZ:6:GLN:HE21  | 51:DZ:50:ARG:H    | 1.53        | 0.56     |
| 35:DV:63:ILE:N    | 35:DV:63:ILE:HD12 | 2.20        | 0.56     |
| 23:DB:2547:A:H5'  | 23:DB:2566:A:C2   | 2.41        | 0.56     |
| 33:B1:8:ILE:HD11  | 33:B1:52:LYS:HB2  | 1.87        | 0.56     |
| 24:DI:49:GLU:CB   | 24:DI:52:LEU:HD12 | 2.36        | 0.56     |
| 24:DI:54:ILE:HD13 | 24:DI:55:PRO:N    | 2.21        | 0.56     |
| 38:BM:35:ALA:HB2  | 38:BM:100:LYS:HB2 | 1.87        | 0.56     |
| 10:AK:92:ARG:HH21 | 21:AU:24:LYS:HG2  | 1.71        | 0.56     |
| 1:CA:919:A:O2'    | 1:CA:920:U:H5'    | 2.05        | 0.56     |
| 18:CS:29:PRO:HA   | 18:CS:47:THR:O    | 2.06        | 0.56     |
| 23:BB:2749:A:OP1  | 23:BB:2751:G:H5'' | 2.06        | 0.56     |
| 46:BU:46:LYS:NZ   | 46:BU:47:PRO:HG2  | 2.21        | 0.56     |
| 1:AA:719:C:O2     | 17:AR:37:LYS:HA   | 2.05        | 0.56     |
| 15:AP:4:ILE:HB    | 15:AP:67:ILE:HD12 | 1.86        | 0.56     |
| 13:CN:12:ARG:HG2  | 13:CN:53:ASP:HB3  | 1.88        | 0.56     |
| 45:BS:55:ILE:HD12 | 45:BS:69:LEU:HD23 | 1.88        | 0.56     |
| 23:DB:1794:A:H2'  | 23:DB:1795:C:C6   | 2.40        | 0.56     |
| 6:CG:145:GLU:C    | 6:CG:147:ASN:H    | 2.07        | 0.56     |
| 23:DB:1442:U:H2'  | 23:DB:1443:U:H6   | 1.70        | 0.56     |
| 40:DH:72:ILE:CD1  | 40:DH:140:ALA:HB3 | 2.35        | 0.56     |
| 23:BB:1338:G:H4'  | 50:BT:18:GLU:CG   | 2.36        | 0.56     |
| 9:CJ:17:LEU:HD22  | 9:CJ:96:VAL:CG1   | 2.35        | 0.56     |
| 46:DU:78:LYS:CD   | 46:DU:79:ALA:H    | 2.19        | 0.56     |
| 23:DB:558:U:O3'   | 41:DJ:111:LYS:HD3 | 2.06        | 0.56     |
| 41:BJ:103:ILE:HA  | 41:BJ:106:LYS:HB3 | 1.88        | 0.56     |
| 7:CH:66:GLN:C     | 7:CH:68:LYS:H     | 2.09        | 0.56     |
| 23:DB:264:C:C2'   | 23:DB:265:A:H5''  | 2.35        | 0.56     |
| 43:BO:24:THR:OG1  | 43:BO:90:VAL:HG12 | 2.06        | 0.56     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2284:A:OP2   | 33:D1:5:ARG:HG3    | 2.04        | 0.56     |
| 1:AA:796:C:OP1     | 10:AK:127:ARG:HB3  | 2.05        | 0.56     |
| 23:DB:1258:U:H2'   | 23:DB:1259:G:H8    | 1.68        | 0.56     |
| 1:CA:1463:U:OP1    | 28:DP:108:ARG:HD2  | 2.06        | 0.56     |
| 51:BZ:70:GLU:O     | 51:BZ:72:ARG:N     | 2.39        | 0.56     |
| 1:AA:1465:A:H2'    | 1:AA:1466:C:C6     | 2.41        | 0.56     |
| 1:CA:818:G:C3'     | 1:CA:819:A:H5''    | 2.36        | 0.56     |
| 23:DB:479:A:O2'    | 23:DB:481:G:H5'    | 2.06        | 0.56     |
| 23:BB:1899:A:O2'   | 23:BB:1900:A:H5''  | 2.05        | 0.56     |
| 23:BB:441:U:H2'    | 23:BB:442:G:C8     | 2.41        | 0.56     |
| 23:BB:1640:A:H2'   | 23:BB:1641:A:C8    | 2.40        | 0.56     |
| 23:DB:807:U:H2'    | 23:DB:808:G:H8     | 1.70        | 0.56     |
| 23:DB:564:C:H1'    | 44:DQ:36:GLN:OE1   | 2.06        | 0.56     |
| 23:DB:289:G:H2'    | 23:DB:290:U:C6     | 2.40        | 0.56     |
| 23:BB:135:U:H2'    | 23:BB:136:G:C8     | 2.40        | 0.56     |
| 23:BB:2729:G:H2'   | 23:BB:2730:C:C6    | 2.41        | 0.56     |
| 23:BB:17:G:H2'     | 23:BB:18:U:C6      | 2.41        | 0.56     |
| 48:BG:88:LEU:HD13  | 48:BG:93:TYR:HB3   | 1.87        | 0.56     |
| 26:BD:109:VAL:HG11 | 26:BD:193:VAL:HG11 | 1.86        | 0.56     |
| 53:B6:92:PRO:HB3   | 53:B6:100:TYR:O    | 2.05        | 0.56     |
| 50:BT:50:LEU:H     | 50:BT:50:LEU:HD22  | 1.70        | 0.56     |
| 40:DH:85:GLY:HA2   | 40:DH:91:PHE:CZ    | 2.40        | 0.56     |
| 35:BV:48:MET:O     | 35:BV:51:GLN:HG3   | 2.05        | 0.56     |
| 1:AA:1313:U:OP1    | 18:AS:6:LYS:HD3    | 2.06        | 0.56     |
| 50:DT:47:VAL:HG13  | 50:DT:51:PHE:HD1   | 1.71        | 0.56     |
| 23:DB:1566:A:H5'   | 25:DC:213:ARG:NH2  | 2.21        | 0.56     |
| 23:DB:9:G:N2       | 23:DB:10:A:H62     | 2.01        | 0.56     |
| 23:BB:10:A:H61     | 23:BB:2895:G:H1'   | 1.70        | 0.56     |
| 23:BB:279:A:H2'    | 23:BB:280:U:H5'    | 1.88        | 0.56     |
| 1:AA:1057:G:H5''   | 2:AC:153:SER:HB2   | 1.87        | 0.56     |
| 23:BB:1487:U:H2'   | 23:BB:1488:C:H6    | 1.69        | 0.56     |
| 23:DB:37:C:O2'     | 23:DB:38:A:H5'     | 2.06        | 0.56     |
| 23:DB:355:U:H2'    | 23:DB:356:G:C8     | 2.41        | 0.56     |
| 1:AA:634:C:H2'     | 1:AA:635:A:C8      | 2.39        | 0.56     |
| 28:BP:38:ARG:HH21  | 28:BP:38:ARG:HB2   | 1.70        | 0.56     |
| 19:CT:38:ILE:O     | 19:CT:38:ILE:HD13  | 2.05        | 0.56     |
| 19:CT:53:MET:O     | 19:CT:57:VAL:HG22  | 2.06        | 0.56     |
| 23:BB:1353:A:H2'   | 23:BB:1354:A:C8    | 2.41        | 0.56     |
| 7:CH:44:PHE:HA     | 7:CH:70:VAL:HG11   | 1.87        | 0.56     |
| 1:CA:1140:C:O2'    | 1:CA:1141:C:H5'    | 2.05        | 0.56     |
| 23:BB:2537:U:H2'   | 23:BB:2538:C:H6    | 1.71        | 0.56     |
| 16:AQ:80:LYS:CD    | 16:AQ:80:LYS:H     | 2.18        | 0.56     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:2570:G:H2'   | 23:BB:2571:U:O4'   | 2.06        | 0.56     |
| 23:DB:2678:C:H2'   | 23:DB:2679:A:H8    | 1.71        | 0.56     |
| 1:CA:204:G:H2'     | 1:CA:205:A:H8      | 1.71        | 0.56     |
| 23:DB:2814:A:H4'   | 31:D0:25:THR:HG21  | 1.88        | 0.56     |
| 23:DB:1716:U:H2'   | 23:DB:1717:A:C8    | 2.41        | 0.56     |
| 22:BA:91:C:H2'     | 22:BA:92:C:C6      | 2.41        | 0.56     |
| 1:CA:250:A:H1'     | 1:CA:252:U:C5      | 2.41        | 0.56     |
| 1:CA:1186:G:H21    | 13:CN:100:TRP:C    | 2.09        | 0.56     |
| 29:DE:72:SER:C     | 29:DE:74:LYS:H     | 2.09        | 0.56     |
| 29:DE:122:GLU:O    | 29:DE:123:LYS:HB2  | 2.05        | 0.56     |
| 49:DR:36:ALA:HA    | 49:DR:58:VAL:HA    | 1.88        | 0.56     |
| 1:CA:45:G:H2'      | 1:CA:46:G:H8       | 1.70        | 0.56     |
| 23:DB:1534:U:O5'   | 23:DB:1534:U:H6    | 1.89        | 0.56     |
| 23:BB:2359:C:H2'   | 23:BB:2360:G:C8    | 2.41        | 0.56     |
| 2:AC:190:THR:HG22  | 2:AC:191:THR:N     | 2.19        | 0.56     |
| 21:AU:40:PRO:O     | 21:AU:44:ARG:HB2   | 2.06        | 0.56     |
| 53:D6:39:LEU:HA    | 53:D6:52:LEU:HB3   | 1.87        | 0.56     |
| 47:DF:65:LEU:O     | 47:DF:86:CYS:HA    | 2.06        | 0.56     |
| 20:CB:69:VAL:HB    | 20:CB:162:VAL:HB   | 1.88        | 0.56     |
| 35:BV:63:ILE:HD13  | 35:BV:72:VAL:HG22  | 1.88        | 0.56     |
| 50:BT:54:GLU:HG3   | 50:BT:90:GLY:N     | 2.21        | 0.56     |
| 23:DB:1060:U:C5    | 24:DI:131:THR:HG22 | 2.41        | 0.56     |
| 23:BB:2885:G:H2'   | 23:BB:2886:A:O4'   | 2.05        | 0.56     |
| 3:CD:122:ILE:O     | 3:CD:128:VAL:HG23  | 2.06        | 0.56     |
| 31:D0:38:LEU:HD23  | 31:D0:39:ARG:H     | 1.71        | 0.56     |
| 42:DN:72:ASP:OD1   | 42:DN:75:ILE:HG23  | 2.06        | 0.56     |
| 27:DK:115:ILE:HG23 | 27:DK:116:ILE:N    | 2.21        | 0.56     |
| 23:DB:1793:C:H2'   | 23:DB:1794:A:C8    | 2.40        | 0.56     |
| 48:DG:67:ALA:O     | 48:DG:71:LEU:HD23  | 2.05        | 0.56     |
| 23:BB:1105:U:O2'   | 23:BB:1106:G:H5'   | 2.06        | 0.56     |
| 1:CA:36:C:O3'      | 11:CL:119:LYS:HA   | 2.06        | 0.56     |
| 23:BB:63:A:H2'     | 23:BB:63:A:OP2     | 2.05        | 0.56     |
| 5:AF:68:GLN:O      | 5:AF:71:ILE:HG23   | 2.05        | 0.56     |
| 46:BU:26:ASN:N     | 46:BU:26:ASN:ND2   | 2.53        | 0.56     |
| 26:BD:116:LYS:HB2  | 26:BD:165:MET:HB3  | 1.88        | 0.56     |
| 15:AP:23:ASP:O     | 15:AP:26:ASN:HB2   | 2.06        | 0.56     |
| 1:AA:253:A:H2'     | 1:AA:254:G:H8      | 1.71        | 0.56     |
| 13:AN:2:LYS:O      | 13:AN:6:LYS:HB2    | 2.05        | 0.56     |
| 1:AA:926:G:H21     | 1:AA:1505:G:H2'    | 1.70        | 0.56     |
| 1:CA:502:A:H4'     | 1:CA:550:G:H4'     | 1.88        | 0.56     |
| 23:DB:833:A:H2'    | 23:DB:834:G:C8     | 2.41        | 0.56     |
| 23:DB:899:A:H2'    | 23:DB:900:A:O4'    | 2.05        | 0.56     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:DD:125:TRP:CD2 | 26:DD:160:LYS:HB3 | 2.42        | 0.56     |
| 21:AU:11:PHE:O    | 21:AU:13:VAL:HG12 | 2.06        | 0.56     |
| 23:BB:1061:U:O4'  | 23:BB:1070:A:H1'  | 2.06        | 0.56     |
| 23:BB:1716:U:H2'  | 23:BB:1717:A:C8   | 2.41        | 0.56     |
| 31:B0:33:SER:C    | 31:B0:35:GLU:H    | 2.09        | 0.56     |
| 23:DB:1205:A:H4'  | 23:DB:1206:G:OP2  | 2.04        | 0.56     |
| 23:BB:1015:U:H2'  | 23:BB:1016:G:C8   | 2.41        | 0.56     |
| 1:CA:83:C:O2'     | 1:CA:84:U:H2'     | 2.06        | 0.56     |
| 20:AB:10:LYS:O    | 20:AB:13:VAL:HG23 | 2.06        | 0.56     |
| 23:BB:1821:A:H2'  | 23:BB:1822:C:H6   | 1.70        | 0.55     |
| 53:B6:95:LYS:HB3  | 53:B6:100:TYR:CE2 | 2.37        | 0.55     |
| 8:CI:62:LEU:HD22  | 8:CI:62:LEU:N     | 2.21        | 0.55     |
| 23:DB:2393:U:H5'  | 37:DL:60:ARG:O    | 2.05        | 0.55     |
| 50:BT:39:THR:HG22 | 50:BT:42:GLU:CG   | 2.32        | 0.55     |
| 50:BT:43:ILE:O    | 50:BT:46:ALA:HB3  | 2.06        | 0.55     |
| 41:BJ:6:ALA:HB3   | 41:BJ:45:THR:HG21 | 1.87        | 0.55     |
| 12:CM:52:ILE:HG23 | 12:CM:56:ARG:NH1  | 2.16        | 0.55     |
| 33:D1:8:ILE:HD12  | 33:D1:51:ALA:HA   | 1.88        | 0.55     |
| 23:DB:513:A:O5'   | 23:DB:513:A:H8    | 1.89        | 0.55     |
| 1:AA:719:C:O2'    | 17:AR:37:LYS:HB2  | 2.05        | 0.55     |
| 37:DL:17:LYS:HD2  | 37:DL:19:LEU:HD11 | 1.88        | 0.55     |
| 23:BB:2834:G:H2'  | 23:BB:2879:A:N6   | 2.21        | 0.55     |
| 23:BB:45:G:C5'    | 23:BB:46:G:H5'    | 2.35        | 0.55     |
| 15:CP:52:LEU:HD21 | 15:CP:75:ILE:HG12 | 1.88        | 0.55     |
| 23:DB:2820:A:OP1  | 42:DN:4:ARG:HA    | 2.07        | 0.55     |
| 42:DN:31:HIS:O    | 42:DN:33:ILE:HG13 | 2.06        | 0.55     |
| 15:CP:23:ASP:O    | 15:CP:26:ASN:HB2  | 2.06        | 0.55     |
| 23:BB:2899:A:H2'  | 23:BB:2900:A:H8   | 1.71        | 0.55     |
| 23:DB:453:A:H4'   | 23:DB:472:A:N6    | 2.21        | 0.55     |
| 48:BG:67:ALA:O    | 48:BG:71:LEU:HD23 | 2.06        | 0.55     |
| 37:BL:93:ASN:O    | 37:BL:95:LEU:N    | 2.39        | 0.55     |
| 20:CB:119:GLN:HA  | 20:CB:124:THR:CG2 | 2.36        | 0.55     |
| 45:DS:51:LEU:C    | 45:DS:53:SER:H    | 2.10        | 0.55     |
| 26:BD:113:SER:HB3 | 26:BD:167:ASN:CA  | 2.37        | 0.55     |
| 14:AO:24:SER:HB3  | 14:AO:27:VAL:CG2  | 2.35        | 0.55     |
| 28:DP:38:ARG:HH21 | 28:DP:38:ARG:HB2  | 1.70        | 0.55     |
| 28:DP:31:VAL:HG11 | 28:DP:38:ARG:HG3  | 1.88        | 0.55     |
| 8:CI:7:GLY:HA3    | 8:CI:81:GLY:O     | 2.06        | 0.55     |
| 2:CC:61:LYS:O     | 2:CC:96:VAL:HB    | 2.06        | 0.55     |
| 3:AD:18:LEU:HD12  | 3:AD:63:ILE:HG12  | 1.88        | 0.55     |
| 24:BI:89:SER:HB2  | 24:BI:136:GLY:HA3 | 1.87        | 0.55     |
| 1:CA:1062:U:H2'   | 1:CA:1063:C:C6    | 2.40        | 0.55     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 39:DX:33:ALA:HB1   | 50:DT:14:PRO:HD2   | 1.88        | 0.55     |
| 23:DB:871:U:H2'    | 23:DB:872:U:H6     | 1.72        | 0.55     |
| 23:BB:818:G:H3'    | 23:BB:1187:G:H22   | 1.70        | 0.55     |
| 1:AA:611:C:H2'     | 1:AA:612:C:H6      | 1.71        | 0.55     |
| 10:AK:52:ARG:HH11  | 10:AK:53:GLY:H     | 1.54        | 0.55     |
| 44:BQ:43:GLN:NE2   | 49:BR:77:PHE:HB3   | 2.20        | 0.55     |
| 1:AA:204:G:H2'     | 1:AA:205:A:H8      | 1.71        | 0.55     |
| 23:DB:659:G:H4'    | 29:DE:95:LYS:HD2   | 1.88        | 0.55     |
| 37:DL:132:ARG:O    | 37:DL:136:GLU:HG3  | 2.06        | 0.55     |
| 1:CA:761:G:H2'     | 1:CA:762:U:C6      | 2.41        | 0.55     |
| 23:BB:780:G:H1     | 25:BC:228:ASP:CG   | 2.10        | 0.55     |
| 3:AD:146:GLU:HA    | 3:AD:149:LYS:HG2   | 1.86        | 0.55     |
| 37:BL:143:GLU:HG2  | 37:BL:144:GLU:N    | 2.17        | 0.55     |
| 38:DM:35:ALA:HB2   | 38:DM:100:LYS:HB2  | 1.88        | 0.55     |
| 42:BN:83:LEU:CA    | 42:BN:86:ARG:HB2   | 2.30        | 0.55     |
| 1:AA:922:G:H2'     | 1:AA:923:A:C8      | 2.41        | 0.55     |
| 1:CA:1079:G:H2'    | 1:CA:1080:A:C8     | 2.41        | 0.55     |
| 18:CS:39:ILE:HB    | 18:CS:66:VAL:HA    | 1.88        | 0.55     |
| 53:D6:12:SER:O     | 53:D6:16:LYS:HD2   | 2.06        | 0.55     |
| 20:CB:221:ARG:CB   | 20:CB:221:ARG:HH11 | 2.18        | 0.55     |
| 17:AR:55:ALA:HA    | 17:AR:58:ILE:HD12  | 1.88        | 0.55     |
| 23:BB:2834:G:H2'   | 23:BB:2879:A:H61   | 1.70        | 0.55     |
| 23:BB:2645:G:H3'   | 23:BB:2646:C:C5'   | 2.35        | 0.55     |
| 3:CD:116:LEU:O     | 3:CD:121:ALA:HB3   | 2.07        | 0.55     |
| 1:CA:308:C:H2'     | 1:CA:309:A:C8      | 2.41        | 0.55     |
| 1:CA:1390:U:H2'    | 1:CA:1391:U:C6     | 2.41        | 0.55     |
| 50:BT:18:GLU:C     | 50:BT:20:ALA:H     | 2.10        | 0.55     |
| 23:DB:322:A:H5'    | 23:DB:340:A:H1'    | 1.87        | 0.55     |
| 42:BN:47:VAL:C     | 42:BN:50:PRO:HD2   | 2.26        | 0.55     |
| 23:BB:1592:C:H2'   | 23:BB:1593:A:H8    | 1.70        | 0.55     |
| 25:DC:123:ILE:HD12 | 25:DC:191:LEU:HD11 | 1.87        | 0.55     |
| 1:CA:1154:G:O2'    | 1:CA:1155:A:H5'    | 2.06        | 0.55     |
| 48:DG:91:VAL:HG23  | 48:DG:92:GLY:H     | 1.72        | 0.55     |
| 23:BB:1720:U:O2'   | 23:BB:1721:G:H5'   | 2.05        | 0.55     |
| 1:CA:1483:A:H2'    | 1:CA:1484:C:O4'    | 2.06        | 0.55     |
| 1:CA:62:U:H2'      | 1:CA:63:C:C6       | 2.41        | 0.55     |
| 37:DL:25:SER:O     | 37:DL:27:LEU:HD12  | 2.06        | 0.55     |
| 23:BB:408:G:O2'    | 23:BB:409:G:H5'    | 2.07        | 0.55     |
| 25:BC:124:LYS:HG3  | 25:BC:125:PRO:HD2  | 1.88        | 0.55     |
| 23:DB:660:C:H2'    | 23:DB:661:A:H8     | 1.70        | 0.55     |
| 48:DG:10:VAL:HG12  | 48:DG:10:VAL:O     | 2.05        | 0.55     |
| 41:DJ:38:GLY:O     | 41:DJ:43:GLU:HB2   | 2.06        | 0.55     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BC:71:ASP:OD2  | 25:BC:118:GLY:HA2  | 2.06        | 0.55     |
| 41:BJ:4:PHE:CG    | 41:BJ:5:THR:N      | 2.74        | 0.55     |
| 3:CD:26:ALA:HA    | 3:CD:30:LYS:CE     | 2.36        | 0.55     |
| 30:BY:8:GLN:CG    | 30:BY:31:ILE:HA    | 2.31        | 0.55     |
| 47:DF:7:TYR:HA    | 47:DF:11:VAL:CG2   | 2.36        | 0.55     |
| 10:AK:88:PRO:HD3  | 21:AU:28:LEU:HD11  | 1.89        | 0.55     |
| 23:BB:1256:G:H21  | 29:BE:77:ILE:HG22  | 1.71        | 0.55     |
| 25:DC:209:ALA:HA  | 25:DC:212:TRP:NE1  | 2.21        | 0.55     |
| 10:CK:22:ILE:HD13 | 10:CK:95:THR:CG2   | 2.34        | 0.55     |
| 26:BD:29:VAL:O    | 26:BD:185:ASN:HB3  | 2.07        | 0.55     |
| 23:DB:1785:A:O2'  | 23:DB:1786:A:H5'   | 2.06        | 0.55     |
| 20:CB:60:ALA:HB1  | 20:CB:220:VAL:HG13 | 1.87        | 0.55     |
| 23:BB:1553:A:O2'  | 23:BB:1554:U:H2'   | 2.07        | 0.55     |
| 38:DM:114:ARG:HA  | 38:DM:130:PHE:CE1  | 2.41        | 0.55     |
| 43:DO:5:SER:HA    | 43:DO:8:ILE:CD1    | 2.34        | 0.55     |
| 23:BB:1656:C:H2'  | 23:BB:1657:U:C6    | 2.41        | 0.55     |
| 23:BB:1792:G:O2'  | 23:BB:1793:C:H5'   | 2.06        | 0.55     |
| 12:AM:89:ARG:HB2  | 12:AM:96:VAL:HG22  | 1.88        | 0.55     |
| 38:BM:114:ARG:HA  | 38:BM:130:PHE:CE1  | 2.42        | 0.55     |
| 48:DG:174:LYS:NZ  | 48:DG:176:LYS:HG2  | 2.22        | 0.55     |
| 23:DB:2840:C:H2'  | 23:DB:2841:C:H6    | 1.72        | 0.55     |
| 1:CA:499:A:H4'    | 1:CA:500:G:H5'     | 1.88        | 0.55     |
| 1:CA:524:G:H2'    | 1:CA:525:C:H6      | 1.70        | 0.55     |
| 40:BH:57:LYS:NZ   | 40:BH:58:LEU:HD22  | 2.22        | 0.55     |
| 23:DB:1349:C:H2'  | 23:DB:1350:C:H6    | 1.71        | 0.55     |
| 1:CA:1405:G:O2'   | 1:CA:1406:U:H5'    | 2.06        | 0.55     |
| 1:CA:1512:U:H2'   | 1:CA:1513:A:C8     | 2.42        | 0.55     |
| 1:CA:213:G:H3'    | 1:CA:214:C:C6      | 2.42        | 0.55     |
| 29:BE:21:ARG:HG3  | 29:BE:22:ASP:N     | 2.19        | 0.55     |
| 3:CD:18:LEU:HD12  | 3:CD:63:ILE:HG12   | 1.87        | 0.55     |
| 23:BB:3:U:HO2'    | 23:BB:4:U:H6       | 1.54        | 0.55     |
| 33:B1:10:LEU:O    | 33:B1:19:PHE:HB2   | 2.07        | 0.55     |
| 23:DB:1047:G:O3'  | 23:DB:1048:A:H8    | 1.89        | 0.55     |
| 23:BB:993:G:H1'   | 49:BR:91:GLN:NE2   | 2.22        | 0.55     |
| 2:CC:13:ILE:O     | 2:CC:14:VAL:HG22   | 2.06        | 0.55     |
| 7:CH:26:MET:HB2   | 7:CH:27:PRO:HD2    | 1.89        | 0.55     |
| 23:BB:1520:U:H2'  | 23:BB:1521:G:O4'   | 2.06        | 0.55     |
| 15:AP:73:ALA:O    | 15:AP:77:GLU:HG3   | 2.07        | 0.55     |
| 34:D3:7:ARG:HG3   | 34:D3:7:ARG:HH11   | 1.71        | 0.55     |
| 24:BI:14:ALA:HB1  | 24:BI:50:LYS:HA    | 1.87        | 0.55     |
| 49:DR:14:VAL:HG22 | 49:DR:15:SER:N     | 2.22        | 0.55     |
| 1:CA:358:U:H2'    | 1:CA:359:G:C8      | 2.41        | 0.55     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:638:U:H2'     | 1:CA:639:G:O4'     | 2.06        | 0.55     |
| 1:CA:1458:G:H5''   | 19:CT:25:SER:HB2   | 1.88        | 0.55     |
| 1:AA:761:G:H2'     | 1:AA:762:U:C6      | 2.42        | 0.55     |
| 1:CA:642:A:H2'     | 1:CA:643:C:H6      | 1.71        | 0.55     |
| 23:BB:1473:G:O2'   | 23:BB:1474:U:H5'   | 2.06        | 0.55     |
| 6:CG:72:VAL:HG12   | 6:CG:89:GLU:HG3    | 1.87        | 0.55     |
| 45:DS:40:ASN:O     | 45:DS:41:LYS:HG3   | 2.05        | 0.55     |
| 1:CA:95:C:O2       | 1:CA:95:C:H2'      | 2.05        | 0.55     |
| 23:DB:2835:A:N6    | 23:DB:2878:U:H2'   | 2.21        | 0.55     |
| 23:DB:2053:G:O2'   | 23:DB:2054:A:H5'   | 2.06        | 0.55     |
| 23:BB:2385:C:H2'   | 23:BB:2386:A:H8    | 1.71        | 0.55     |
| 23:BB:2384:U:H5''  | 23:BB:2386:A:OP1   | 2.05        | 0.55     |
| 25:DC:128:THR:HG23 | 25:DC:190:THR:HG22 | 1.89        | 0.55     |
| 44:BQ:26:ALA:HB1   | 44:BQ:30:VAL:HG11  | 1.88        | 0.55     |
| 22:DA:42:C:O4'     | 47:DF:65:LEU:HB2   | 2.06        | 0.55     |
| 8:CI:55:ASP:HB2    | 8:CI:59:LYS:HG3    | 1.88        | 0.55     |
| 8:CI:79:ARG:O      | 8:CI:83:THR:HG22   | 2.06        | 0.55     |
| 51:DZ:35:SER:HA    | 51:DZ:49:LEU:O     | 2.05        | 0.55     |
| 48:DG:34:ARG:HD3   | 48:DG:34:ARG:N     | 2.20        | 0.55     |
| 50:BT:17:SER:N     | 50:BT:21:SER:OG    | 2.39        | 0.55     |
| 29:BE:5:LEU:CD1    | 29:BE:10:SER:HB2   | 2.31        | 0.55     |
| 12:CM:106:ARG:HD3  | 12:CM:110:GLY:O    | 2.06        | 0.55     |
| 28:BP:91:VAL:O     | 28:BP:92:ARG:HB3   | 2.07        | 0.55     |
| 26:BD:148:GLN:CB   | 26:BD:152:PRO:HG2  | 2.36        | 0.55     |
| 25:DC:156:SER:HB3  | 25:DC:159:THR:HG21 | 1.88        | 0.55     |
| 1:CA:674:G:H2'     | 1:CA:675:A:C8      | 2.39        | 0.55     |
| 29:DE:148:ILE:HD13 | 29:DE:187:VAL:CG2  | 2.36        | 0.55     |
| 1:CA:1342:C:H2'    | 1:CA:1343:G:H8     | 1.72        | 0.55     |
| 27:BK:59:LYS:HD3   | 27:BK:89:ASN:HA    | 1.88        | 0.55     |
| 11:AL:33:CYS:HA    | 11:AL:54:VAL:HA    | 1.87        | 0.55     |
| 23:BB:264:C:C2'    | 23:BB:265:A:H5''   | 2.36        | 0.55     |
| 23:BB:453:A:H4'    | 23:BB:472:A:N6     | 2.21        | 0.55     |
| 1:CA:635:A:H2'     | 1:CA:636:U:C6      | 2.42        | 0.55     |
| 23:DB:693:A:H2'    | 23:DB:694:U:H6     | 1.69        | 0.55     |
| 23:DB:2195:U:O2'   | 23:DB:2196:C:H5'   | 2.07        | 0.55     |
| 31:D0:8:THR:HG23   | 31:D0:11:LYS:H     | 1.70        | 0.55     |
| 1:CA:784:A:H2'     | 1:CA:785:G:H8      | 1.72        | 0.55     |
| 23:DB:2230:G:H2'   | 23:DB:2231:U:H6    | 1.71        | 0.55     |
| 51:BZ:63:GLY:O     | 51:BZ:67:VAL:HG23  | 2.07        | 0.55     |
| 1:AA:533:A:H5''    | 57:AA:1892:HOH:O   | 2.06        | 0.55     |
| 23:BB:2814:A:H2'   | 23:BB:2815:C:H6    | 1.71        | 0.55     |
| 10:CK:52:ARG:HH11  | 10:CK:53:GLY:H     | 1.53        | 0.55     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:285:C:H2'    | 1:AA:286:C:C6      | 2.41        | 0.55     |
| 23:DB:1014:A:O2'  | 23:DB:1015:U:H5'   | 2.05        | 0.55     |
| 23:DB:2636:C:H2'  | 23:DB:2637:U:C6    | 2.42        | 0.55     |
| 23:BB:1164:C:H2'  | 23:BB:1165:A:C8    | 2.42        | 0.55     |
| 42:DN:7:GLY:HA2   | 42:DN:46:ARG:HH11  | 1.72        | 0.55     |
| 23:BB:2197:U:O2'  | 23:BB:2198:A:H2'   | 2.06        | 0.55     |
| 23:DB:2520:C:O2'  | 23:DB:2521:C:H5'   | 2.06        | 0.55     |
| 38:DM:67:VAL:HG11 | 38:DM:102:LEU:HD13 | 1.89        | 0.55     |
| 23:DB:452:G:OP1   | 29:DE:53:THR:HG23  | 2.07        | 0.55     |
| 1:CA:449:G:H2'    | 1:CA:450:G:C8      | 2.41        | 0.55     |
| 1:AA:104:G:O2'    | 1:AA:105:G:H5'     | 2.07        | 0.55     |
| 4:CE:87:VAL:HG23  | 4:CE:91:SER:O      | 2.07        | 0.55     |
| 23:DB:598:U:H2'   | 23:DB:599:A:H8     | 1.71        | 0.55     |
| 45:BS:10:ALA:HB3  | 45:BS:101:SER:OG   | 2.06        | 0.55     |
| 23:BB:83:A:N1     | 23:BB:101:A:H5'    | 2.21        | 0.55     |
| 30:BY:21:ALA:O    | 30:BY:24:LEU:HB3   | 2.06        | 0.55     |
| 5:AF:86:ARG:NH1   | 17:AR:64:LEU:HD12  | 2.21        | 0.55     |
| 23:DB:2573:C:H3'  | 57:DB:3629:HOH:O   | 2.04        | 0.55     |
| 43:DO:94:ARG:O    | 43:DO:97:PHE:HB2   | 2.06        | 0.55     |
| 23:DB:2666:C:O2   | 23:DB:2666:C:O4'   | 2.23        | 0.55     |
| 23:DB:106:C:H2'   | 23:DB:107:G:H8     | 1.71        | 0.55     |
| 40:BH:27:ARG:HG2  | 40:BH:27:ARG:HH21  | 1.71        | 0.55     |
| 23:BB:1822:C:O2'  | 23:BB:1823:G:H5'   | 2.07        | 0.55     |
| 48:BG:6:ALA:HB3   | 48:BG:68:ARG:NE    | 2.22        | 0.55     |
| 8:CI:50:PRO:O     | 8:CI:54:VAL:HG22   | 2.06        | 0.55     |
| 8:AI:22:PRO:HA    | 8:AI:60:LEU:CB     | 2.35        | 0.55     |
| 8:AI:79:ARG:HA    | 8:AI:82:ILE:HD12   | 1.87        | 0.55     |
| 48:DG:24:THR:C    | 48:DG:25:ILE:HD12  | 2.27        | 0.55     |
| 40:DH:80:ILE:O    | 40:DH:80:ILE:HD12  | 2.07        | 0.55     |
| 47:DF:168:LEU:O   | 47:DF:169:LEU:HB2  | 2.06        | 0.55     |
| 16:AQ:45:VAL:HG12 | 16:AQ:46:HIS:N     | 2.22        | 0.55     |
| 23:BB:589:U:H2'   | 23:BB:590:A:C8     | 2.42        | 0.55     |
| 20:CB:16:GLY:CA   | 20:CB:40:ILE:H     | 2.19        | 0.55     |
| 1:AA:314:C:O2'    | 1:AA:315:A:H5'     | 2.07        | 0.55     |
| 27:BK:71:ARG:HB3  | 27:BK:72:PRO:HD2   | 1.88        | 0.55     |
| 49:BR:3:ALA:O     | 49:BR:4:VAL:HG13   | 2.06        | 0.55     |
| 1:AA:1301:U:O2    | 1:AA:1301:U:H2'    | 2.04        | 0.55     |
| 23:BB:9:G:N2      | 23:BB:10:A:H62     | 2.04        | 0.55     |
| 23:DB:1784:A:H4'  | 23:DB:1785:A:O5'   | 2.07        | 0.55     |
| 26:DD:9:VAL:O     | 28:DP:4:ILE:HD11   | 2.06        | 0.55     |
| 27:BK:59:LYS:HD2  | 27:BK:89:ASN:ND2   | 2.22        | 0.55     |
| 23:BB:2590:A:H2'  | 23:BB:2591:C:C6    | 2.41        | 0.55     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:484:G:H4'    | 1:AA:485:U:C5'     | 2.37        | 0.55     |
| 23:BB:608:A:H2'   | 23:BB:609:A:C8     | 2.41        | 0.55     |
| 1:CA:484:G:H4'    | 1:CA:485:U:C5'     | 2.37        | 0.55     |
| 28:BP:50:ARG:HD3  | 28:BP:56:SER:HB3   | 1.89        | 0.55     |
| 45:BS:51:LEU:C    | 45:BS:53:SER:H     | 2.10        | 0.55     |
| 39:BX:8:GLU:HB2   | 39:BX:13:GLU:OE1   | 2.06        | 0.55     |
| 23:DB:2537:U:H2'  | 23:DB:2538:C:H6    | 1.71        | 0.55     |
| 23:BB:350:G:H2'   | 23:BB:351:C:H6     | 1.71        | 0.55     |
| 23:BB:2708:G:O2'  | 23:BB:2709:G:H5'   | 2.06        | 0.55     |
| 1:CA:505:G:H2'    | 1:CA:506:G:H8      | 1.72        | 0.55     |
| 1:CA:545:C:H5''   | 3:CD:68:GLU:HG2    | 1.88        | 0.55     |
| 23:DB:1640:A:H2'  | 23:DB:1641:A:C8    | 2.41        | 0.55     |
| 23:BB:2102:G:N3   | 23:BB:2102:G:H2'   | 2.22        | 0.55     |
| 1:AA:608:A:H3'    | 57:AA:1895:HOH:O   | 2.05        | 0.55     |
| 50:BT:5:GLU:HA    | 50:BT:8:LEU:CB     | 2.19        | 0.55     |
| 20:AB:204:ASP:CG  | 20:AB:205:ALA:H    | 2.10        | 0.55     |
| 23:DB:2352:A:H2'  | 23:DB:2353:G:O4'   | 2.07        | 0.55     |
| 47:DF:71:LYS:O    | 47:DF:73:VAL:HG23  | 2.06        | 0.55     |
| 23:DB:987:C:H2'   | 23:DB:988:A:O4'    | 2.07        | 0.55     |
| 38:DM:34:LYS:HB3  | 38:DM:129:THR:HG22 | 1.87        | 0.55     |
| 50:BT:39:THR:CG2  | 50:BT:42:GLU:H     | 2.20        | 0.55     |
| 25:BC:109:LEU:H   | 25:BC:109:LEU:CD2  | 2.20        | 0.55     |
| 30:BY:8:GLN:OE1   | 30:BY:23:LEU:HD11  | 2.07        | 0.55     |
| 1:CA:865:A:H2'    | 1:CA:866:C:C6      | 2.41        | 0.55     |
| 43:DO:39:VAL:HB   | 43:DO:49:VAL:HG22  | 1.88        | 0.55     |
| 23:DB:28:A:H61    | 23:DB:512:G:H1'    | 1.71        | 0.55     |
| 29:DE:117:ARG:HA  | 29:DE:185:LYS:HG2  | 1.88        | 0.55     |
| 23:BB:590:A:H2'   | 23:BB:591:U:H6     | 1.69        | 0.55     |
| 23:BB:1199:U:H2'  | 23:BB:1200:C:H6    | 1.72        | 0.55     |
| 1:CA:1339:A:H2'   | 1:CA:1340:A:O4'    | 2.06        | 0.55     |
| 23:DB:1792:G:O2'  | 23:DB:1793:C:H5'   | 2.07        | 0.55     |
| 23:BB:1439:A:N7   | 23:BB:1440:U:N1    | 2.54        | 0.55     |
| 25:BC:156:SER:HB3 | 25:BC:159:THR:HG21 | 1.88        | 0.55     |
| 20:CB:103:TRP:O   | 20:CB:107:ARG:HG2  | 2.07        | 0.55     |
| 28:DP:50:ARG:HD3  | 28:DP:56:SER:HB3   | 1.88        | 0.55     |
| 23:BB:1793:C:H2'  | 23:BB:1794:A:C8    | 2.41        | 0.55     |
| 1:CA:1343:G:H4'   | 8:CI:123:ARG:O     | 2.06        | 0.55     |
| 13:AN:1:ALA:HB1   | 13:AN:6:LYS:HE2    | 1.89        | 0.55     |
| 1:AA:617:G:H4'    | 15:AP:46:LYS:NZ    | 2.22        | 0.55     |
| 46:DU:53:GLN:HG2  | 46:DU:53:GLN:O     | 2.07        | 0.55     |
| 28:BP:31:VAL:HG11 | 28:BP:38:ARG:HG3   | 1.87        | 0.55     |
| 35:BV:53:LYS:HB3  | 35:BV:55:GLU:OE1   | 2.06        | 0.55     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:1329:A:O2'    | 1:CA:1330:U:H5'    | 2.05        | 0.55     |
| 23:BB:665:U:O2'    | 23:BB:666:A:H5'    | 2.07        | 0.55     |
| 2:CC:82:ASP:O      | 2:CC:86:LEU:HG     | 2.06        | 0.55     |
| 1:CA:373:A:H1'     | 1:CA:481:G:N3      | 2.22        | 0.55     |
| 23:BB:2341:G:H2'   | 23:BB:2342:C:H6    | 1.71        | 0.55     |
| 23:DB:2859:G:H2'   | 23:DB:2860:A:C8    | 2.42        | 0.55     |
| 23:DB:1109:C:H3'   | 23:DB:1110:G:C8    | 2.41        | 0.55     |
| 1:CA:182:A:N3      | 1:CA:182:A:H5''    | 2.21        | 0.55     |
| 31:B0:8:THR:HG23   | 31:B0:11:LYS:H     | 1.72        | 0.55     |
| 1:AA:696:A:H2'     | 1:AA:697:U:H6      | 1.71        | 0.55     |
| 35:BV:6:ALA:O      | 35:BV:65:VAL:HG12  | 2.06        | 0.55     |
| 23:BB:244:A:H1'    | 23:BB:255:A:N6     | 2.22        | 0.55     |
| 17:CR:56:ARG:O     | 17:CR:60:ARG:HG2   | 2.07        | 0.55     |
| 42:DN:2:ARG:HA     | 42:DN:5:LYS:HD3    | 1.88        | 0.55     |
| 47:BF:121:PHE:HB3  | 47:BF:127:TYR:CZ   | 2.41        | 0.55     |
| 38:DM:78:LEU:O     | 38:DM:80:VAL:HG12  | 2.06        | 0.55     |
| 17:AR:36:GLY:HA3   | 17:AR:70:THR:HA    | 1.89        | 0.55     |
| 1:CA:384:G:H2'     | 1:CA:385:C:C6      | 2.42        | 0.55     |
| 23:DB:2660:A:H2'   | 23:DB:2661:G:C8    | 2.42        | 0.55     |
| 1:CA:104:G:O2'     | 1:CA:105:G:H5'     | 2.06        | 0.55     |
| 21:CU:8:ASN:O      | 21:CU:9:GLU:HB3    | 2.06        | 0.55     |
| 6:AG:109:LYS:HA    | 6:AG:109:LYS:HE2   | 1.89        | 0.55     |
| 44:BQ:16:ILE:O     | 44:BQ:18:LYS:N     | 2.40        | 0.55     |
| 48:BG:89:VAL:CB    | 48:BG:159:LYS:HA   | 2.25        | 0.55     |
| 48:DG:97:VAL:HA    | 48:DG:102:ILE:HA   | 1.88        | 0.55     |
| 48:DG:84:LYS:CG    | 48:DG:85:LYS:H     | 2.16        | 0.55     |
| 40:BH:78:VAL:HG11  | 40:BH:103:VAL:HG12 | 1.88        | 0.55     |
| 1:CA:1250:A:H2'    | 1:CA:1251:A:C8     | 2.42        | 0.55     |
| 44:DQ:94:LEU:CD1   | 49:DR:13:ARG:HB2   | 2.37        | 0.55     |
| 8:AI:61:ASP:C      | 8:AI:62:LEU:HD13   | 2.27        | 0.55     |
| 7:CH:86:LYS:HB3    | 7:CH:90:GLU:HB3    | 1.89        | 0.55     |
| 50:BT:25:GLU:HA    | 50:BT:29:THR:O     | 2.06        | 0.55     |
| 25:DC:93:VAL:HG13  | 25:DC:94:LEU:N     | 2.22        | 0.55     |
| 41:BJ:45:THR:HG21  | 41:BJ:50:THR:HG21  | 1.89        | 0.55     |
| 51:BZ:35:SER:HA    | 51:BZ:49:LEU:O     | 2.06        | 0.55     |
| 1:CA:978:A:H5'     | 1:CA:1362:A:H62    | 1.71        | 0.55     |
| 53:D6:180:GLU:O    | 53:D6:184:LEU:HG   | 2.06        | 0.55     |
| 37:BL:116:VAL:HG13 | 37:BL:117:THR:N    | 2.19        | 0.55     |
| 23:DB:818:G:H3'    | 23:DB:1187:G:H22   | 1.71        | 0.55     |
| 20:AB:221:ARG:CB   | 20:AB:221:ARG:HH11 | 2.18        | 0.55     |
| 48:DG:152:ARG:HH22 | 48:DG:162:ARG:HA   | 1.70        | 0.55     |
| 48:BG:152:ARG:NH2  | 48:BG:162:ARG:HA   | 2.21        | 0.55     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 45:BS:29:VAL:HG23 | 45:BS:70:LYS:HA    | 1.87        | 0.55     |
| 24:BI:17:ALA:O    | 24:BI:18:ASN:HB3   | 2.06        | 0.55     |
| 23:BB:365:U:H2'   | 23:BB:366:C:C6     | 2.42        | 0.55     |
| 20:CB:144:GLU:O   | 20:CB:148:GLY:HA3  | 2.07        | 0.55     |
| 23:BB:2740:A:H2'  | 23:BB:2741:A:C8    | 2.41        | 0.55     |
| 23:BB:63:A:H8     | 23:BB:63:A:OP2     | 1.90        | 0.55     |
| 43:BO:4:LYS:O     | 43:BO:8:ILE:HG13   | 2.07        | 0.55     |
| 14:CO:77:ARG:O    | 14:CO:81:LEU:HB2   | 2.07        | 0.55     |
| 23:BB:616:A:H4'   | 29:BE:101:TYR:CE2  | 2.42        | 0.55     |
| 19:CT:66:ILE:HG22 | 19:CT:67:HIS:N     | 2.22        | 0.55     |
| 1:AA:473:U:H2'    | 1:AA:474:G:H8      | 1.72        | 0.55     |
| 12:CM:2:ARG:HG3   | 12:CM:6:ILE:N      | 2.21        | 0.55     |
| 2:AC:78:LYS:HG3   | 2:AC:81:GLU:HB2    | 1.89        | 0.55     |
| 23:DB:1915:U:H5'' | 57:DB:3486:HOH:O   | 2.05        | 0.55     |
| 23:DB:2415:G:C4'  | 37:DL:66:PHE:HB2   | 2.37        | 0.55     |
| 1:CA:1384:C:H2'   | 1:CA:1385:G:C8     | 2.42        | 0.55     |
| 23:BB:2540:C:H2'  | 23:BB:2541:A:H8    | 1.72        | 0.55     |
| 23:BB:741:U:H2'   | 23:BB:742:A:C8     | 2.41        | 0.55     |
| 23:DB:2676:C:O2'  | 23:DB:2677:G:H5'   | 2.07        | 0.55     |
| 24:BI:112:LYS:O   | 24:BI:116:MET:HG3  | 2.06        | 0.55     |
| 23:DB:575:A:O2'   | 23:DB:576:U:H5'    | 2.06        | 0.55     |
| 22:DA:94:A:OP1    | 35:DV:19:ARG:HD3   | 2.05        | 0.55     |
| 23:DB:596:U:H2'   | 23:DB:597:G:C8     | 2.42        | 0.55     |
| 23:DB:2729:G:H2'  | 23:DB:2730:C:C6    | 2.42        | 0.55     |
| 23:DB:176:A:O2'   | 23:DB:177:G:H5'    | 2.07        | 0.55     |
| 41:BJ:130:HIS:HD2 | 41:BJ:132:HIS:HB2  | 1.71        | 0.55     |
| 23:DB:1849:G:H2'  | 23:DB:1850:G:H8    | 1.72        | 0.55     |
| 23:BB:234:U:H2'   | 23:BB:235:U:H6     | 1.71        | 0.55     |
| 25:BC:149:LYS:HD3 | 25:BC:152:GLN:HE22 | 1.71        | 0.55     |
| 52:DW:33:GLY:O    | 52:DW:34:SER:HB2   | 2.06        | 0.55     |
| 48:BG:84:LYS:HG3  | 48:BG:132:LEU:N    | 2.22        | 0.55     |
| 53:D6:86:SER:HB3  | 53:D6:88:LEU:HD13  | 1.87        | 0.55     |
| 8:CI:27:ILE:HD13  | 8:CI:34:LEU:HD22   | 1.89        | 0.55     |
| 41:BJ:56:VAL:HG12 | 41:BJ:57:LEU:N     | 2.22        | 0.55     |
| 8:AI:24:ASN:HD21  | 8:AI:26:LYS:HG3    | 1.72        | 0.55     |
| 7:CH:87:ARG:N     | 7:CH:90:GLU:HB3    | 2.22        | 0.55     |
| 22:BA:27:C:N4     | 22:BA:28:C:N4      | 2.55        | 0.55     |
| 24:BI:77:VAL:HA   | 24:BI:80:LYS:CE    | 2.37        | 0.55     |
| 47:BF:168:LEU:O   | 47:BF:169:LEU:HB2  | 2.06        | 0.55     |
| 40:DH:90:LEU:CD1  | 40:DH:90:LEU:H     | 2.15        | 0.55     |
| 35:BV:26:PHE:CE2  | 35:BV:44:HIS:HA    | 2.42        | 0.55     |
| 12:AM:44:ILE:HA   | 12:AM:47:LEU:CD1   | 2.37        | 0.55     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1314:C:H2'    | 1:AA:1315:U:C6     | 2.42        | 0.55     |
| 23:DB:141:G:C6     | 50:DT:2:ILE:HG23   | 2.42        | 0.55     |
| 17:AR:38:ILE:H     | 17:AR:38:ILE:HD13  | 1.72        | 0.55     |
| 22:DA:107:G:O2'    | 22:DA:108:A:H5'    | 2.07        | 0.55     |
| 3:AD:187:ARG:O     | 3:AD:191:SER:HB3   | 2.06        | 0.55     |
| 23:DB:969:G:H2'    | 23:DB:970:U:H6     | 1.72        | 0.55     |
| 53:B6:118:VAL:HG21 | 53:B6:183:ILE:HG21 | 1.88        | 0.55     |
| 1:CA:843:U:OP2     | 1:CA:843:U:H4'     | 2.05        | 0.55     |
| 23:BB:116:C:O2'    | 23:BB:117:G:H5'    | 2.06        | 0.55     |
| 11:AL:20:VAL:HG23  | 11:AL:20:VAL:O     | 2.07        | 0.55     |
| 23:DB:63:A:OP2     | 23:DB:63:A:H8      | 1.90        | 0.55     |
| 23:BB:2722:G:H2'   | 23:BB:2723:C:H6    | 1.72        | 0.55     |
| 1:CA:1070:U:H2'    | 1:CA:1071:C:C6     | 2.41        | 0.55     |
| 23:DB:1309:G:OP1   | 36:D2:9:VAL:HG12   | 2.07        | 0.55     |
| 6:AG:104:VAL:O     | 6:AG:108:ARG:HG3   | 2.07        | 0.55     |
| 23:DB:740:C:O2'    | 23:DB:741:U:H5'    | 2.07        | 0.55     |
| 23:DB:2340:A:H2'   | 23:DB:2341:G:H8    | 1.71        | 0.55     |
| 24:BI:58:ILE:N     | 24:BI:58:ILE:HD12  | 2.21        | 0.55     |
| 23:BB:1353:A:H2'   | 23:BB:1354:A:H8    | 1.72        | 0.55     |
| 23:BB:2801:G:H2'   | 23:BB:2802:G:H8    | 1.70        | 0.55     |
| 42:BN:61:ALA:C     | 42:BN:63:ARG:H     | 2.09        | 0.55     |
| 1:CA:1464:U:H2'    | 1:CA:1465:A:C8     | 2.42        | 0.55     |
| 20:AB:25:LYS:HD3   | 20:AB:193:ASP:OD1  | 2.06        | 0.55     |
| 23:DB:286:U:H2'    | 23:DB:287:G:C8     | 2.42        | 0.55     |
| 23:DB:460:A:H4'    | 50:DT:72:GLN:HB2   | 1.88        | 0.55     |
| 23:BB:2728:U:H2'   | 23:BB:2729:G:H8    | 1.72        | 0.55     |
| 23:BB:355:U:H2'    | 23:BB:356:G:H8     | 1.71        | 0.55     |
| 1:CA:721:G:H4'     | 1:CA:722:G:O4'     | 2.06        | 0.55     |
| 1:CA:649:A:H2'     | 1:CA:650:G:O4'     | 2.07        | 0.55     |
| 7:CH:17:GLN:HE21   | 7:CH:17:GLN:HA     | 1.70        | 0.55     |
| 1:CA:1132:C:H2'    | 1:CA:1133:G:C8     | 2.42        | 0.55     |
| 1:CA:696:A:H2'     | 1:CA:697:U:C6      | 2.42        | 0.55     |
| 52:BW:48:ALA:HB3   | 52:BW:81:ILE:O     | 2.06        | 0.55     |
| 48:BG:97:VAL:HA    | 48:BG:102:ILE:HA   | 1.89        | 0.55     |
| 44:DQ:26:ALA:HB1   | 44:DQ:30:VAL:HG11  | 1.88        | 0.55     |
| 10:CK:73:VAL:O     | 10:CK:76:TYR:HB2   | 2.07        | 0.55     |
| 51:DZ:51:VAL:HG11  | 51:DZ:56:MET:HG3   | 1.87        | 0.55     |
| 45:BS:3:THR:HB     | 45:BS:62:ASP:CB    | 2.29        | 0.55     |
| 23:DB:2645:G:H3'   | 23:DB:2646:C:C5'   | 2.37        | 0.55     |
| 25:BC:90:ILE:CD1   | 25:BC:102:TYR:HB3  | 2.37        | 0.55     |
| 47:BF:84:ILE:HG22  | 47:BF:84:ILE:O     | 2.07        | 0.55     |
| 1:AA:1079:G:H2'    | 1:AA:1080:A:C8     | 2.41        | 0.55     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:923:A:H2'    | 1:CA:924:C:C6     | 2.42        | 0.55     |
| 13:AN:29:ILE:HB   | 13:AN:30:ILE:HD12 | 1.89        | 0.55     |
| 23:DB:972:A:OP2   | 23:DB:974:G:H5''  | 2.07        | 0.55     |
| 10:CK:91:GLY:O    | 10:CK:95:THR:HG22 | 2.06        | 0.55     |
| 23:DB:45:G:C5'    | 23:DB:46:G:H5'    | 2.33        | 0.55     |
| 40:DH:4:ILE:HG22  | 40:DH:17:ASP:H    | 1.71        | 0.55     |
| 23:BB:1728:C:H2'  | 23:BB:1730:C:O2   | 2.06        | 0.55     |
| 23:BB:1789:A:H2'  | 23:BB:1790:C:C6   | 2.41        | 0.55     |
| 26:BD:118:PHE:HE2 | 42:BN:1:MET:SD    | 2.29        | 0.55     |
| 12:AM:95:PRO:CD   | 12:AM:108:ARG:HG2 | 2.36        | 0.55     |
| 39:BX:20:ASN:ND2  | 39:BX:20:ASN:N    | 2.55        | 0.55     |
| 1:CA:551:U:H2'    | 1:CA:552:U:C6     | 2.42        | 0.55     |
| 1:CA:254:G:O2'    | 1:CA:255:G:H5'    | 2.07        | 0.55     |
| 23:BB:1582:C:H3'  | 23:BB:1583:A:C2   | 2.41        | 0.55     |
| 6:CG:50:ALA:CB    | 6:CG:57:GLU:HG3   | 2.37        | 0.55     |
| 23:BB:2577:A:H5'' | 23:BB:2578:G:H5'  | 1.88        | 0.55     |
| 1:AA:1225:A:H3'   | 1:AA:1226:C:H6    | 1.72        | 0.55     |
| 23:DB:545:U:H2'   | 23:DB:546:U:H4'   | 1.89        | 0.55     |
| 23:BB:479:A:O2'   | 23:BB:481:G:H5'   | 2.07        | 0.55     |
| 23:BB:937:C:H2'   | 23:BB:938:G:C8    | 2.41        | 0.55     |
| 23:BB:1682:G:H2'  | 23:BB:1683:U:C6   | 2.41        | 0.55     |
| 1:CA:591:U:H2'    | 1:CA:592:G:H8     | 1.71        | 0.55     |
| 23:BB:528:A:N1    | 23:BB:2042:A:H2'  | 2.21        | 0.55     |
| 23:DB:1047:G:H1'  | 23:DB:1110:G:H22  | 1.71        | 0.55     |
| 2:CC:14:VAL:O     | 2:CC:15:LYS:HD2   | 2.07        | 0.55     |
| 34:D3:7:ARG:NH1   | 34:D3:7:ARG:HG3   | 2.22        | 0.55     |
| 1:CA:157:U:O2'    | 1:CA:158:G:H5'    | 2.07        | 0.55     |
| 1:AA:476:U:O2'    | 1:AA:477:C:H5'    | 2.07        | 0.55     |
| 1:AA:487:A:H2'    | 1:AA:488:C:O4'    | 2.07        | 0.55     |
| 12:AM:43:LYS:HB2  | 12:AM:46:GLU:HG3  | 1.87        | 0.55     |
| 1:AA:779:C:H5''   | 10:AK:123:PRO:HB3 | 1.89        | 0.55     |
| 23:DB:1477:A:H2'  | 23:DB:1478:G:O4'  | 2.07        | 0.55     |
| 1:CA:852:G:H2'    | 1:CA:853:C:C6     | 2.42        | 0.55     |
| 12:AM:92:ARG:HE   | 12:AM:92:ARG:HA   | 1.72        | 0.55     |
| 23:DB:1395:A:H4'  | 23:DB:1397:U:C5   | 2.42        | 0.55     |
| 1:AA:28:A:N3      | 1:AA:296:U:H4'    | 2.21        | 0.55     |
| 1:CA:1507:A:H2'   | 1:CA:1508:A:C8    | 2.41        | 0.55     |
| 23:DB:1117:C:H2'  | 23:DB:1118:C:H6   | 1.71        | 0.55     |
| 23:DB:1117:C:H2'  | 23:DB:1118:C:C6   | 2.42        | 0.55     |
| 23:DB:1100:C:H2'  | 23:DB:1101:U:C6   | 2.42        | 0.55     |
| 23:DB:1100:C:OP2  | 24:DI:2:LYS:HB3   | 2.06        | 0.55     |
| 23:DB:1822:C:O2'  | 23:DB:1823:G:H5'  | 2.06        | 0.55     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 21:CU:40:PRO:O     | 21:CU:44:ARG:HB2   | 2.07        | 0.55     |
| 48:BG:106:LEU:HD12 | 48:BG:151:ARG:HD3  | 1.89        | 0.55     |
| 30:DY:8:GLN:HB3    | 30:DY:31:ILE:C     | 2.26        | 0.55     |
| 47:BF:115:GLY:CA   | 47:BF:177:ARG:HD2  | 2.32        | 0.55     |
| 41:BJ:38:GLY:O     | 41:BJ:43:GLU:HB2   | 2.07        | 0.55     |
| 44:BQ:91:ARG:HB2   | 49:BR:11:GLN:NE2   | 2.21        | 0.55     |
| 47:BF:101:ARG:HA   | 47:BF:105:ILE:HD12 | 1.88        | 0.55     |
| 47:BF:109:ARG:CB   | 47:BF:135:ILE:HD12 | 2.35        | 0.55     |
| 42:DN:80:PHE:O     | 42:DN:85:PRO:HD3   | 2.07        | 0.55     |
| 47:DF:16:MET:O     | 47:DF:20:ASN:HA    | 2.07        | 0.55     |
| 20:CB:46:VAL:HA    | 20:CB:49:PHE:CD2   | 2.41        | 0.55     |
| 1:AA:1360:A:H2'    | 1:AA:1361:G:O4'    | 2.07        | 0.55     |
| 25:DC:16:VAL:CB    | 25:DC:203:VAL:HB   | 2.34        | 0.55     |
| 40:BH:8:LYS:O      | 40:BH:13:GLY:HA3   | 2.07        | 0.55     |
| 46:BU:73:ASN:C     | 46:BU:75:ALA:H     | 2.09        | 0.55     |
| 31:B0:39:ARG:HH11  | 31:B0:39:ARG:HG3   | 1.71        | 0.55     |
| 23:DB:549:G:H2'    | 41:DJ:2:LYS:HE3    | 1.89        | 0.55     |
| 13:CN:7:ALA:O      | 13:CN:11:LYS:HG2   | 2.06        | 0.55     |
| 43:BO:26:LEU:HB2   | 43:BO:39:VAL:HG22  | 1.88        | 0.55     |
| 48:BG:153:PRO:HG3  | 48:BG:162:ARG:CB   | 2.37        | 0.55     |
| 27:BK:54:LYS:HD2   | 27:BK:54:LYS:N     | 2.20        | 0.55     |
| 26:DD:141:ARG:O    | 26:DD:142:VAL:HG13 | 2.07        | 0.55     |
| 48:BG:74:MET:O     | 48:BG:78:VAL:HG13  | 2.06        | 0.55     |
| 49:DR:68:ARG:NH2   | 49:DR:90:ARG:HB2   | 2.21        | 0.55     |
| 1:CA:869:G:H5'     | 1:CA:872:A:O4'     | 2.07        | 0.55     |
| 3:AD:118:SER:HA    | 3:AD:130:ASN:HB2   | 1.89        | 0.55     |
| 23:DB:1487:U:H2'   | 23:DB:1488:C:H6    | 1.72        | 0.55     |
| 1:CA:634:C:H2'     | 1:CA:635:A:C8      | 2.41        | 0.55     |
| 1:CA:57:G:H2'      | 1:CA:58:C:H6       | 1.69        | 0.55     |
| 23:BB:1937:A:N7    | 23:BB:1939:U:H2'   | 2.22        | 0.55     |
| 22:BA:6:G:H2'      | 22:BA:7:G:H8       | 1.70        | 0.55     |
| 1:AA:784:A:H2'     | 1:AA:785:G:H8      | 1.72        | 0.55     |
| 23:DB:285:G:H2'    | 23:DB:286:U:O4'    | 2.07        | 0.55     |
| 41:DJ:103:ILE:HD12 | 41:DJ:104:ALA:N    | 2.22        | 0.55     |
| 23:DB:2677:G:H2'   | 23:DB:2678:C:C6    | 2.41        | 0.55     |
| 23:BB:134:G:H2'    | 23:BB:135:U:C6     | 2.42        | 0.55     |
| 1:AA:649:A:H2'     | 1:AA:650:G:O4'     | 2.07        | 0.55     |
| 1:AA:1499:A:O2'    | 1:AA:1500:A:H5'    | 2.07        | 0.55     |
| 1:CA:28:A:N3       | 1:CA:296:U:H4'     | 2.22        | 0.55     |
| 1:CA:1486:G:H2'    | 1:CA:1487:G:O4'    | 2.06        | 0.55     |
| 9:CJ:66:GLU:HB3    | 13:CN:98:ALA:HB2   | 1.88        | 0.55     |
| 1:AA:628:G:O2'     | 1:AA:629:A:H5'     | 2.07        | 0.55     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:71:A:O2'      | 1:CA:72:A:H5''     | 2.07        | 0.55     |
| 37:BL:131:ALA:C    | 37:BL:133:ALA:H    | 2.09        | 0.55     |
| 44:BQ:34:ALA:O     | 44:BQ:37:ALA:HB3   | 2.07        | 0.54     |
| 23:DB:572:A:H3'    | 23:DB:573:U:O4'    | 2.07        | 0.54     |
| 44:DQ:26:ALA:HB1   | 44:DQ:30:VAL:CG1   | 2.36        | 0.54     |
| 20:AB:164:ASP:CG   | 20:AB:203:ASP:HB2  | 2.27        | 0.54     |
| 26:BD:4:LEU:HD23   | 26:BD:101:PHE:CE1  | 2.42        | 0.54     |
| 26:BD:106:LYS:HB3  | 26:BD:206:ALA:CB   | 2.38        | 0.54     |
| 44:DQ:63:ARG:NH1   | 44:DQ:96:ASP:HB2   | 2.09        | 0.54     |
| 23:DB:2394:C:OP1   | 37:DL:63:LYS:HG2   | 2.07        | 0.54     |
| 50:BT:38:ALA:HB1   | 50:BT:43:ILE:HD11  | 1.89        | 0.54     |
| 1:CA:1296:C:C4'    | 1:CA:1302:C:H41    | 2.11        | 0.54     |
| 44:BQ:91:ARG:NH1   | 49:BR:10:LYS:HB3   | 2.22        | 0.54     |
| 48:BG:17:LYS:HZ2   | 48:BG:18:ILE:H     | 1.53        | 0.54     |
| 47:BF:71:LYS:O     | 47:BF:73:VAL:HG23  | 2.07        | 0.54     |
| 1:CA:1060:U:H2'    | 1:CA:1061:G:H8     | 1.72        | 0.54     |
| 37:BL:113:ALA:HB3  | 37:BL:115:GLU:OE1  | 2.06        | 0.54     |
| 45:DS:13:SER:OG    | 45:DS:14:ALA:N     | 2.40        | 0.54     |
| 47:DF:7:TYR:O      | 47:DF:12:VAL:HG23  | 2.06        | 0.54     |
| 35:BV:44:HIS:CE1   | 35:BV:85:LYS:HB2   | 2.43        | 0.54     |
| 13:AN:7:ALA:O      | 13:AN:11:LYS:HG2   | 2.06        | 0.54     |
| 32:D4:5:ALA:HA     | 32:D4:37:GLN:HE21  | 1.72        | 0.54     |
| 23:DB:1656:C:H2'   | 23:DB:1657:U:C6    | 2.42        | 0.54     |
| 22:BA:107:G:O2'    | 22:BA:108:A:H5'    | 2.06        | 0.54     |
| 31:D0:38:LEU:HB3   | 31:D0:41:HIS:NE2   | 2.22        | 0.54     |
| 11:CL:20:VAL:O     | 11:CL:20:VAL:HG23  | 2.07        | 0.54     |
| 2:AC:51:VAL:HA     | 2:AC:69:THR:HA     | 1.89        | 0.54     |
| 23:DB:967:U:H2'    | 23:DB:968:C:C6     | 2.42        | 0.54     |
| 7:AH:49:LYS:O      | 7:AH:59:GLU:N      | 2.39        | 0.54     |
| 1:CA:272:C:H2'     | 1:CA:273:U:C6      | 2.41        | 0.54     |
| 1:AA:551:U:H2'     | 1:AA:552:U:C6      | 2.41        | 0.54     |
| 12:AM:90:HIS:HA    | 12:AM:108:ARG:HH22 | 1.71        | 0.54     |
| 12:CM:95:PRO:N     | 12:CM:108:ARG:HG2  | 2.21        | 0.54     |
| 23:DB:2529:G:H4'   | 48:DG:174:LYS:CG   | 2.36        | 0.54     |
| 1:CA:926:G:N2      | 1:CA:1505:G:H2'    | 2.22        | 0.54     |
| 4:CE:152:VAL:HG21  | 7:CH:98:LEU:HB3    | 1.88        | 0.54     |
| 35:DV:31:TYR:HB3   | 35:DV:37:PRO:HG3   | 1.89        | 0.54     |
| 6:CG:50:ALA:HB2    | 6:CG:57:GLU:HG3    | 1.88        | 0.54     |
| 25:BC:123:ILE:HD12 | 25:BC:191:LEU:CD1  | 2.36        | 0.54     |
| 1:CA:736:C:H2'     | 1:CA:737:C:H6      | 1.67        | 0.54     |
| 1:AA:1329:A:O2'    | 1:AA:1330:U:H5'    | 2.07        | 0.54     |
| 44:DQ:65:ASN:HB2   | 44:DQ:75:TYR:HB2   | 1.89        | 0.54     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:BB:1205:A:H4'   | 23:BB:1206:G:OP2  | 2.05        | 0.54     |
| 23:DB:2041:U:H2'   | 23:DB:2042:A:H8   | 1.72        | 0.54     |
| 23:BB:962:G:H21    | 23:BB:2250:G:H22  | 1.55        | 0.54     |
| 23:DB:1513:U:H2'   | 23:DB:1514:G:C8   | 2.43        | 0.54     |
| 48:BG:87:GLN:HE21  | 48:BG:164:ALA:HA  | 1.72        | 0.54     |
| 23:DB:564:C:O2'    | 23:DB:565:C:H5'   | 2.07        | 0.54     |
| 23:BB:136:G:H2'    | 23:BB:137:U:C6    | 2.41        | 0.54     |
| 23:DB:596:U:H2'    | 23:DB:597:G:H8    | 1.72        | 0.54     |
| 1:AA:818:G:H3'     | 1:AA:819:A:H5''   | 1.88        | 0.54     |
| 1:CA:171:A:H2'     | 1:CA:172:A:C8     | 2.42        | 0.54     |
| 1:AA:74:A:O2'      | 1:AA:75:G:H5'     | 2.07        | 0.54     |
| 23:DB:445:C:O2'    | 23:DB:446:G:H5'   | 2.06        | 0.54     |
| 1:CA:470:C:H2'     | 1:CA:471:U:C6     | 2.42        | 0.54     |
| 22:BA:78:A:H2'     | 22:BA:79:G:O4'    | 2.06        | 0.54     |
| 24:DI:63:ASP:O     | 24:DI:64:ARG:HB2  | 2.06        | 0.54     |
| 1:CA:317:U:H2'     | 1:CA:318:G:H8     | 1.72        | 0.54     |
| 1:AA:903:G:O2'     | 1:AA:904:U:H5'    | 2.07        | 0.54     |
| 26:BD:51:THR:HG22  | 26:BD:52:THR:N    | 2.23        | 0.54     |
| 53:D6:76:LEU:HD21  | 53:D6:97:ASP:O    | 2.07        | 0.54     |
| 25:BC:93:VAL:HG13  | 25:BC:94:LEU:N    | 2.22        | 0.54     |
| 29:BE:105:LEU:HD21 | 29:BE:177:PRO:HA  | 1.87        | 0.54     |
| 48:BG:34:ARG:HG2   | 48:BG:34:ARG:HH11 | 1.71        | 0.54     |
| 47:BF:131:VAL:C    | 47:BF:133:GLU:H   | 2.10        | 0.54     |
| 43:BO:88:LYS:HG2   | 43:BO:89:ASP:H    | 1.72        | 0.54     |
| 1:CA:17:U:O2'      | 1:CA:18:C:H5'     | 2.06        | 0.54     |
| 23:DB:139:U:H3     | 50:DT:49:LYS:CE   | 2.20        | 0.54     |
| 6:AG:110:ARG:HB2   | 6:AG:118:ARG:HB3  | 1.89        | 0.54     |
| 40:BH:105:ALA:HB3  | 40:BH:108:VAL:CG2 | 2.36        | 0.54     |
| 23:BB:2487:G:H2'   | 23:BB:2488:G:H8   | 1.72        | 0.54     |
| 25:BC:202:ARG:NH1  | 25:BC:213:ARG:NE  | 2.55        | 0.54     |
| 20:AB:16:GLY:CA    | 20:AB:40:ILE:H    | 2.20        | 0.54     |
| 5:CF:6:ILE:HG13    | 5:CF:6:ILE:O      | 2.07        | 0.54     |
| 1:AA:21:G:H2'      | 1:AA:22:G:H8      | 1.70        | 0.54     |
| 23:DB:10:A:H61     | 23:DB:2895:G:H1'  | 1.72        | 0.54     |
| 48:DG:74:MET:O     | 48:DG:78:VAL:HG13 | 2.07        | 0.54     |
| 26:DD:8:LYS:CD     | 26:DD:197:THR:H   | 2.20        | 0.54     |
| 28:DP:3:ILE:HG23   | 28:DP:4:ILE:HG13  | 1.88        | 0.54     |
| 9:AJ:17:LEU:HD22   | 9:AJ:96:VAL:CG1   | 2.36        | 0.54     |
| 4:AE:152:VAL:HA    | 4:AE:155:LYS:HD3  | 1.89        | 0.54     |
| 1:AA:1343:G:H4'    | 8:AI:123:ARG:O    | 2.07        | 0.54     |
| 1:AA:321:A:O2'     | 1:AA:322:C:H5'    | 2.07        | 0.54     |
| 1:AA:1000:A:H2'    | 1:AA:1001:C:C6    | 2.43        | 0.54     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 9:AJ:36:VAL:HA    | 9:AJ:76:ILE:HA     | 1.89        | 0.54     |
| 23:BB:784:G:N1    | 25:BC:227:VAL:HG11 | 2.21        | 0.54     |
| 1:CA:617:G:H4'    | 15:CP:46:LYS:NZ    | 2.22        | 0.54     |
| 27:DK:88:ASN:ND2  | 27:DK:88:ASN:C     | 2.61        | 0.54     |
| 23:BB:98:G:C2'    | 23:BB:99:U:H5''    | 2.37        | 0.54     |
| 6:AG:21:LEU:HG    | 6:AG:22:LEU:N      | 2.21        | 0.54     |
| 30:BY:40:THR:HG22 | 30:BY:42:ALA:H     | 1.72        | 0.54     |
| 46:BU:53:GLN:O    | 46:BU:53:GLN:HG2   | 2.07        | 0.54     |
| 7:CH:100:ILE:HD11 | 7:CH:128:VAL:HB    | 1.90        | 0.54     |
| 23:BB:1915:U:H2'  | 23:BB:1916:A:C8    | 2.42        | 0.54     |
| 22:BA:49:C:H2'    | 22:BA:50:A:C8      | 2.42        | 0.54     |
| 23:DB:2290:G:H2'  | 23:DB:2291:U:C6    | 2.42        | 0.54     |
| 1:CA:425:G:H2'    | 1:CA:426:U:C6      | 2.42        | 0.54     |
| 23:BB:1571:A:H2'  | 23:BB:1572:A:H8    | 1.71        | 0.54     |
| 48:BG:38:ASP:CG   | 48:BG:39:ALA:H     | 2.10        | 0.54     |
| 26:DD:122:VAL:HA  | 26:DD:127:PHE:H    | 1.72        | 0.54     |
| 1:AA:45:G:H2'     | 1:AA:46:G:C8       | 2.42        | 0.54     |
| 23:DB:813:U:H2'   | 23:DB:814:C:C6     | 2.42        | 0.54     |
| 19:CT:48:LYS:O    | 19:CT:52:GLU:HB3   | 2.07        | 0.54     |
| 23:BB:794:A:H2'   | 23:BB:795:C:H6     | 1.71        | 0.54     |
| 23:DB:2815:C:H2'  | 23:DB:2816:G:H8    | 1.71        | 0.54     |
| 1:CA:1451:U:H5''  | 1:CA:1452:C:OP2    | 2.08        | 0.54     |
| 1:CA:1484:C:O2'   | 1:CA:1485:U:H5'    | 2.07        | 0.54     |
| 23:DB:1300:G:H4'  | 23:DB:1301:A:O5'   | 2.05        | 0.54     |
| 1:AA:731:G:O2'    | 1:AA:732:C:H5'     | 2.06        | 0.54     |
| 23:DB:2494:G:H4'  | 38:DM:79:ALA:HB2   | 1.89        | 0.54     |
| 23:DB:2095:A:H3'  | 23:DB:2096:C:H6    | 1.71        | 0.54     |
| 53:D6:93:SER:HB3  | 53:D6:100:TYR:O    | 2.07        | 0.54     |
| 23:DB:1276:A:O2'  | 23:DB:1277:G:H5'   | 2.06        | 0.54     |
| 7:AH:17:GLN:HA    | 7:AH:17:GLN:HE21   | 1.70        | 0.54     |
| 1:CA:404:G:O2'    | 1:CA:405:U:H5'     | 2.07        | 0.54     |
| 23:DB:2384:U:H5'' | 23:DB:2386:A:OP1   | 2.08        | 0.54     |
| 52:DW:37:VAL:HG12 | 52:DW:38:ARG:N     | 2.18        | 0.54     |
| 44:BQ:34:ALA:O    | 44:BQ:38:VAL:HG23  | 2.07        | 0.54     |
| 21:CU:42:THR:O    | 21:CU:46:ARG:HG3   | 2.08        | 0.54     |
| 40:BH:124:THR:O   | 40:BH:125:THR:CB   | 2.54        | 0.54     |
| 1:CA:1370:G:O2'   | 1:CA:1371:G:H5'    | 2.07        | 0.54     |
| 44:DQ:83:LYS:NZ   | 44:DQ:87:VAL:HA    | 2.23        | 0.54     |
| 47:BF:115:GLY:CA  | 47:BF:177:ARG:HH11 | 2.21        | 0.54     |
| 47:BF:1:ALA:O     | 47:BF:4:HIS:HB3    | 2.07        | 0.54     |
| 23:BB:322:A:H5'   | 23:BB:340:A:H1'    | 1.89        | 0.54     |
| 40:DH:86:ASP:HB2  | 40:DH:89:LYS:HD3   | 1.89        | 0.54     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1060:U:H2'    | 1:AA:1061:G:H8     | 1.72        | 0.54     |
| 45:DS:8:ARG:HB3    | 45:DS:102:HIS:CE1  | 2.42        | 0.54     |
| 33:D1:34:GLU:HA    | 33:D1:48:TYR:O     | 2.07        | 0.54     |
| 23:BB:674:G:O3'    | 29:BE:60:TRP:CZ2   | 2.61        | 0.54     |
| 15:CP:66:THR:O     | 15:CP:67:ILE:HB    | 2.07        | 0.54     |
| 45:BS:52:GLU:HA    | 45:BS:55:ILE:CG2   | 2.36        | 0.54     |
| 1:AA:1468:A:O2'    | 1:AA:1469:C:H5'    | 2.08        | 0.54     |
| 25:BC:16:VAL:H     | 25:BC:203:VAL:HG12 | 1.73        | 0.54     |
| 25:BC:18:VAL:HG11  | 25:BC:202:ARG:HD2  | 1.90        | 0.54     |
| 23:BB:1198:U:H2'   | 23:BB:1199:U:C6    | 2.42        | 0.54     |
| 11:CL:24:GLU:HB2   | 11:CL:26:CYS:SG    | 2.48        | 0.54     |
| 49:DR:39:LEU:CB    | 49:DR:49:ILE:HG12  | 2.37        | 0.54     |
| 23:DB:1553:A:O2'   | 23:DB:1554:U:H2'   | 2.07        | 0.54     |
| 9:AJ:14:ASP:OD1    | 9:AJ:17:LEU:HB2    | 2.07        | 0.54     |
| 43:DO:4:LYS:O      | 43:DO:8:ILE:HG13   | 2.07        | 0.54     |
| 28:DP:88:ARG:HG3   | 28:DP:112:ARG:HB3  | 1.88        | 0.54     |
| 23:BB:2073:C:C5'   | 25:BC:227:VAL:HG12 | 2.37        | 0.54     |
| 28:BP:112:ARG:HB2  | 28:BP:112:ARG:HH11 | 1.72        | 0.54     |
| 23:BB:714:U:H1'    | 23:BB:717:C:H5     | 1.72        | 0.54     |
| 39:DX:18:LEU:HA    | 39:DX:21:LEU:HD12  | 1.89        | 0.54     |
| 6:AG:57:GLU:H      | 6:AG:57:GLU:CD     | 2.10        | 0.54     |
| 45:DS:30:SER:O     | 45:DS:33:LEU:HB2   | 2.07        | 0.54     |
| 1:AA:213:G:H3'     | 1:AA:214:C:C6      | 2.42        | 0.54     |
| 23:BB:184:C:H2'    | 23:BB:185:G:C8     | 2.43        | 0.54     |
| 23:DB:1563:U:H2'   | 23:DB:1564:C:C6    | 2.42        | 0.54     |
| 23:DB:1292:G:H2'   | 23:DB:1293:C:C6    | 2.43        | 0.54     |
| 53:B6:181:GLN:O    | 53:B6:185:GLY:HA3  | 2.08        | 0.54     |
| 23:BB:2814:A:H4'   | 31:B0:25:THR:HG21  | 1.88        | 0.54     |
| 23:BB:904:G:H2'    | 23:BB:905:A:C8     | 2.42        | 0.54     |
| 23:BB:831:G:H2'    | 23:BB:832:U:O4'    | 2.08        | 0.54     |
| 23:DB:955:U:H5''   | 38:DM:86:LYS:HD2   | 1.89        | 0.54     |
| 2:CC:13:ILE:N      | 2:CC:13:ILE:HD13   | 2.23        | 0.54     |
| 23:DB:1341:G:H3'   | 23:DB:1397:U:O2    | 2.06        | 0.54     |
| 43:BO:105:ALA:C    | 43:BO:107:ALA:H    | 2.11        | 0.54     |
| 27:BK:25:LEU:HD13  | 27:BK:38:ILE:HG22  | 1.90        | 0.54     |
| 17:AR:61:ALA:HB3   | 17:AR:67:LEU:HD12  | 1.89        | 0.54     |
| 23:BB:1299:G:H4'   | 23:BB:1301:A:H1'   | 1.88        | 0.54     |
| 1:AA:975:A:H4'     | 1:AA:976:G:OP2     | 2.07        | 0.54     |
| 25:DC:175:LEU:HD11 | 25:DC:181:ARG:HG3  | 1.90        | 0.54     |
| 48:DG:132:LEU:O    | 48:DG:132:LEU:HD12 | 2.08        | 0.54     |
| 53:D6:59:THR:HG22  | 53:D6:67:VAL:HG23  | 1.89        | 0.54     |
| 53:D6:98:ALA:O     | 53:D6:99:LEU:HD23  | 2.08        | 0.54     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 20:CB:204:ASP:CG  | 20:CB:205:ALA:H    | 2.10        | 0.54     |
| 24:DI:79:LEU:HD11 | 24:DI:131:THR:OG1  | 2.07        | 0.54     |
| 23:BB:1459:G:H5'' | 23:BB:1460:U:OP1   | 2.06        | 0.54     |
| 40:DH:88:GLY:HA3  | 40:DH:125:THR:OG1  | 2.07        | 0.54     |
| 1:CA:950:U:H2'    | 1:CA:951:G:H8      | 1.73        | 0.54     |
| 4:CE:136:VAL:HG13 | 4:CE:137:ARG:N     | 2.22        | 0.54     |
| 18:AS:51:HIS:HA   | 18:AS:55:GLN:O     | 2.07        | 0.54     |
| 8:AI:94:ARG:CB    | 8:AI:94:ARG:HH11   | 2.17        | 0.54     |
| 23:BB:2834:G:H1'  | 23:BB:2883:A:N6    | 2.23        | 0.54     |
| 48:DG:145:ALA:HA  | 48:DG:148:ARG:CG   | 2.38        | 0.54     |
| 24:DI:17:ALA:O    | 24:DI:18:ASN:CB    | 2.55        | 0.54     |
| 47:BF:162:ASP:O   | 47:BF:166:ARG:HD2  | 2.06        | 0.54     |
| 23:DB:784:G:N1    | 25:DC:227:VAL:HG11 | 2.21        | 0.54     |
| 1:AA:1392:G:O2'   | 1:AA:1393:U:H5'    | 2.07        | 0.54     |
| 26:DD:148:GLN:CB  | 26:DD:152:PRO:HG2  | 2.37        | 0.54     |
| 26:DD:9:VAL:HA    | 26:DD:197:THR:HG23 | 1.89        | 0.54     |
| 36:B2:21:ARG:HG2  | 36:B2:31:LEU:CG    | 2.38        | 0.54     |
| 23:DB:1080:A:O2'  | 24:DI:126:ARG:HD2  | 2.08        | 0.54     |
| 23:BB:1441:G:H2'  | 23:BB:1442:U:C6    | 2.43        | 0.54     |
| 53:D6:109:GLU:O   | 53:D6:112:LYS:HB2  | 2.07        | 0.54     |
| 43:BO:5:SER:HA    | 43:BO:8:ILE:CD1    | 2.35        | 0.54     |
| 3:AD:185:PRO:HB2  | 3:AD:190:LEU:HG    | 1.89        | 0.54     |
| 12:CM:89:ARG:HB2  | 12:CM:96:VAL:HG22  | 1.88        | 0.54     |
| 24:DI:85:ILE:CD1  | 24:DI:137:LEU:HD21 | 2.37        | 0.54     |
| 23:BB:2840:C:H2'  | 23:BB:2841:C:H6    | 1.71        | 0.54     |
| 13:CN:1:ALA:HB1   | 13:CN:6:LYS:HE2    | 1.89        | 0.54     |
| 10:CK:80:ASN:HB3  | 10:CK:105:ARG:HB3  | 1.90        | 0.54     |
| 11:AL:64:SER:OG   | 11:AL:96:THR:HG23  | 2.06        | 0.54     |
| 50:DT:80:TRP:CZ3  | 50:DT:82:LYS:HG2   | 2.42        | 0.54     |
| 23:DB:1508:A:H5'  | 23:DB:1509:A:C6    | 2.43        | 0.54     |
| 1:CA:1314:C:H2'   | 1:CA:1315:U:C6     | 2.42        | 0.54     |
| 11:CL:33:CYS:HA   | 11:CL:54:VAL:HA    | 1.90        | 0.54     |
| 1:AA:1141:C:H2'   | 1:AA:1142:G:C8     | 2.42        | 0.54     |
| 23:DB:1637:A:H2'  | 23:DB:1638:C:C6    | 2.42        | 0.54     |
| 37:BL:23:ILE:HG13 | 49:BR:82:HIS:CE1   | 2.42        | 0.54     |
| 1:AA:1451:U:H5''  | 1:AA:1452:C:OP2    | 2.07        | 0.54     |
| 49:DR:91:GLN:HG3  | 49:DR:92:TRP:H     | 1.72        | 0.54     |
| 23:BB:575:A:O2'   | 23:BB:576:U:H5'    | 2.07        | 0.54     |
| 1:AA:730:G:O2'    | 1:AA:766:A:H5'     | 2.07        | 0.54     |
| 23:BB:1849:G:H2'  | 23:BB:1850:G:H8    | 1.72        | 0.54     |
| 23:BB:443:A:OP1   | 29:BE:40:ARG:HD2   | 2.07        | 0.54     |
| 23:DB:1464:G:H2'  | 23:DB:1465:G:H8    | 1.71        | 0.54     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1104:C:H2'   | 23:DB:1105:U:C6    | 2.43        | 0.54     |
| 23:BB:1885:A:H3'   | 23:BB:1886:U:C6    | 2.42        | 0.54     |
| 52:DW:32:ALA:C     | 52:DW:34:SER:H     | 2.10        | 0.54     |
| 48:BG:51:PHE:CD2   | 48:BG:68:ARG:HG2   | 2.43        | 0.54     |
| 44:BQ:26:ALA:HB1   | 44:BQ:30:VAL:CG1   | 2.38        | 0.54     |
| 22:BA:43:C:H2'     | 22:BA:44:G:H5''    | 1.90        | 0.54     |
| 26:BD:111:GLY:H    | 26:BD:194:PRO:HG3  | 1.72        | 0.54     |
| 37:DL:113:ALA:HB3  | 37:DL:115:GLU:OE1  | 2.07        | 0.54     |
| 7:AH:87:ARG:N      | 7:AH:90:GLU:HB3    | 2.23        | 0.54     |
| 30:DY:7:THR:HG23   | 30:DY:34:THR:OG1   | 2.08        | 0.54     |
| 50:BT:47:VAL:HG13  | 50:BT:51:PHE:HD1   | 1.72        | 0.54     |
| 48:BG:26:LYS:HA    | 48:BG:32:LEU:HA    | 1.90        | 0.54     |
| 51:BZ:51:VAL:HG11  | 51:BZ:56:MET:HG3   | 1.90        | 0.54     |
| 47:BF:7:TYR:HA     | 47:BF:11:VAL:CG2   | 2.38        | 0.54     |
| 29:BE:154:ASP:OD1  | 29:BE:156:ASN:HB3  | 2.07        | 0.54     |
| 1:CA:1317:C:OP1    | 13:CN:56:PRO:HD2   | 2.06        | 0.54     |
| 25:DC:16:VAL:N     | 25:DC:203:VAL:HG12 | 2.23        | 0.54     |
| 21:CU:3:ILE:HD11   | 21:CU:23:GLU:HB2   | 1.87        | 0.54     |
| 15:AP:54:LEU:HD22  | 15:AP:80:LYS:HE3   | 1.89        | 0.54     |
| 32:D4:8:LYS:O      | 32:D4:25:VAL:HG21  | 2.08        | 0.54     |
| 48:DG:148:ARG:HB2  | 48:DG:152:ARG:HH21 | 1.73        | 0.54     |
| 27:DK:8:LEU:H      | 27:DK:8:LEU:HD12   | 1.73        | 0.54     |
| 20:AB:40:ILE:HG21  | 20:AB:200:PRO:O    | 2.07        | 0.54     |
| 42:BN:34:ILE:O     | 42:BN:112:TYR:HA   | 2.08        | 0.54     |
| 10:CK:83:VAL:CB    | 10:CK:109:ILE:HG23 | 2.37        | 0.54     |
| 23:DB:1549:A:H2'   | 23:DB:1550:C:C6    | 2.43        | 0.54     |
| 28:BP:3:ILE:HG23   | 28:BP:4:ILE:HG13   | 1.88        | 0.54     |
| 1:AA:1073:U:H4'    | 20:AB:104:LYS:HE3  | 1.89        | 0.54     |
| 3:AD:89:LEU:HD23   | 3:AD:199:ILE:HD11  | 1.90        | 0.54     |
| 20:CB:95:TRP:CZ2   | 20:CB:100:LEU:HD13 | 2.43        | 0.54     |
| 33:B1:47:ILE:H     | 33:B1:47:ILE:HD12  | 1.73        | 0.54     |
| 20:CB:172:ILE:HG22 | 20:CB:176:ASN:ND2  | 2.23        | 0.54     |
| 23:DB:1401:G:H2'   | 23:DB:1402:U:C6    | 2.42        | 0.54     |
| 45:BS:30:SER:O     | 45:BS:33:LEU:HB2   | 2.07        | 0.54     |
| 1:AA:373:A:H1'     | 1:AA:481:G:N3      | 2.23        | 0.54     |
| 50:BT:44:LYS:O     | 50:BT:48:GLN:HG2   | 2.08        | 0.54     |
| 41:DJ:72:LYS:HB2   | 41:DJ:89:PHE:HB2   | 1.89        | 0.54     |
| 23:BB:2491:U:H5''  | 23:BB:2570:G:H5''  | 1.90        | 0.54     |
| 1:AA:692:U:H2'     | 1:AA:694:A:OP2     | 2.08        | 0.54     |
| 23:BB:2728:U:H2'   | 23:BB:2729:G:C8    | 2.42        | 0.54     |
| 26:BD:174:SER:O    | 26:BD:175:LEU:HB2  | 2.07        | 0.54     |
| 1:AA:477:C:H2'     | 1:AA:478:A:C8      | 2.43        | 0.54     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 12:AM:43:LYS:O     | 12:AM:46:GLU:HG3   | 2.08        | 0.54     |
| 23:BB:861:A:H2'    | 23:BB:862:G:O4'    | 2.07        | 0.54     |
| 23:BB:1010:A:N3    | 23:BB:1153:C:H1'   | 2.23        | 0.54     |
| 25:BC:261:ARG:HG2  | 25:BC:261:ARG:O    | 2.08        | 0.54     |
| 1:AA:54:C:H2'      | 1:AA:352:C:H41     | 1.72        | 0.54     |
| 23:BB:813:U:H2'    | 23:BB:814:C:C6     | 2.43        | 0.54     |
| 3:CD:87:GLU:OE1    | 3:CD:91:ALA:HB2    | 2.08        | 0.54     |
| 23:BB:1276:A:O2'   | 23:BB:1277:G:H5'   | 2.07        | 0.54     |
| 23:DB:2543:G:H2'   | 23:DB:2544:G:O4'   | 2.07        | 0.54     |
| 23:BB:2677:G:H2'   | 23:BB:2678:C:C6    | 2.43        | 0.54     |
| 5:AF:43:GLY:HA2    | 5:AF:58:HIS:NE2    | 2.21        | 0.54     |
| 23:BB:806:C:O2'    | 23:BB:807:U:H5'    | 2.08        | 0.54     |
| 23:DB:1295:C:H2'   | 23:DB:1296:G:C8    | 2.43        | 0.54     |
| 28:BP:30:TRP:HD1   | 28:BP:39:LEU:HG    | 1.73        | 0.54     |
| 23:BB:2543:G:H2'   | 23:BB:2544:G:O4'   | 2.07        | 0.54     |
| 40:DH:27:ARG:H     | 40:DH:31:VAL:HG21  | 1.71        | 0.54     |
| 25:BC:143:VAL:HG12 | 25:BC:144:GLU:H    | 1.71        | 0.54     |
| 23:DB:2355:G:H4'   | 52:DW:20:LEU:CD1   | 2.37        | 0.54     |
| 23:DB:1821:A:H2'   | 23:DB:1822:C:H6    | 1.69        | 0.54     |
| 25:DC:141:HIS:HB3  | 25:DC:190:THR:OG1  | 2.07        | 0.54     |
| 11:CL:38:THR:OG1   | 53:D6:84:ARG:HG2   | 2.07        | 0.54     |
| 23:DB:856:G:C1'    | 52:DW:23:LYS:HB3   | 2.38        | 0.54     |
| 53:B6:58:VAL:HG12  | 53:B6:59:THR:H     | 1.73        | 0.54     |
| 40:BH:121:VAL:HG21 | 40:BH:128:HIS:NE2  | 2.23        | 0.54     |
| 40:BH:81:ALA:CB    | 40:BH:147:VAL:HG23 | 2.37        | 0.54     |
| 1:AA:1219:A:H2'    | 1:AA:1220:G:H8     | 1.73        | 0.54     |
| 48:DG:26:LYS:HA    | 48:DG:32:LEU:HA    | 1.90        | 0.54     |
| 47:BF:103:ILE:HD11 | 47:BF:174:PHE:CA   | 2.36        | 0.54     |
| 47:DF:133:GLU:HA   | 47:DF:150:GLY:HA2  | 1.90        | 0.54     |
| 10:AK:92:ARG:NH2   | 21:AU:24:LYS:HG2   | 2.22        | 0.54     |
| 1:AA:979:C:H1'     | 1:AA:1317:C:H41    | 1.72        | 0.54     |
| 29:BE:28:VAL:O     | 29:BE:32:VAL:HG13  | 2.07        | 0.54     |
| 15:AP:75:ILE:HG22  | 15:AP:80:LYS:HD2   | 1.89        | 0.54     |
| 29:DE:134:LEU:HD21 | 29:DE:161:ALA:HB2  | 1.89        | 0.54     |
| 20:AB:60:ALA:HB1   | 20:AB:220:VAL:HG13 | 1.89        | 0.54     |
| 20:CB:15:PHE:HA    | 20:CB:42:LEU:HD21  | 1.90        | 0.54     |
| 38:BM:126:ILE:HD12 | 38:BM:126:ILE:N    | 2.20        | 0.54     |
| 44:BQ:86:SER:HB2   | 49:BR:50:GLY:O     | 2.08        | 0.54     |
| 49:DR:39:LEU:HB2   | 49:DR:49:ILE:HG12  | 1.88        | 0.54     |
| 50:DT:18:GLU:C     | 50:DT:20:ALA:H     | 2.11        | 0.54     |
| 29:DE:176:ASP:OD1  | 29:DE:178:VAL:HG12 | 2.07        | 0.54     |
| 1:AA:551:U:H2'     | 1:AA:552:U:H6      | 1.72        | 0.54     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 27:BK:88:ASN:HD22 | 27:BK:89:ASN:N    | 2.05        | 0.54     |
| 1:CA:254:G:H4'    | 16:CQ:19:SER:OG   | 2.08        | 0.54     |
| 20:CB:95:TRP:CH2  | 20:CB:100:LEU:HB2 | 2.41        | 0.54     |
| 23:BB:2419:U:H2'  | 23:BB:2420:C:C6   | 2.43        | 0.54     |
| 23:BB:1583:A:H4'  | 23:BB:1585:C:C4   | 2.43        | 0.54     |
| 39:DX:21:LEU:HA   | 39:DX:25:GLN:HB3  | 1.89        | 0.54     |
| 24:BI:100:ILE:O   | 24:BI:139:VAL:HA  | 2.07        | 0.54     |
| 23:DB:1249:U:H4'  | 44:DQ:3:VAL:HG11  | 1.90        | 0.54     |
| 7:AH:51:GLU:HG2   | 7:AH:52:GLY:N     | 2.23        | 0.54     |
| 23:DB:2852:G:H2'  | 23:DB:2853:C:H6   | 1.71        | 0.54     |
| 19:CT:50:PHE:O    | 19:CT:53:MET:HG3  | 2.08        | 0.54     |
| 11:CL:33:CYS:HB2  | 11:CL:77:SER:O    | 2.07        | 0.54     |
| 23:DB:528:A:N1    | 23:DB:2042:A:H2'  | 2.22        | 0.54     |
| 29:DE:18:THR:HA   | 29:DE:106:LYS:HD3 | 1.90        | 0.54     |
| 23:DB:904:G:H2'   | 23:DB:905:A:C8    | 2.43        | 0.54     |
| 23:DB:2570:G:H2'  | 23:DB:2571:U:O4'  | 2.07        | 0.54     |
| 23:BB:355:U:H2'   | 23:BB:356:G:C8    | 2.43        | 0.54     |
| 23:BB:877:A:H2    | 23:BB:900:A:N7    | 2.05        | 0.54     |
| 23:DB:1742:U:H2'  | 23:DB:1743:G:C8   | 2.43        | 0.54     |
| 22:DA:10:G:H2'    | 22:DA:11:C:O4'    | 2.08        | 0.54     |
| 4:AE:22:LYS:HB3   | 4:AE:29:ILE:HB    | 1.90        | 0.54     |
| 23:BB:2210:U:N3   | 23:BB:2212:A:N7   | 2.54        | 0.54     |
| 1:CA:462:G:H2'    | 1:CA:463:U:C6     | 2.43        | 0.54     |
| 23:BB:394:C:H2'   | 23:BB:395:U:O4'   | 2.08        | 0.54     |
| 1:CA:1013:G:H2'   | 1:CA:1015:G:OP2   | 2.07        | 0.54     |
| 23:DB:1577:C:H2'  | 23:DB:1578:U:C6   | 2.42        | 0.54     |
| 1:AA:721:G:H4'    | 1:AA:722:G:O4'    | 2.07        | 0.54     |
| 25:DC:65:ASP:CG   | 25:DC:65:ASP:O    | 2.46        | 0.54     |
| 53:B6:58:VAL:HG22 | 53:B6:68:VAL:HA   | 1.89        | 0.54     |
| 53:B6:68:VAL:HG21 | 53:B6:99:LEU:HD12 | 1.90        | 0.54     |
| 8:CI:20:ILE:HG23  | 8:CI:60:LEU:HD11  | 1.88        | 0.54     |
| 41:DJ:4:PHE:CG    | 41:DJ:5:THR:N     | 2.75        | 0.54     |
| 8:AI:50:PRO:O     | 8:AI:54:VAL:HG22  | 2.07        | 0.54     |
| 43:DO:35:ILE:HG21 | 43:DO:71:ALA:CB   | 2.38        | 0.54     |
| 23:BB:996:A:H4'   | 44:BQ:91:ARG:HH11 | 1.71        | 0.54     |
| 42:BN:80:PHE:O    | 42:BN:85:PRO:HD3  | 2.08        | 0.54     |
| 47:BF:7:TYR:O     | 47:BF:12:VAL:HG23 | 2.08        | 0.54     |
| 43:BO:88:LYS:HG2  | 43:BO:89:ASP:N    | 2.23        | 0.54     |
| 12:AM:79:LEU:CD2  | 12:AM:86:ARG:HH21 | 2.21        | 0.54     |
| 23:BB:675:A:H4'   | 29:BE:60:TRP:HZ2  | 1.71        | 0.54     |
| 50:DT:50:LEU:HD22 | 50:DT:50:LEU:N    | 2.23        | 0.54     |
| 45:DS:66:ILE:HD13 | 45:DS:66:ILE:N    | 2.20        | 0.54     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 26:BD:9:VAL:O      | 28:BP:4:ILE:HD11   | 2.08        | 0.54     |
| 28:BP:3:ILE:HG23   | 28:BP:4:ILE:N      | 2.23        | 0.54     |
| 1:CA:1058:G:OP1    | 2:CC:198:LYS:HE3   | 2.07        | 0.54     |
| 23:BB:37:C:O2'     | 23:BB:38:A:H5'     | 2.08        | 0.54     |
| 39:DX:20:ASN:N     | 39:DX:20:ASN:ND2   | 2.54        | 0.54     |
| 1:CA:1343:G:H2'    | 1:CA:1344:C:H6     | 1.73        | 0.54     |
| 19:CT:68:LYS:HA    | 19:CT:68:LYS:HE2   | 1.90        | 0.54     |
| 37:BL:47:ARG:HG3   | 37:BL:48:ARG:N     | 2.22        | 0.54     |
| 1:CA:1254:A:O4'    | 1:CA:1356:G:H5''   | 2.08        | 0.54     |
| 1:AA:1533:C:O2'    | 1:AA:1534:A:H5''   | 2.07        | 0.54     |
| 1:AA:1512:U:H2'    | 1:AA:1513:A:H8     | 1.73        | 0.54     |
| 23:DB:2415:G:H2'   | 23:DB:2416:C:H6    | 1.72        | 0.54     |
| 25:DC:71:ASP:OD2   | 25:DC:118:GLY:HA2  | 2.08        | 0.54     |
| 23:DB:2700:A:H2'   | 23:DB:2701:U:H6    | 1.73        | 0.54     |
| 51:DZ:69:ALA:HA    | 51:DZ:72:ARG:NH1   | 2.23        | 0.54     |
| 50:DT:44:LYS:O     | 50:DT:48:GLN:HG2   | 2.08        | 0.54     |
| 23:DB:2369:A:H2'   | 23:DB:2370:G:H8    | 1.71        | 0.54     |
| 1:AA:284:C:H2'     | 1:AA:285:C:H6      | 1.72        | 0.54     |
| 1:CA:730:G:O2'     | 1:CA:766:A:H5'     | 2.07        | 0.54     |
| 23:BB:441:U:H2'    | 23:BB:442:G:H8     | 1.73        | 0.54     |
| 1:CA:98:A:H2'      | 1:CA:99:C:C6       | 2.43        | 0.54     |
| 12:AM:58:GLU:O     | 12:AM:61:LYS:HG2   | 2.08        | 0.54     |
| 23:DB:189:G:H2'    | 23:DB:205:G:H22    | 1.73        | 0.54     |
| 23:DB:1676:A:H2'   | 23:DB:1677:A:O4'   | 2.07        | 0.54     |
| 48:BG:132:LEU:O    | 48:BG:132:LEU:HD12 | 2.08        | 0.54     |
| 52:DW:49:ASN:HA    | 52:DW:61:LYS:HB2   | 1.90        | 0.54     |
| 8:CI:23:GLY:N      | 8:CI:60:LEU:HA     | 2.20        | 0.54     |
| 20:CB:14:HIS:HD2   | 20:CB:202:ASN:H    | 1.53        | 0.54     |
| 41:BJ:44:TYR:CE2   | 44:BQ:59:LEU:HD11  | 2.43        | 0.54     |
| 23:BB:2199:A:H3'   | 23:BB:2200:C:H6    | 1.71        | 0.54     |
| 47:BF:134:GLN:O    | 47:BF:136:ILE:N    | 2.40        | 0.54     |
| 40:DH:87:GLU:HB2   | 40:DH:89:LYS:NZ    | 2.23        | 0.54     |
| 47:DF:174:PHE:HB3  | 47:DF:176:PHE:CD1  | 2.43        | 0.54     |
| 18:AS:39:ILE:HG12  | 18:AS:70:LEU:HD12  | 1.89        | 0.54     |
| 10:CK:88:PRO:HD3   | 21:CU:28:LEU:CD1   | 2.37        | 0.54     |
| 30:DY:2:LYS:HE3    | 30:DY:58:GLU:HB3   | 1.89        | 0.54     |
| 11:CL:26:CYS:SG    | 11:CL:29:LYS:HE2   | 2.48        | 0.54     |
| 27:BK:115:ILE:HG23 | 27:BK:116:ILE:N    | 2.22        | 0.54     |
| 1:AA:1239:A:N6     | 1:AA:1299:A:H62    | 2.05        | 0.54     |
| 23:DB:1439:A:N7    | 23:DB:1440:U:N1    | 2.55        | 0.54     |
| 36:B2:10:LEU:HD11  | 36:B2:14:ARG:CZ    | 2.38        | 0.54     |
| 40:DH:113:SER:HB2  | 40:DH:132:PHE:CZ   | 2.43        | 0.54     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:337:G:H2'    | 1:AA:338:A:H8      | 1.71        | 0.54     |
| 14:AO:81:LEU:HD23 | 14:AO:85:LEU:HD13  | 1.89        | 0.54     |
| 23:BB:1796:U:O2'  | 23:BB:1797:G:H5'   | 2.07        | 0.54     |
| 41:BJ:99:ARG:O    | 41:BJ:103:ILE:HG13 | 2.08        | 0.54     |
| 1:AA:706:A:C4'    | 10:AK:30:ILE:HD11  | 2.38        | 0.54     |
| 27:BK:87:LEU:HD12 | 27:BK:92:GLU:HA    | 1.89        | 0.54     |
| 23:BB:1488:C:O2'  | 23:BB:1489:C:H5'   | 2.07        | 0.54     |
| 1:CA:253:A:H2'    | 1:CA:254:G:C8      | 2.42        | 0.54     |
| 23:BB:1688:U:O2   | 23:BB:1700:A:H5'   | 2.08        | 0.54     |
| 45:DS:31:GLN:C    | 45:DS:33:LEU:H     | 2.09        | 0.54     |
| 1:CA:734:G:O2'    | 17:CR:59:LYS:HD3   | 2.08        | 0.54     |
| 6:CG:21:LEU:HG    | 6:CG:22:LEU:N      | 2.21        | 0.54     |
| 23:BB:1387:A:H2'  | 23:BB:1388:G:C8    | 2.41        | 0.54     |
| 1:CA:677:U:H1'    | 10:CK:120:CYS:SG   | 2.48        | 0.54     |
| 53:D6:33:ALA:CB   | 53:D6:63:PRO:HA    | 2.38        | 0.54     |
| 17:CR:31:TYR:CG   | 17:CR:54:LEU:HD11  | 2.43        | 0.54     |
| 23:BB:2415:G:H2'  | 23:BB:2416:C:H6    | 1.72        | 0.54     |
| 23:BB:2635:A:H4'  | 26:BD:79:LEU:HB2   | 1.90        | 0.54     |
| 23:DB:831:G:H2'   | 23:DB:832:U:O4'    | 2.07        | 0.54     |
| 1:CA:477:C:H2'    | 1:CA:478:A:C8      | 2.43        | 0.54     |
| 23:BB:1395:A:H4'  | 23:BB:1397:U:C5    | 2.42        | 0.54     |
| 2:AC:13:ILE:HD13  | 2:AC:13:ILE:N      | 2.23        | 0.54     |
| 23:BB:2196:C:H2'  | 23:BB:2197:U:C6    | 2.43        | 0.54     |
| 23:DB:1119:U:O2'  | 23:DB:1120:G:H5'   | 2.08        | 0.54     |
| 1:AA:55:A:OP2     | 1:AA:352:C:N4      | 2.40        | 0.54     |
| 23:BB:423:A:H5''  | 23:BB:424:G:H5'    | 1.89        | 0.54     |
| 22:BA:16:G:O2'    | 22:BA:17:C:H5'     | 2.07        | 0.54     |
| 52:BW:75:ASN:O    | 52:BW:76:ARG:HB2   | 2.08        | 0.54     |
| 25:DC:124:LYS:HG3 | 25:DC:125:PRO:HD2  | 1.89        | 0.54     |
| 22:BA:35:C:H2'    | 22:BA:36:C:C5'     | 2.37        | 0.54     |
| 23:DB:1339:G:N2   | 23:DB:1603:A:H1'   | 2.22        | 0.54     |
| 23:DB:2822:G:H2'  | 23:DB:2823:A:H5''  | 1.90        | 0.54     |
| 2:CC:181:ILE:HD12 | 2:CC:181:ILE:N     | 2.23        | 0.54     |
| 23:BB:2666:C:O4'  | 23:BB:2666:C:O2    | 2.24        | 0.54     |
| 42:BN:7:GLY:HA2   | 42:BN:46:ARG:HH11  | 1.73        | 0.54     |
| 40:BH:1:MET:HB3   | 40:BH:21:VAL:O     | 2.08        | 0.54     |
| 1:AA:113:G:O4'    | 1:AA:354:G:H4'     | 2.07        | 0.54     |
| 19:AT:14:GLU:OE2  | 19:AT:18:LYS:HE2   | 2.08        | 0.54     |
| 19:AT:19:HIS:O    | 19:AT:23:ARG:HG2   | 2.08        | 0.54     |
| 48:BG:93:TYR:C    | 48:BG:94:ARG:HG3   | 2.27        | 0.54     |
| 20:AB:187:ASP:H   | 20:AB:190:SER:HB2  | 1.73        | 0.54     |
| 48:DG:84:LYS:HG3  | 48:DG:132:LEU:N    | 2.23        | 0.54     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 26:BD:105:LYS:N   | 26:BD:106:LYS:HZ3  | 2.03        | 0.54     |
| 53:B6:72:ASP:HB3  | 53:B6:75:ALA:HB2   | 1.88        | 0.54     |
| 47:DF:115:GLY:CA  | 47:DF:177:ARG:HH11 | 2.20        | 0.54     |
| 41:DJ:45:THR:N    | 41:DJ:46:PRO:HD3   | 2.21        | 0.54     |
| 44:DQ:77:LYS:HA   | 44:DQ:80:ASN:HB3   | 1.90        | 0.54     |
| 35:DV:72:VAL:HB   | 35:DV:92:VAL:O     | 2.08        | 0.54     |
| 48:DG:34:ARG:HH11 | 48:DG:34:ARG:HG2   | 1.72        | 0.54     |
| 44:BQ:57:ARG:NH1  | 44:BQ:57:ARG:HG2   | 2.22        | 0.54     |
| 25:BC:65:ASP:CG   | 25:BC:65:ASP:O     | 2.46        | 0.54     |
| 1:AA:429:U:H1'    | 1:AA:430:A:H5''    | 1.90        | 0.54     |
| 1:AA:978:A:H5'    | 1:AA:1362:A:H61    | 1.73        | 0.54     |
| 11:AL:86:VAL:HB   | 11:AL:89:LEU:HB2   | 1.88        | 0.54     |
| 1:AA:332:G:O2'    | 1:AA:333:U:H5'     | 2.08        | 0.54     |
| 15:AP:6:LEU:HD23  | 15:AP:17:TYR:HB2   | 1.90        | 0.54     |
| 13:CN:51:PRO:HG2  | 13:CN:52:ARG:H     | 1.73        | 0.54     |
| 43:DO:58:ILE:HG22 | 43:DO:62:LEU:CD2   | 2.36        | 0.54     |
| 1:AA:1339:A:H2'   | 1:AA:1340:A:O4'    | 2.08        | 0.54     |
| 42:BN:72:ASP:OD1  | 42:BN:75:ILE:HG23  | 2.07        | 0.54     |
| 23:BB:1566:A:H5'  | 25:BC:213:ARG:NH2  | 2.23        | 0.54     |
| 27:BK:20:MET:C    | 27:BK:41:ILE:HD12  | 2.28        | 0.54     |
| 27:DK:105:ARG:HD2 | 27:DK:122:VAL:HG11 | 1.90        | 0.54     |
| 1:CA:1414:U:H2'   | 1:CA:1415:G:C8     | 2.43        | 0.54     |
| 10:CK:23:HIS:O    | 10:CK:29:THR:HA    | 2.08        | 0.54     |
| 27:BK:58:LEU:CD1  | 27:BK:86:LEU:HB3   | 2.38        | 0.54     |
| 23:BB:8:C:O2'     | 23:BB:9:G:H5'      | 2.08        | 0.54     |
| 23:DB:1197:G:O2'  | 23:DB:1198:U:H5'   | 2.07        | 0.54     |
| 20:CB:65:LYS:HB2  | 20:CB:158:ASP:H    | 1.73        | 0.54     |
| 23:BB:125:A:H3'   | 23:BB:126:A:H5''   | 1.90        | 0.54     |
| 1:CA:1239:A:N6    | 1:CA:1299:A:H62    | 2.06        | 0.54     |
| 20:CB:119:GLN:NE2 | 20:CB:124:THR:HG23 | 2.22        | 0.54     |
| 1:AA:272:C:H2'    | 1:AA:273:U:C6      | 2.42        | 0.54     |
| 23:BB:2822:G:H2'  | 23:BB:2823:A:H5''  | 1.90        | 0.54     |
| 1:AA:254:G:H4'    | 16:AQ:19:SER:OG    | 2.08        | 0.54     |
| 1:CA:239:U:C5'    | 1:CA:239:U:H6      | 2.21        | 0.54     |
| 11:AL:106:VAL:CG2 | 11:AL:116:TYR:HB3  | 2.38        | 0.54     |
| 23:DB:64:A:H2'    | 23:DB:65:U:H6      | 1.68        | 0.54     |
| 23:DB:1582:C:H3'  | 23:DB:1583:A:C2    | 2.42        | 0.54     |
| 11:CL:79:ILE:HD12 | 11:CL:96:THR:HG22  | 1.90        | 0.54     |
| 19:AT:53:MET:O    | 19:AT:57:VAL:HG22  | 2.08        | 0.54     |
| 1:CA:1499:A:O2'   | 1:CA:1500:A:H5'    | 2.08        | 0.54     |
| 38:BM:4:PRO:HG3   | 38:BM:68:PHE:HE2   | 1.73        | 0.54     |
| 1:AA:1494:G:O2'   | 1:AA:1495:U:H5'    | 2.08        | 0.54     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:DB:2455:G:H2'   | 23:DB:2456:C:H6   | 1.72        | 0.54     |
| 23:BB:871:U:H2'    | 23:BB:872:U:H6    | 1.73        | 0.54     |
| 20:CB:129:THR:C    | 20:CB:131:LYS:H   | 2.10        | 0.54     |
| 1:AA:1332:A:H2'    | 1:AA:1333:A:H8    | 1.73        | 0.54     |
| 23:DB:2569:G:O2'   | 23:DB:2570:G:H5'  | 2.07        | 0.54     |
| 1:CA:168:G:O2'     | 1:CA:169:C:H5'    | 2.08        | 0.54     |
| 23:DB:1301:A:O2'   | 23:DB:1302:A:H2'  | 2.08        | 0.54     |
| 23:DB:1499:C:H2'   | 23:DB:1500:G:H8   | 1.73        | 0.54     |
| 23:BB:1897:G:O2'   | 23:BB:1898:U:H5'  | 2.08        | 0.54     |
| 34:D3:56:LEU:O     | 34:D3:59:ALA:HB3  | 2.08        | 0.54     |
| 1:CA:1175:G:O2'    | 1:CA:1176:A:H5'   | 2.07        | 0.54     |
| 23:DB:2097:A:H2'   | 23:DB:2098:U:C6   | 2.42        | 0.54     |
| 23:BB:1464:G:H2'   | 23:BB:1465:G:H8   | 1.73        | 0.54     |
| 25:BC:175:LEU:HD11 | 25:BC:181:ARG:HG3 | 1.90        | 0.54     |
| 23:DB:429:A:H2'    | 23:DB:430:A:C8    | 2.43        | 0.54     |
| 23:BB:657:U:H2'    | 23:BB:658:U:C6    | 2.43        | 0.54     |
| 34:B3:50:SER:C     | 34:B3:52:GLY:H    | 2.12        | 0.54     |
| 17:AR:19:GLU:HG3   | 17:AR:54:LEU:HD12 | 1.90        | 0.54     |
| 23:BB:2636:C:H2'   | 23:BB:2637:U:C6   | 2.42        | 0.54     |
| 23:BB:564:C:O2'    | 23:BB:565:C:H5'   | 2.08        | 0.54     |
| 23:DB:1825:U:H2'   | 23:DB:1826:G:H8   | 1.73        | 0.54     |
| 48:DG:93:TYR:C     | 48:DG:94:ARG:HG3  | 2.28        | 0.54     |
| 40:BH:80:ILE:HD12  | 40:BH:144:VAL:CG2 | 2.34        | 0.54     |
| 20:CB:69:VAL:HB    | 20:CB:162:VAL:CB  | 2.38        | 0.54     |
| 1:AA:1219:A:H2'    | 1:AA:1220:G:C8    | 2.43        | 0.54     |
| 30:DY:40:THR:HG22  | 30:DY:42:ALA:H    | 1.73        | 0.54     |
| 44:BQ:91:ARG:HE    | 49:BR:11:GLN:HB2  | 1.73        | 0.54     |
| 40:DH:127:GLU:H    | 40:DH:127:GLU:CD  | 2.12        | 0.54     |
| 43:BO:35:ILE:HG22  | 43:BO:53:THR:HG23 | 1.89        | 0.54     |
| 47:BF:141:ASP:CB   | 47:BF:144:LYS:HB2 | 2.38        | 0.54     |
| 42:DN:83:LEU:CA    | 42:DN:86:ARG:HB2  | 2.31        | 0.54     |
| 1:AA:923:A:H2'     | 1:AA:924:C:C6     | 2.43        | 0.54     |
| 47:DF:101:ARG:NH1  | 47:DF:138:PRO:HB2 | 2.22        | 0.54     |
| 12:AM:82:LEU:HD22  | 18:AS:73:PHE:HE2  | 1.72        | 0.54     |
| 23:BB:2868:A:H2'   | 23:BB:2869:G:C8   | 2.43        | 0.54     |
| 23:BB:2468:A:H2'   | 23:BB:2476:A:C6   | 2.43        | 0.54     |
| 53:B6:113:ASP:HA   | 53:B6:116:ARG:NE  | 2.22        | 0.54     |
| 11:CL:86:VAL:HG11  | 11:CL:89:LEU:HD23 | 1.89        | 0.54     |
| 13:CN:41:TRP:O     | 13:CN:44:VAL:HG12 | 2.08        | 0.54     |
| 49:BR:39:LEU:HD22  | 49:BR:53:PHE:HD1  | 1.73        | 0.54     |
| 5:AF:6:ILE:O       | 5:AF:6:ILE:HG13   | 2.07        | 0.54     |
| 4:AE:45:VAL:O      | 4:AE:71:ILE:HG22  | 2.08        | 0.54     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:1386:C:H2'   | 23:BB:1387:A:H8    | 1.71        | 0.54     |
| 23:BB:2243:U:H2'   | 23:BB:2244:U:H6    | 1.73        | 0.54     |
| 23:DB:1353:A:H2'   | 23:DB:1354:A:C8    | 2.43        | 0.54     |
| 23:DB:665:U:O2'    | 23:DB:666:A:H5'    | 2.08        | 0.54     |
| 14:CO:7:ALA:O      | 14:CO:11:ILE:HG22  | 2.08        | 0.54     |
| 20:AB:172:ILE:HG22 | 20:AB:176:ASN:ND2  | 2.23        | 0.54     |
| 5:AF:47:LEU:HD21   | 5:AF:57:ALA:CB     | 2.38        | 0.54     |
| 1:CA:87:C:C2'      | 1:CA:88:U:H5''     | 2.38        | 0.54     |
| 1:AA:677:U:H2'     | 1:AA:678:U:C6      | 2.43        | 0.54     |
| 1:AA:1170:A:H2'    | 1:AA:1171:A:O4'    | 2.08        | 0.54     |
| 43:DO:79:ALA:HA    | 43:DO:115:LEU:HD23 | 1.90        | 0.54     |
| 23:BB:2835:A:H61   | 23:BB:2878:U:H2'   | 1.72        | 0.54     |
| 23:DB:2814:A:H2'   | 23:DB:2815:C:H6    | 1.72        | 0.54     |
| 2:AC:13:ILE:H      | 2:AC:13:ILE:HD13   | 1.73        | 0.54     |
| 23:BB:2322:A:N6    | 23:BB:2333:A:N6    | 2.55        | 0.54     |
| 23:BB:2678:C:H2'   | 23:BB:2679:A:C8    | 2.42        | 0.54     |
| 12:CM:64:VAL:HA    | 12:CM:68:LEU:CD1   | 2.38        | 0.54     |
| 23:BB:445:C:O2'    | 23:BB:446:G:H5'    | 2.08        | 0.54     |
| 23:DB:423:A:H5''   | 23:DB:424:G:H5'    | 1.89        | 0.54     |
| 1:CA:820:U:H4'     | 1:CA:821:G:OP2     | 2.08        | 0.54     |
| 51:DZ:41:GLU:O     | 51:DZ:44:LYS:HD2   | 2.07        | 0.54     |
| 1:CA:487:A:H2'     | 1:CA:488:C:O4'     | 2.08        | 0.54     |
| 23:BB:1965:C:H5''  | 23:BB:1966:A:H2'   | 1.88        | 0.54     |
| 26:DD:38:LYS:HD3   | 26:DD:45:TYR:OH    | 2.08        | 0.54     |
| 26:DD:45:TYR:HD2   | 26:DD:83:ARG:HD3   | 1.71        | 0.54     |
| 23:DB:1495:A:H2'   | 23:DB:1496:A:C8    | 2.43        | 0.54     |
| 23:BB:1820:U:OP1   | 25:BC:176:ARG:HD2  | 2.08        | 0.53     |
| 48:BG:9:VAL:H      | 48:BG:48:THR:HB    | 1.73        | 0.53     |
| 20:AB:210:THR:HA   | 20:AB:213:LEU:HB2  | 1.89        | 0.53     |
| 40:BH:133:GLN:HA   | 40:BH:139:PHE:HB3  | 1.90        | 0.53     |
| 27:BK:35:VAL:HG12  | 27:BK:69:VAL:CG2   | 2.37        | 0.53     |
| 53:B6:42:LYS:HA    | 53:B6:51:PRO:CA    | 2.28        | 0.53     |
| 1:CA:1351:U:O2'    | 1:CA:1352:C:H5'    | 2.08        | 0.53     |
| 44:DQ:57:ARG:HG2   | 44:DQ:57:ARG:HH11  | 1.73        | 0.53     |
| 5:AF:93:LYS:O      | 5:AF:94:HIS:HB2    | 2.07        | 0.53     |
| 50:BT:50:LEU:N     | 50:BT:50:LEU:HD22  | 2.23        | 0.53     |
| 41:BJ:45:THR:N     | 41:BJ:46:PRO:HD3   | 2.22        | 0.53     |
| 47:BF:43:ILE:HG13  | 47:BF:44:ALA:N     | 2.23        | 0.53     |
| 29:BE:117:ARG:HA   | 29:BE:185:LYS:HG2  | 1.90        | 0.53     |
| 47:DF:103:ILE:HD11 | 47:DF:174:PHE:CA   | 2.37        | 0.53     |
| 13:AN:41:TRP:O     | 13:AN:44:VAL:HG12  | 2.07        | 0.53     |
| 1:AA:1320:C:H41    | 18:AS:36:ARG:HB3   | 1.74        | 0.53     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 20:AB:15:PHE:HA    | 20:AB:42:LEU:HD11  | 1.89        | 0.53     |
| 26:DD:124:ARG:HA   | 26:DD:165:MET:HE3  | 1.89        | 0.53     |
| 29:DE:188:MET:HE3  | 29:DE:193:VAL:HG13 | 1.89        | 0.53     |
| 42:DN:32:GLU:O     | 42:DN:114:GLU:HA   | 2.08        | 0.53     |
| 38:BM:18:ARG:C     | 38:BM:38:ARG:HH22  | 2.11        | 0.53     |
| 1:AA:86:G:O2'      | 1:AA:88:U:H5       | 1.91        | 0.53     |
| 1:AA:1070:U:H2'    | 1:AA:1071:C:C6     | 2.42        | 0.53     |
| 37:BL:95:LEU:HB2   | 37:BL:101:ILE:HG13 | 1.88        | 0.53     |
| 23:BB:2747:G:O6    | 23:BB:2755:C:H5''  | 2.07        | 0.53     |
| 4:CE:148:SER:HB2   | 4:CE:150:GLU:OE1   | 2.08        | 0.53     |
| 35:BV:29:ILE:HD13  | 35:BV:31:TYR:CE2   | 2.44        | 0.53     |
| 1:CA:662:U:H2'     | 1:CA:663:A:C8      | 2.42        | 0.53     |
| 26:BD:33:ARG:NE    | 26:BD:74:GLU:HB3   | 2.23        | 0.53     |
| 23:BB:1593:A:H2'   | 23:BB:1594:U:H6    | 1.71        | 0.53     |
| 2:CC:46:LEU:HB3    | 2:CC:49:ALA:CB     | 2.38        | 0.53     |
| 24:BI:89:SER:HA    | 24:BI:97:VAL:CG2   | 2.38        | 0.53     |
| 23:DB:269:C:H2'    | 23:DB:270:A:C8     | 2.43        | 0.53     |
| 42:BN:51:LEU:HD11  | 42:BN:69:ARG:HG3   | 1.90        | 0.53     |
| 23:DB:2496:C:OP1   | 38:DM:82:MET:HB2   | 2.09        | 0.53     |
| 1:AA:389:A:H2'     | 1:AA:389:A:N3      | 2.23        | 0.53     |
| 27:DK:98:ARG:HE    | 27:DK:98:ARG:N     | 2.06        | 0.53     |
| 43:DO:66:GLY:HA2   | 43:DO:102:ARG:NE   | 2.23        | 0.53     |
| 23:DB:1475:G:H4'   | 23:DB:1476:U:O5'   | 2.07        | 0.53     |
| 53:D6:144:ALA:HA   | 53:D6:149:LEU:HG   | 1.90        | 0.53     |
| 6:AG:72:VAL:HG12   | 6:AG:89:GLU:HG3    | 1.89        | 0.53     |
| 1:CA:542:G:O2'     | 1:CA:543:U:H5'     | 2.08        | 0.53     |
| 52:DW:75:ASN:O     | 52:DW:76:ARG:HB2   | 2.07        | 0.53     |
| 23:DB:1528:A:H2'   | 23:DB:1529:G:O4'   | 2.08        | 0.53     |
| 45:BS:90:LYS:HD2   | 45:BS:92:ARG:NH1   | 2.23        | 0.53     |
| 1:AA:328:C:H4'     | 1:AA:329:A:H5''    | 1.90        | 0.53     |
| 25:DC:66:PHE:HB2   | 25:DC:150:GLY:O    | 2.09        | 0.53     |
| 20:AB:69:VAL:HG12  | 20:AB:168:GLU:HG3  | 1.90        | 0.53     |
| 20:AB:14:HIS:HD2   | 20:AB:202:ASN:H    | 1.55        | 0.53     |
| 22:DA:43:C:H2'     | 22:DA:44:G:H5''    | 1.91        | 0.53     |
| 23:BB:1022:G:N2    | 23:BB:1142:A:N1    | 2.55        | 0.53     |
| 20:CB:69:VAL:O     | 20:CB:163:ILE:HG22 | 2.07        | 0.53     |
| 5:AF:3:HIS:N       | 5:AF:3:HIS:CD2     | 2.76        | 0.53     |
| 26:DD:106:LYS:O    | 26:DD:107:VAL:HB   | 2.08        | 0.53     |
| 37:DL:110:VAL:HG23 | 37:DL:126:ARG:O    | 2.08        | 0.53     |
| 47:DF:40:GLY:HA2   | 47:DF:84:ILE:CG2   | 2.36        | 0.53     |
| 47:DF:78:ILE:N     | 47:DF:79:ARG:HH11  | 2.05        | 0.53     |
| 25:BC:80:LEU:HD11  | 25:BC:109:LEU:HG   | 1.91        | 0.53     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 33:B1:33:LEU:HB3  | 33:B1:51:ALA:CB    | 2.38        | 0.53     |
| 23:BB:673:C:H2'   | 23:BB:674:G:H5'    | 1.90        | 0.53     |
| 23:BB:675:A:OP1   | 29:BE:60:TRP:NE1   | 2.41        | 0.53     |
| 50:DT:47:VAL:HG13 | 50:DT:51:PHE:CD1   | 2.42        | 0.53     |
| 46:BU:27:VAL:CG2  | 46:BU:33:VAL:HG12  | 2.35        | 0.53     |
| 21:CU:16:ARG:NE   | 21:CU:16:ARG:HA    | 2.24        | 0.53     |
| 52:DW:10:ARG:O    | 52:DW:11:ASN:HB2   | 2.07        | 0.53     |
| 9:CJ:36:VAL:HA    | 9:CJ:76:ILE:HA     | 1.89        | 0.53     |
| 23:DB:1657:U:O2'  | 26:DD:138:LEU:HD12 | 2.08        | 0.53     |
| 1:AA:699:C:C2'    | 1:AA:700:G:H5''    | 2.35        | 0.53     |
| 23:BB:967:U:H2'   | 23:BB:968:C:C6     | 2.43        | 0.53     |
| 1:CA:332:G:O2'    | 1:CA:333:U:H5'     | 2.08        | 0.53     |
| 31:D0:38:LEU:HB3  | 31:D0:41:HIS:CD2   | 2.43        | 0.53     |
| 23:BB:171:U:H2'   | 23:BB:172:A:H8     | 1.72        | 0.53     |
| 38:DM:40:ARG:HB2  | 38:DM:93:VAL:HG22  | 1.89        | 0.53     |
| 2:CC:51:VAL:HA    | 2:CC:69:THR:HA     | 1.89        | 0.53     |
| 26:BD:8:LYS:CD    | 26:BD:197:THR:H    | 2.21        | 0.53     |
| 2:AC:26:LYS:HG3   | 2:AC:27:GLU:N      | 2.23        | 0.53     |
| 23:DB:62:U:H2'    | 23:DB:63:A:O4'     | 2.09        | 0.53     |
| 23:DB:559:G:H21   | 44:DQ:51:GLN:HE22  | 1.56        | 0.53     |
| 22:BA:74:U:O5'    | 22:BA:74:U:H6      | 1.90        | 0.53     |
| 41:BJ:72:LYS:HB2  | 41:BJ:89:PHE:HB2   | 1.90        | 0.53     |
| 23:DB:1236:G:H1'  | 23:DB:1237:A:C8    | 2.43        | 0.53     |
| 39:BX:21:LEU:HA   | 39:BX:25:GLN:HB3   | 1.89        | 0.53     |
| 23:DB:1429:G:O2'  | 23:DB:1430:G:H5'   | 2.08        | 0.53     |
| 6:CG:19:SER:OG    | 6:CG:22:LEU:HB2    | 2.07        | 0.53     |
| 1:AA:737:C:H2'    | 1:AA:738:C:C6      | 2.43        | 0.53     |
| 23:BB:1889:A:H2'  | 23:BB:1890:A:H8    | 1.71        | 0.53     |
| 19:AT:50:PHE:O    | 19:AT:53:MET:HG3   | 2.08        | 0.53     |
| 23:BB:2700:A:H2'  | 23:BB:2701:U:H6    | 1.73        | 0.53     |
| 23:DB:1166:G:H2'  | 23:DB:1167:C:H6    | 1.72        | 0.53     |
| 26:DD:159:LYS:O   | 26:DD:161:MET:HG2  | 2.08        | 0.53     |
| 50:DT:32:LEU:O    | 50:DT:83:ALA:HB2   | 2.08        | 0.53     |
| 23:BB:1316:U:O2'  | 23:BB:1317:G:H5'   | 2.07        | 0.53     |
| 41:DJ:29:ALA:O    | 41:DJ:32:LEU:HB2   | 2.07        | 0.53     |
| 23:DB:680:C:H2'   | 23:DB:681:G:H8     | 1.73        | 0.53     |
| 23:BB:1347:A:H2'  | 23:BB:1348:C:O4'   | 2.08        | 0.53     |
| 19:AT:48:LYS:O    | 19:AT:52:GLU:HB3   | 2.08        | 0.53     |
| 23:BB:833:A:H2'   | 23:BB:834:G:C8     | 2.42        | 0.53     |
| 35:DV:16:ALA:HA   | 35:DV:19:ARG:HE    | 1.73        | 0.53     |
| 23:DB:1299:G:H4'  | 23:DB:1301:A:H1'   | 1.90        | 0.53     |
| 20:CB:93:HIS:CD2  | 20:CB:145:ASN:HB3  | 2.43        | 0.53     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1154:G:O2'    | 1:AA:1155:A:H5'    | 2.08        | 0.53     |
| 1:AA:386:C:O2'     | 1:AA:387:U:H5'     | 2.08        | 0.53     |
| 47:DF:119:LYS:HA   | 47:DF:121:PHE:CE1  | 2.42        | 0.53     |
| 23:DB:244:A:H1'    | 23:DB:255:A:N6     | 2.23        | 0.53     |
| 25:DC:131:MET:HE1  | 25:DC:143:VAL:HG13 | 1.91        | 0.53     |
| 23:BB:2033:A:O2'   | 23:BB:2035:G:OP2   | 2.24        | 0.53     |
| 37:BL:141:LYS:HZ3  | 37:BL:143:GLU:HA   | 1.74        | 0.53     |
| 5:CF:93:LYS:O      | 5:CF:94:HIS:HB2    | 2.08        | 0.53     |
| 20:CB:163:ILE:CG2  | 20:CB:164:ASP:H    | 2.12        | 0.53     |
| 25:BC:76:VAL:HA    | 25:BC:113:ASP:O    | 2.09        | 0.53     |
| 13:CN:79:SER:OG    | 13:CN:82:LYS:HG2   | 2.07        | 0.53     |
| 47:BF:135:ILE:HD11 | 47:BF:137:PHE:CD1  | 2.42        | 0.53     |
| 21:AU:16:ARG:HA    | 21:AU:16:ARG:NE    | 2.24        | 0.53     |
| 18:CS:51:HIS:HA    | 18:CS:55:GLN:O     | 2.08        | 0.53     |
| 50:DT:17:SER:N     | 50:DT:21:SER:OG    | 2.40        | 0.53     |
| 50:DT:25:GLU:HA    | 50:DT:29:THR:O     | 2.08        | 0.53     |
| 53:D6:174:GLN:CD   | 53:D6:178:LYS:HE2  | 2.28        | 0.53     |
| 41:BJ:81:ILE:HG23  | 41:BJ:82:GLY:N     | 2.20        | 0.53     |
| 29:DE:5:LEU:CD1    | 29:DE:10:SER:HB2   | 2.37        | 0.53     |
| 53:B6:162:GLN:HA   | 53:B6:162:GLN:NE2  | 2.18        | 0.53     |
| 13:CN:40:ARG:HH12  | 18:CS:6:LYS:HB2    | 1.73        | 0.53     |
| 43:BO:39:VAL:HB    | 43:BO:49:VAL:HG22  | 1.89        | 0.53     |
| 35:DV:44:HIS:CE1   | 35:DV:85:LYS:HB2   | 2.43        | 0.53     |
| 44:BQ:4:LYS:HZ3    | 44:BQ:7:VAL:HG22   | 1.73        | 0.53     |
| 11:AL:24:GLU:HB2   | 11:AL:26:CYS:SG    | 2.48        | 0.53     |
| 23:BB:2722:G:O2'   | 23:BB:2723:C:H5'   | 2.07        | 0.53     |
| 3:CD:197:HIS:ND1   | 3:CD:198:LEU:N     | 2.57        | 0.53     |
| 6:CG:57:GLU:H      | 6:CG:57:GLU:CD     | 2.12        | 0.53     |
| 23:DB:281:C:H2'    | 23:DB:282:A:H8     | 1.73        | 0.53     |
| 23:DB:741:U:H2'    | 23:DB:742:A:C8     | 2.43        | 0.53     |
| 26:DD:14:ILE:HA    | 28:DP:11:GLN:HE22  | 1.72        | 0.53     |
| 19:AT:57:VAL:HG23  | 19:AT:58:ASP:N     | 2.22        | 0.53     |
| 52:DW:46:ALA:HB2   | 52:DW:78:PHE:HD1   | 1.73        | 0.53     |
| 6:AG:134:VAL:HB    | 6:AG:137:ARG:NH2   | 2.24        | 0.53     |
| 50:BT:69:ARG:HG2   | 50:BT:73:ARG:C     | 2.29        | 0.53     |
| 23:BB:1563:U:H2'   | 23:BB:1564:C:C6    | 2.43        | 0.53     |
| 23:BB:1220:G:H2'   | 23:BB:1221:C:C6    | 2.43        | 0.53     |
| 23:BB:4:U:H2'      | 23:BB:5:A:H8       | 1.74        | 0.53     |
| 23:BB:1947:C:H2'   | 23:BB:1948:G:C8    | 2.44        | 0.53     |
| 23:BB:1315:C:H2'   | 23:BB:1316:U:H6    | 1.73        | 0.53     |
| 1:AA:182:A:H5''    | 1:AA:182:A:N3      | 2.23        | 0.53     |
| 1:AA:612:C:H2'     | 1:AA:613:C:C6      | 2.43        | 0.53     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:285:G:O2'   | 23:DB:286:U:H5'    | 2.08        | 0.53     |
| 23:BB:813:U:H2'   | 23:BB:814:C:H6     | 1.71        | 0.53     |
| 42:BN:7:GLY:HA2   | 42:BN:46:ARG:NH1   | 2.23        | 0.53     |
| 47:DF:121:PHE:HB3 | 47:DF:127:TYR:CZ   | 2.43        | 0.53     |
| 1:CA:607:A:H2'    | 1:CA:608:A:C8      | 2.44        | 0.53     |
| 23:BB:1528:A:H2'  | 23:BB:1529:G:O4'   | 2.08        | 0.53     |
| 23:BB:250:G:H2'   | 23:BB:251:A:C8     | 2.42        | 0.53     |
| 1:AA:898:G:N2     | 1:AA:900:A:H3'     | 2.23        | 0.53     |
| 46:BU:13:LEU:HD12 | 46:BU:68:ASN:O     | 2.08        | 0.53     |
| 7:CH:55:LYS:HZ1   | 7:CH:55:LYS:HA     | 1.73        | 0.53     |
| 1:CA:825:A:H2'    | 1:CA:826:C:H6      | 1.74        | 0.53     |
| 22:BA:64:G:H2'    | 22:BA:65:U:C6      | 2.44        | 0.53     |
| 1:CA:386:C:O2'    | 1:CA:387:U:H5'     | 2.08        | 0.53     |
| 48:BG:154:GLU:OE2 | 48:BG:156:TYR:HB2  | 2.08        | 0.53     |
| 23:DB:39:G:O2'    | 23:DB:40:U:H5'     | 2.09        | 0.53     |
| 48:DG:154:GLU:C   | 48:DG:156:TYR:H    | 2.12        | 0.53     |
| 23:DB:1827:U:C2'  | 23:DB:1828:G:H5'   | 2.39        | 0.53     |
| 37:DL:125:LEU:H   | 37:DL:143:GLU:HG3  | 1.74        | 0.53     |
| 20:CB:164:ASP:CG  | 20:CB:203:ASP:HB2  | 2.29        | 0.53     |
| 37:DL:79:LEU:CG   | 37:DL:112:LEU:HA   | 2.32        | 0.53     |
| 41:DJ:36:LEU:HD12 | 41:DJ:118:MET:O    | 2.09        | 0.53     |
| 7:AH:44:PHE:HA    | 7:AH:70:VAL:HG11   | 1.90        | 0.53     |
| 24:BI:11:GLN:O    | 24:BI:11:GLN:HG3   | 2.07        | 0.53     |
| 23:BB:321:U:H4'   | 29:BE:159:LEU:O    | 2.09        | 0.53     |
| 17:AR:34:GLU:HB2  | 21:AU:18:PHE:HZ    | 1.72        | 0.53     |
| 1:AA:1317:C:H3'   | 1:AA:1318:A:H8     | 1.73        | 0.53     |
| 1:AA:719:C:H2'    | 17:AR:38:ILE:CD1   | 2.38        | 0.53     |
| 23:BB:2884:U:H4'  | 31:B0:49:ARG:NH2   | 2.24        | 0.53     |
| 24:BI:18:ASN:N    | 24:BI:19:PRO:CD    | 2.71        | 0.53     |
| 37:DL:95:LEU:HD13 | 37:DL:101:ILE:HG13 | 1.90        | 0.53     |
| 48:DG:30:GLY:H    | 48:DG:78:VAL:HA    | 1.73        | 0.53     |
| 24:DI:45:THR:HA   | 24:DI:48:ILE:CG2   | 2.38        | 0.53     |
| 28:DP:3:ILE:C     | 28:DP:3:ILE:HD13   | 2.28        | 0.53     |
| 28:DP:3:ILE:HG23  | 28:DP:4:ILE:N      | 2.24        | 0.53     |
| 23:DB:559:G:P     | 41:DJ:111:LYS:HD3  | 2.48        | 0.53     |
| 23:BB:2155:U:H2'  | 23:BB:2156:G:C8    | 2.43        | 0.53     |
| 23:DB:322:A:H3'   | 29:DE:163:ASN:HD21 | 1.72        | 0.53     |
| 23:DB:2529:G:O2'  | 48:DG:174:LYS:HE2  | 2.09        | 0.53     |
| 1:AA:1254:A:O4'   | 1:AA:1356:G:H5''   | 2.08        | 0.53     |
| 27:DK:59:LYS:HD2  | 27:DK:89:ASN:ND2   | 2.22        | 0.53     |
| 27:DK:88:ASN:HD22 | 27:DK:89:ASN:N     | 2.06        | 0.53     |
| 1:CA:1123:U:O2'   | 1:CA:1124:G:H5'    | 2.07        | 0.53     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1240:U:O2'   | 23:DB:1241:A:H5'   | 2.09        | 0.53     |
| 5:AF:80:PHE:CE1    | 25:BC:123:ILE:HG12 | 2.43        | 0.53     |
| 40:BH:57:LYS:O     | 40:BH:61:VAL:HG12  | 2.08        | 0.53     |
| 23:DB:545:U:H2'    | 23:DB:548:G:OP2    | 2.09        | 0.53     |
| 1:CA:452:A:H2'     | 1:CA:453:G:O4'     | 2.09        | 0.53     |
| 23:BB:2455:G:H2'   | 23:BB:2456:C:H6    | 1.74        | 0.53     |
| 23:DB:1315:C:H2'   | 23:DB:1316:U:H6    | 1.71        | 0.53     |
| 43:BO:28:VAL:O     | 43:BO:28:VAL:HG13  | 2.09        | 0.53     |
| 23:BB:680:C:H2'    | 23:BB:681:G:C8     | 2.43        | 0.53     |
| 1:CA:693:G:H2'     | 1:CA:694:A:O4'     | 2.08        | 0.53     |
| 23:BB:1429:G:O2'   | 23:BB:1430:G:H5'   | 2.07        | 0.53     |
| 23:DB:2816:G:O2'   | 23:DB:2817:U:H5'   | 2.08        | 0.53     |
| 25:BC:177:SER:O    | 25:BC:270:ARG:HG3  | 2.08        | 0.53     |
| 23:DB:2888:C:H2'   | 23:DB:2889:C:H6    | 1.73        | 0.53     |
| 42:DN:7:GLY:HA2    | 42:DN:46:ARG:NH1   | 2.24        | 0.53     |
| 23:DB:303:G:H2'    | 23:DB:304:U:C6     | 2.43        | 0.53     |
| 2:AC:174:LEU:HD12  | 2:AC:174:LEU:H     | 1.73        | 0.53     |
| 53:B6:7:TYR:CE1    | 53:B6:160:GLU:HG2  | 2.44        | 0.53     |
| 19:AT:54:GLN:N     | 19:AT:55:PRO:HD2   | 2.23        | 0.53     |
| 15:CP:73:ALA:O     | 15:CP:77:GLU:HG3   | 2.08        | 0.53     |
| 5:CF:85:ILE:HG22   | 5:CF:86:ARG:N      | 2.24        | 0.53     |
| 23:BB:1109:C:H3'   | 23:BB:1110:G:C8    | 2.43        | 0.53     |
| 26:BD:40:LEU:HD12  | 26:BD:41:ALA:N     | 2.24        | 0.53     |
| 26:BD:45:TYR:HD2   | 26:BD:83:ARG:HD3   | 1.73        | 0.53     |
| 23:DB:464:U:H2'    | 23:DB:465:G:O4'    | 2.08        | 0.53     |
| 40:BH:130:VAL:HG21 | 40:BH:144:VAL:CG2  | 2.38        | 0.53     |
| 40:BH:80:ILE:H     | 40:BH:145:ASN:H    | 1.56        | 0.53     |
| 8:AI:56:MET:C      | 8:AI:58:GLU:H      | 2.11        | 0.53     |
| 23:BB:141:G:H1     | 50:BT:2:ILE:CD1    | 2.12        | 0.53     |
| 41:DJ:59:ALA:C     | 41:DJ:61:LYS:H     | 2.11        | 0.53     |
| 29:DE:58:LYS:HE2   | 29:DE:60:TRP:CD1   | 2.43        | 0.53     |
| 23:DB:2733:A:H2'   | 23:DB:2734:A:O4'   | 2.08        | 0.53     |
| 23:BB:1060:U:C4    | 24:BI:131:THR:HG22 | 2.43        | 0.53     |
| 45:DS:14:ALA:O     | 45:DS:18:ARG:HG2   | 2.09        | 0.53     |
| 1:AA:1317:C:OP1    | 13:AN:56:PRO:HD2   | 2.09        | 0.53     |
| 50:DT:39:THR:CG2   | 50:DT:42:GLU:H     | 2.21        | 0.53     |
| 23:DB:851:C:O2'    | 30:DY:45:GLY:HA3   | 2.09        | 0.53     |
| 23:DB:45:G:H5'     | 23:DB:46:G:OP1     | 2.09        | 0.53     |
| 1:AA:1351:U:O2'    | 1:AA:1352:C:H5'    | 2.08        | 0.53     |
| 26:DD:170:VAL:O    | 26:DD:170:VAL:HG23 | 2.08        | 0.53     |
| 1:AA:313:A:H2'     | 1:AA:314:C:C6      | 2.44        | 0.53     |
| 42:DN:72:ASP:OD2   | 42:DN:74:GLU:HB3   | 2.09        | 0.53     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:706:A:C4'     | 10:CK:30:ILE:HD11 | 2.39        | 0.53     |
| 47:BF:163:GLU:HA   | 47:BF:166:ARG:HD3 | 1.90        | 0.53     |
| 7:AH:66:GLN:C      | 7:AH:68:LYS:H     | 2.10        | 0.53     |
| 46:DU:34:ILE:HG12  | 46:DU:63:ALA:CB   | 2.38        | 0.53     |
| 3:CD:89:LEU:HD23   | 3:CD:199:ILE:HD11 | 1.89        | 0.53     |
| 12:AM:80:MET:HA    | 12:AM:87:GLY:HA3  | 1.91        | 0.53     |
| 3:AD:197:HIS:ND1   | 3:AD:198:LEU:N    | 2.56        | 0.53     |
| 23:DB:1726:C:H2'   | 23:DB:1727:C:C6   | 2.43        | 0.53     |
| 23:BB:1150:C:O2'   | 23:BB:1151:A:H5'  | 2.08        | 0.53     |
| 4:AE:110:MET:SD    | 4:AE:126:ALA:HB2  | 2.49        | 0.53     |
| 26:BD:133:THR:HG23 | 26:BD:134:HIS:N   | 2.24        | 0.53     |
| 23:DB:2460:U:H2'   | 23:DB:2461:A:H8   | 1.73        | 0.53     |
| 19:CT:57:VAL:HG23  | 19:CT:58:ASP:N    | 2.23        | 0.53     |
| 23:DB:1405:U:H2'   | 23:DB:1406:U:C6   | 2.44        | 0.53     |
| 1:CA:1516:G:H2'    | 1:CA:1518:A:OP2   | 2.09        | 0.53     |
| 1:AA:1140:C:O2'    | 1:AA:1141:C:H5'   | 2.08        | 0.53     |
| 23:BB:1258:U:H2'   | 23:BB:1259:G:H8   | 1.72        | 0.53     |
| 50:BT:69:ARG:HG3   | 50:BT:70:HIS:N    | 2.24        | 0.53     |
| 1:AA:677:U:H1'     | 10:AK:120:CYS:SG  | 2.49        | 0.53     |
| 23:BB:540:C:H2'    | 23:BB:541:A:C8    | 2.43        | 0.53     |
| 23:DB:2825:G:H5''  | 23:DB:2825:G:N3   | 2.23        | 0.53     |
| 23:DB:649:G:H2'    | 23:DB:650:C:H6    | 1.73        | 0.53     |
| 23:DB:807:U:H2'    | 23:DB:808:G:C8    | 2.43        | 0.53     |
| 1:AA:607:A:H2'     | 1:AA:608:A:C8     | 2.43        | 0.53     |
| 1:AA:607:A:H2'     | 1:AA:608:A:H8     | 1.73        | 0.53     |
| 1:AA:818:G:C3'     | 1:AA:819:A:H5''   | 2.38        | 0.53     |
| 23:BB:1300:G:H4'   | 23:BB:1301:A:O5'  | 2.07        | 0.53     |
| 26:BD:97:SER:HB3   | 26:BD:99:GLU:HG3  | 1.90        | 0.53     |
| 24:BI:81:LYS:HG3   | 24:BI:82:ALA:N    | 2.23        | 0.53     |
| 45:BS:72:THR:CG2   | 45:BS:108:SER:HB3 | 2.38        | 0.53     |
| 19:CT:54:GLN:N     | 19:CT:55:PRO:HD2  | 2.23        | 0.53     |
| 23:DB:394:C:H2'    | 23:DB:395:U:O4'   | 2.08        | 0.53     |
| 40:DH:27:ARG:NH1   | 51:DZ:60:ASP:HA   | 2.22        | 0.53     |
| 48:BG:16:VAL:HG11  | 48:BG:44:HIS:CE1  | 2.44        | 0.53     |
| 10:AK:51:PHE:CZ    | 10:AK:61:ALA:HA   | 2.44        | 0.53     |
| 21:AU:42:THR:O     | 21:AU:46:ARG:HG3  | 2.09        | 0.53     |
| 48:DG:88:LEU:HD13  | 48:DG:93:TYR:HB3  | 1.89        | 0.53     |
| 40:BH:89:LYS:HZ1   | 40:BH:123:ARG:CB  | 2.21        | 0.53     |
| 8:CI:20:ILE:HD13   | 8:CI:85:ALA:CB    | 2.39        | 0.53     |
| 8:AI:27:ILE:HD13   | 8:AI:34:LEU:HD22  | 1.90        | 0.53     |
| 47:BF:133:GLU:HA   | 47:BF:150:GLY:HA2 | 1.90        | 0.53     |
| 13:AN:40:ARG:HH12  | 18:AS:6:LYS:HB2   | 1.73        | 0.53     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 33:D1:26:LYS:HB2   | 33:D1:52:LYS:HZ2  | 1.73        | 0.53     |
| 23:DB:141:G:N2     | 23:DB:141:G:OP2   | 2.42        | 0.53     |
| 23:BB:2834:G:O6    | 23:BB:2879:A:H2'  | 2.08        | 0.53     |
| 31:B0:41:HIS:HB3   | 42:BN:99:LYS:HB2  | 1.90        | 0.53     |
| 1:AA:1350:A:H2'    | 1:AA:1351:U:C6    | 2.43        | 0.53     |
| 9:CJ:5:ARG:HG2     | 9:CJ:79:PRO:HD3   | 1.91        | 0.53     |
| 1:AA:86:G:N3       | 1:AA:87:C:N4      | 2.56        | 0.53     |
| 14:CO:81:LEU:HD23  | 14:CO:85:LEU:HD13 | 1.90        | 0.53     |
| 46:DU:39:ASN:CG    | 46:DU:62:ALA:HB3  | 2.29        | 0.53     |
| 26:BD:14:ILE:O     | 26:BD:14:ILE:HG23 | 2.09        | 0.53     |
| 23:BB:2592:G:H2'   | 23:BB:2593:U:O4'  | 2.09        | 0.53     |
| 27:DK:59:LYS:HD3   | 27:DK:89:ASN:HA   | 1.90        | 0.53     |
| 35:BV:29:ILE:HG13  | 35:BV:88:HIS:CE1  | 2.40        | 0.53     |
| 6:AG:50:ALA:CB     | 6:AG:57:GLU:HG3   | 2.38        | 0.53     |
| 25:BC:123:ILE:HG13 | 25:BC:123:ILE:O   | 2.07        | 0.53     |
| 23:DB:2136:G:O2'   | 23:DB:2137:U:H5'  | 2.09        | 0.53     |
| 27:DK:2:ILE:HD12   | 27:DK:2:ILE:N     | 2.24        | 0.53     |
| 23:BB:2190:G:O2'   | 23:BB:2191:A:H5'  | 2.09        | 0.53     |
| 50:DT:69:ARG:HG2   | 50:DT:73:ARG:C    | 2.29        | 0.53     |
| 19:AT:78:LEU:O     | 19:AT:82:ILE:HG23 | 2.09        | 0.53     |
| 1:CA:1514:G:H2'    | 1:CA:1515:G:H8    | 1.73        | 0.53     |
| 1:CA:1470:U:O2'    | 1:CA:1471:U:H5'   | 2.08        | 0.53     |
| 23:BB:416:U:H2'    | 23:BB:417:C:C6    | 2.44        | 0.53     |
| 23:BB:572:A:H3'    | 23:BB:573:U:O4'   | 2.08        | 0.53     |
| 23:BB:2784:U:O2'   | 23:BB:2785:C:H5'  | 2.08        | 0.53     |
| 34:D3:38:LYS:HG3   | 34:D3:41:ARG:NH1  | 2.24        | 0.53     |
| 1:AA:451:A:C6      | 1:AA:480:U:H2'    | 2.43        | 0.53     |
| 5:CF:18:VAL:O      | 5:CF:22:ILE:HG13  | 2.07        | 0.53     |
| 23:BB:2888:C:H2'   | 23:BB:2889:C:H6   | 1.72        | 0.53     |
| 23:DB:2834:G:H2'   | 23:DB:2879:A:N6   | 2.23        | 0.53     |
| 12:AM:43:LYS:HB2   | 12:AM:46:GLU:CG   | 2.38        | 0.53     |
| 1:CA:993:G:N2      | 1:CA:996:A:N6     | 2.57        | 0.53     |
| 18:AS:69:LYS:O     | 18:AS:72:GLU:HG2  | 2.08        | 0.53     |
| 23:DB:1520:U:H2'   | 23:DB:1521:G:O4'  | 2.09        | 0.53     |
| 2:CC:174:LEU:H     | 2:CC:174:LEU:HD12 | 1.74        | 0.53     |
| 51:DZ:53:ALA:O     | 51:DZ:55:GLY:N    | 2.38        | 0.53     |
| 23:BB:2691:C:H2'   | 23:BB:2692:G:H8   | 1.74        | 0.53     |
| 23:BB:1107:G:H2'   | 23:BB:1108:U:C6   | 2.44        | 0.53     |
| 34:B3:56:LEU:O     | 34:B3:59:ALA:HB3  | 2.08        | 0.53     |
| 1:AA:162:A:H2'     | 1:AA:163:C:O4'    | 2.09        | 0.53     |
| 23:BB:2252:G:O2'   | 23:BB:2253:G:H5'  | 2.09        | 0.53     |
| 10:AK:73:VAL:O     | 10:AK:76:TYR:HB2  | 2.09        | 0.53     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2030:A:H4'   | 23:DB:2031:A:H5'   | 1.89        | 0.53     |
| 8:AI:42:THR:O      | 8:AI:45:MET:HG2    | 2.09        | 0.53     |
| 8:AI:82:ILE:O      | 8:AI:86:LEU:HD13   | 2.08        | 0.53     |
| 8:AI:113:LYS:HA    | 8:AI:120:ALA:HB2   | 1.91        | 0.53     |
| 50:BT:57:VAL:HG22  | 50:BT:58:VAL:N     | 2.20        | 0.53     |
| 25:DC:76:VAL:HA    | 25:DC:113:ASP:O    | 2.07        | 0.53     |
| 44:BQ:63:ARG:HH12  | 44:BQ:96:ASP:CB    | 2.13        | 0.53     |
| 49:BR:6:GLN:HE22   | 49:BR:10:LYS:H     | 1.56        | 0.53     |
| 48:BG:24:THR:C     | 48:BG:25:ILE:HD12  | 2.29        | 0.53     |
| 23:BB:987:C:H2'    | 23:BB:988:A:O4'    | 2.09        | 0.53     |
| 24:DI:52:LEU:HD22  | 24:DI:81:LYS:HD3   | 1.91        | 0.53     |
| 29:BE:134:LEU:CD2  | 29:BE:161:ALA:HB2  | 2.39        | 0.53     |
| 1:AA:1080:A:H2'    | 1:AA:1081:A:H5'    | 1.90        | 0.53     |
| 20:AB:46:VAL:HA    | 20:AB:49:PHE:CD2   | 2.43        | 0.53     |
| 25:DC:209:ALA:O    | 25:DC:213:ARG:HB2  | 2.07        | 0.53     |
| 24:DI:32:VAL:HG22  | 24:DI:60:VAL:CG2   | 2.39        | 0.53     |
| 13:AN:51:PRO:HG2   | 13:AN:52:ARG:H     | 1.72        | 0.53     |
| 31:B0:38:LEU:HB3   | 31:B0:41:HIS:NE2   | 2.24        | 0.53     |
| 3:CD:138:PRO:HA    | 3:CD:181:PHE:CD2   | 2.35        | 0.53     |
| 45:BS:36:LEU:H     | 45:BS:36:LEU:HD22  | 1.74        | 0.53     |
| 22:BA:32:U:C4'     | 22:BA:52:A:H62     | 2.22        | 0.53     |
| 37:DL:95:LEU:HA    | 37:DL:98:ALA:HB3   | 1.91        | 0.53     |
| 23:DB:1777:U:O2'   | 23:DB:1778:U:H5'   | 2.08        | 0.53     |
| 1:AA:1074:G:O3'    | 20:AB:101:THR:OG1  | 2.21        | 0.53     |
| 20:AB:101:THR:HG22 | 20:AB:174:GLU:OE1  | 2.09        | 0.53     |
| 40:DH:113:SER:N    | 40:DH:132:PHE:CE1  | 2.75        | 0.53     |
| 12:CM:95:PRO:CD    | 12:CM:108:ARG:HG2  | 2.37        | 0.53     |
| 27:DK:89:ASN:C     | 27:DK:89:ASN:HD22  | 2.12        | 0.53     |
| 11:AL:109:ARG:HH21 | 11:AL:112:ALA:HB3  | 1.73        | 0.53     |
| 23:BB:2078:C:H2'   | 23:BB:2079:U:H6    | 1.73        | 0.53     |
| 25:BC:123:ILE:HD12 | 25:BC:191:LEU:HD11 | 1.91        | 0.53     |
| 23:DB:1389:G:O2'   | 23:DB:1390:U:H5'   | 2.08        | 0.53     |
| 5:CF:53:LYS:HD3    | 5:CF:54:LEU:H      | 1.74        | 0.53     |
| 23:DB:1351:C:H4'   | 23:DB:1572:A:O4'   | 2.08        | 0.53     |
| 23:DB:2540:C:H2'   | 23:DB:2541:A:H8    | 1.72        | 0.53     |
| 1:CA:451:A:C6      | 1:CA:480:U:H2'     | 2.44        | 0.53     |
| 44:BQ:65:ASN:HB2   | 44:BQ:75:TYR:HB2   | 1.91        | 0.53     |
| 23:BB:2854:G:H2'   | 23:BB:2855:C:C6    | 2.44        | 0.53     |
| 41:DJ:130:HIS:HD2  | 41:DJ:132:HIS:HB2  | 1.72        | 0.53     |
| 40:DH:135:HIS:CG   | 40:DH:136:SER:N    | 2.77        | 0.53     |
| 22:BA:90:C:OP1     | 38:BM:16:ARG:HB2   | 2.09        | 0.53     |
| 23:BB:2496:C:H5'   | 38:BM:82:MET:HG3   | 1.91        | 0.53     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:DB:2708:G:O2'   | 23:DB:2709:G:H5'  | 2.08        | 0.53     |
| 23:DB:930:G:H1'    | 30:DY:24:LEU:HD11 | 1.91        | 0.53     |
| 23:DB:2543:G:H2'   | 23:DB:2544:G:C8   | 2.44        | 0.53     |
| 23:DB:1295:C:H2'   | 23:DB:1296:G:H8   | 1.73        | 0.53     |
| 23:DB:79:C:O2'     | 23:DB:346:A:H1'   | 2.08        | 0.53     |
| 1:AA:645:G:O2'     | 1:AA:646:G:H5'    | 2.08        | 0.53     |
| 1:AA:1289:A:H2'    | 1:AA:1290:G:H5'   | 1.90        | 0.53     |
| 23:DB:1031:G:H4'   | 32:D4:6:SER:HB3   | 1.90        | 0.53     |
| 24:DI:5:GLN:O      | 24:DI:6:ALA:HB3   | 2.08        | 0.53     |
| 1:CA:560:A:H4'     | 1:CA:561:U:H5''   | 1.90        | 0.53     |
| 23:BB:2324:U:H3'   | 23:BB:2325:G:H5'' | 1.90        | 0.53     |
| 17:AR:63:TYR:CD2   | 17:AR:63:TYR:N    | 2.75        | 0.53     |
| 18:CS:79:TYR:CE1   | 18:CS:80:ARG:HG3  | 2.44        | 0.53     |
| 42:BN:54:LEU:CD1   | 42:BN:62:ASN:HB3  | 2.38        | 0.53     |
| 1:CA:975:A:H4'     | 1:CA:976:G:OP2    | 2.07        | 0.53     |
| 23:DB:1099:G:C8    | 24:DI:3:LYS:HB2   | 2.44        | 0.53     |
| 48:BG:10:VAL:HG23  | 48:BG:48:THR:HA   | 1.89        | 0.53     |
| 23:DB:922:C:H1'    | 52:DW:22:VAL:HG21 | 1.90        | 0.53     |
| 40:BH:97:ARG:O     | 40:BH:101:ASP:HB2 | 2.08        | 0.53     |
| 8:AI:44:ARG:HH11   | 8:AI:44:ARG:HG2   | 1.73        | 0.53     |
| 1:AA:948:C:O2'     | 1:AA:949:A:H5'    | 2.08        | 0.53     |
| 34:D3:36:ALA:O     | 34:D3:39:ARG:HB3  | 2.09        | 0.53     |
| 12:CM:14:ALA:HB1   | 12:CM:33:LEU:HD21 | 1.91        | 0.53     |
| 47:BF:111:ARG:O    | 47:BF:112:ASP:HB2 | 2.08        | 0.53     |
| 40:DH:5:LEU:HD13   | 40:DH:13:GLY:CA   | 2.34        | 0.53     |
| 47:DF:141:ASP:HB2  | 47:DF:144:LYS:HB2 | 1.90        | 0.53     |
| 29:DE:105:LEU:HD21 | 29:DE:177:PRO:HA  | 1.89        | 0.53     |
| 21:AU:24:LYS:CD    | 21:AU:25:ALA:H    | 2.20        | 0.53     |
| 1:CA:1081:A:OP1    | 4:CE:21:SER:O     | 2.26        | 0.53     |
| 1:CA:1320:C:H41    | 18:CS:36:ARG:HB3  | 1.72        | 0.53     |
| 1:CA:979:C:H1'     | 1:CA:1317:C:H41   | 1.74        | 0.53     |
| 33:D1:33:LEU:HB3   | 33:D1:51:ALA:CB   | 2.38        | 0.53     |
| 23:BB:979:A:H3'    | 23:BB:980:A:C5'   | 2.39        | 0.53     |
| 48:DG:153:PRO:HG3  | 48:DG:162:ARG:CB  | 2.39        | 0.53     |
| 28:DP:91:VAL:O     | 28:DP:92:ARG:HB3  | 2.09        | 0.53     |
| 46:DU:32:LYS:HA    | 46:DU:65:GLN:HA   | 1.90        | 0.53     |
| 3:AD:138:PRO:HA    | 3:AD:181:PHE:CD2  | 2.35        | 0.53     |
| 45:BS:70:LYS:HD3   | 45:BS:110:ARG:O   | 2.08        | 0.53     |
| 25:BC:209:ALA:HA   | 25:BC:212:TRP:NE1 | 2.23        | 0.53     |
| 27:BK:8:LEU:H      | 27:BK:8:LEU:HD12  | 1.74        | 0.53     |
| 49:DR:39:LEU:O     | 49:DR:40:MET:HB2  | 2.08        | 0.53     |
| 11:AL:28:GLN:HB2   | 11:AL:80:LEU:HG   | 1.90        | 0.53     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 10:AK:80:ASN:HB3  | 10:AK:105:ARG:HB3  | 1.91        | 0.53     |
| 27:DK:58:LEU:N    | 27:DK:58:LEU:HD23  | 2.23        | 0.53     |
| 1:CA:473:U:H2'    | 1:CA:474:G:H8      | 1.74        | 0.53     |
| 1:AA:237:G:H2'    | 1:AA:238:A:C8      | 2.44        | 0.53     |
| 3:CD:94:GLU:HA    | 3:CD:99:ASN:ND2    | 2.24        | 0.53     |
| 3:AD:129:VAL:HG12 | 3:AD:131:ILE:H     | 1.74        | 0.53     |
| 1:CA:833:G:O2'    | 1:CA:834:U:H5'     | 2.09        | 0.53     |
| 3:CD:118:SER:HA   | 3:CD:130:ASN:HB2   | 1.89        | 0.53     |
| 23:BB:2845:U:O2'  | 23:BB:2846:G:H5'   | 2.08        | 0.53     |
| 23:DB:1181:U:H2'  | 23:DB:1182:G:C8    | 2.41        | 0.53     |
| 1:AA:168:G:O2'    | 1:AA:169:C:H5'     | 2.09        | 0.53     |
| 1:AA:449:G:H2'    | 1:AA:450:G:C8      | 2.43        | 0.53     |
| 23:BB:2604:U:O2'  | 23:BB:2605:U:H5'   | 2.09        | 0.53     |
| 23:BB:2369:A:H2'  | 23:BB:2370:G:H8    | 1.74        | 0.53     |
| 23:BB:934:U:H2'   | 23:BB:935:C:H6     | 1.74        | 0.53     |
| 23:BB:2813:A:H2'  | 23:BB:2814:A:C8    | 2.43        | 0.53     |
| 23:BB:2041:U:H2'  | 23:BB:2042:A:H8    | 1.73        | 0.53     |
| 1:AA:590:U:H2'    | 1:AA:591:U:C6      | 2.44        | 0.53     |
| 5:AF:7:VAL:HG11   | 17:AR:64:LEU:HD21  | 1.90        | 0.53     |
| 23:DB:2821:A:OP2  | 26:DD:115:GLY:HA3  | 2.09        | 0.53     |
| 23:BB:2636:C:H4'  | 26:BD:81:GLU:OE2   | 2.09        | 0.53     |
| 30:DY:13:ILE:HG22 | 30:DY:14:GLY:N     | 2.24        | 0.53     |
| 4:CE:42:ASN:O     | 4:CE:75:LEU:HD12   | 2.09        | 0.53     |
| 23:DB:1835:G:H2'  | 23:DB:1836:C:C6    | 2.44        | 0.53     |
| 23:DB:1153:C:H2'  | 23:DB:1154:G:O4'   | 2.08        | 0.53     |
| 23:DB:1268:A:H2'  | 23:DB:1269:A:O4'   | 2.09        | 0.53     |
| 34:B3:21:PHE:CE1  | 34:B3:58:ILE:HG12  | 2.44        | 0.53     |
| 6:CG:12:LEU:HD22  | 6:CG:13:PRO:HD2    | 1.90        | 0.53     |
| 23:DB:947:A:H2'   | 23:DB:948:C:H6     | 1.74        | 0.53     |
| 26:BD:106:LYS:O   | 26:BD:107:VAL:HB   | 2.08        | 0.53     |
| 53:B6:38:LEU:HD22 | 53:B6:41:LEU:HD22  | 1.91        | 0.53     |
| 8:CI:56:MET:C     | 8:CI:58:GLU:H      | 2.11        | 0.53     |
| 44:DQ:63:ARG:HH22 | 44:DQ:96:ASP:CA    | 2.22        | 0.53     |
| 30:DY:8:GLN:OE1   | 30:DY:23:LEU:HD11  | 2.09        | 0.53     |
| 23:DB:1060:U:OP2  | 24:DI:74:PRO:HA    | 2.09        | 0.53     |
| 29:BE:138:LEU:HB3 | 29:BE:143:LEU:O    | 2.08        | 0.53     |
| 42:DN:52:ILE:HD13 | 42:DN:87:PHE:CD2   | 2.44        | 0.53     |
| 1:AA:764:C:N4     | 1:AA:812:G:N1      | 2.57        | 0.53     |
| 23:DB:1021:A:H61  | 23:DB:1142:A:H61   | 1.56        | 0.53     |
| 47:DF:101:ARG:HA  | 47:DF:105:ILE:HD12 | 1.90        | 0.53     |
| 47:DF:7:TYR:OH    | 47:DF:29:ARG:HG3   | 2.09        | 0.53     |
| 45:BS:14:ALA:O    | 45:BS:18:ARG:HG2   | 2.09        | 0.53     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2471:A:O2'   | 23:DB:2472:G:O5'   | 2.27        | 0.53     |
| 37:DL:56:PRO:O     | 37:DL:59:ARG:HB2   | 2.09        | 0.53     |
| 23:BB:972:A:OP2    | 23:BB:974:G:H5''   | 2.09        | 0.53     |
| 23:DB:1459:G:H5''  | 23:DB:1460:U:OP1   | 2.08        | 0.53     |
| 23:BB:2733:A:H2'   | 23:BB:2734:A:O4'   | 2.08        | 0.53     |
| 48:DG:30:GLY:HA3   | 48:DG:78:VAL:HG12  | 1.90        | 0.53     |
| 23:BB:460:A:H2'    | 23:BB:461:C:O4'    | 2.09        | 0.53     |
| 40:DH:70:GLU:HA    | 40:DH:73:ASN:HB2   | 1.89        | 0.53     |
| 9:AJ:7:ARG:NH1     | 9:AJ:101:SER:HB2   | 2.24        | 0.53     |
| 26:BD:9:VAL:HA     | 26:BD:197:THR:HG23 | 1.91        | 0.53     |
| 37:BL:95:LEU:HB2   | 37:BL:101:ILE:CG1  | 2.39        | 0.53     |
| 20:CB:124:THR:HG23 | 20:CB:124:THR:O    | 2.09        | 0.53     |
| 23:DB:582:A:H2'    | 23:DB:583:G:H8     | 1.74        | 0.53     |
| 29:DE:155:GLU:O    | 29:DE:159:LEU:HB2  | 2.09        | 0.53     |
| 1:CA:1057:G:H5''   | 2:CC:153:SER:HB2   | 1.89        | 0.53     |
| 46:DU:26:ASN:ND2   | 46:DU:26:ASN:N     | 2.52        | 0.53     |
| 1:CA:551:U:H2'     | 1:CA:552:U:H6      | 1.73        | 0.53     |
| 4:CE:155:LYS:O     | 4:CE:158:LYS:HE3   | 2.08        | 0.53     |
| 23:BB:273:G:O2'    | 23:BB:274:C:H5'    | 2.09        | 0.53     |
| 29:DE:46:GLN:HB3   | 29:DE:86:ALA:HA    | 1.91        | 0.53     |
| 29:DE:48:THR:O     | 29:DE:52:VAL:HG23  | 2.09        | 0.53     |
| 44:DQ:2:ARG:HG3    | 44:DQ:3:VAL:H      | 1.74        | 0.53     |
| 1:CA:87:C:C3'      | 1:CA:88:U:H5''     | 2.39        | 0.53     |
| 23:DB:2023:C:H4'   | 23:DB:2617:U:O3'   | 2.09        | 0.53     |
| 23:BB:222:A:H61    | 23:BB:232:G:H1'    | 1.72        | 0.53     |
| 23:BB:2812:G:H2'   | 23:BB:2813:A:C8    | 2.43        | 0.53     |
| 50:BT:32:LEU:O     | 50:BT:83:ALA:HB2   | 2.09        | 0.53     |
| 23:BB:2439:A:N7    | 23:BB:2586:U:H4'   | 2.24        | 0.53     |
| 1:AA:129:A:H1'     | 1:AA:130:A:C8      | 2.44        | 0.53     |
| 1:AA:1152:A:H2'    | 1:AA:1153:G:H8     | 1.72        | 0.53     |
| 23:BB:2889:C:O2'   | 23:BB:2890:G:H5'   | 2.09        | 0.53     |
| 5:AF:18:VAL:HG11   | 5:AF:58:HIS:NE2    | 2.24        | 0.53     |
| 23:DB:1495:A:O2'   | 23:DB:1496:A:H5'   | 2.09        | 0.53     |
| 41:DJ:88:THR:HG22  | 41:DJ:91:GLU:HG3   | 1.91        | 0.53     |
| 2:AC:181:ILE:N     | 2:AC:181:ILE:HD12  | 2.23        | 0.53     |
| 23:DB:2652:C:H2'   | 23:DB:2653:U:O4'   | 2.09        | 0.53     |
| 23:DB:1714:U:H3'   | 23:DB:1715:G:C5'   | 2.39        | 0.53     |
| 25:DC:270:ARG:NH1  | 25:DC:270:ARG:HB3  | 2.24        | 0.53     |
| 1:CA:89:U:H2'      | 1:CA:90:C:C6       | 2.44        | 0.53     |
| 25:DC:109:LEU:H    | 25:DC:109:LEU:CD2  | 2.22        | 0.53     |
| 25:DC:119:VAL:HG13 | 25:DC:133:ASN:HD21 | 1.73        | 0.53     |
| 37:DL:121:THR:HA   | 37:DL:141:LYS:HB3  | 1.91        | 0.53     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 52:DW:22:VAL:O     | 52:DW:23:LYS:HG3   | 2.09        | 0.53     |
| 53:B6:68:VAL:HB    | 53:B6:99:LEU:HG    | 1.90        | 0.53     |
| 1:AA:981:U:C4'     | 13:AN:60:ARG:HD2   | 2.32        | 0.53     |
| 48:DG:34:ARG:HG2   | 48:DG:34:ARG:NH1   | 2.24        | 0.53     |
| 7:AH:44:PHE:HE2    | 7:AH:100:ILE:HG12  | 1.74        | 0.53     |
| 1:CA:597:G:H2'     | 1:CA:598:U:H5'     | 1.90        | 0.53     |
| 44:BQ:59:LEU:HD13  | 44:BQ:60:TRP:N     | 2.24        | 0.53     |
| 44:BQ:93:ILE:O     | 44:BQ:96:ASP:HB3   | 2.09        | 0.53     |
| 23:BB:1203:U:H3'   | 23:BB:1204:A:H5''  | 1.89        | 0.53     |
| 23:BB:2108:A:H2'   | 23:BB:2109:U:C4'   | 2.35        | 0.53     |
| 23:DB:2468:A:H2'   | 23:DB:2476:A:C6    | 2.43        | 0.53     |
| 8:CI:36:GLN:N      | 8:CI:36:GLN:HE21   | 2.07        | 0.53     |
| 31:B0:38:LEU:HB3   | 31:B0:41:HIS:CD2   | 2.44        | 0.53     |
| 13:CN:29:ILE:HB    | 13:CN:30:ILE:HD12  | 1.91        | 0.53     |
| 23:BB:2734:A:C2'   | 23:BB:2735:G:H5'   | 2.37        | 0.53     |
| 29:DE:138:LEU:HB3  | 29:DE:143:LEU:O    | 2.09        | 0.53     |
| 20:AB:65:LYS:HB2   | 20:AB:158:ASP:H    | 1.74        | 0.53     |
| 49:DR:39:LEU:HD22  | 49:DR:53:PHE:HD1   | 1.74        | 0.53     |
| 23:BB:850:U:H2'    | 23:BB:851:C:C6     | 2.44        | 0.53     |
| 24:DI:129:GLU:HB3  | 24:DI:133:ARG:HH12 | 1.73        | 0.53     |
| 4:AE:152:VAL:HG21  | 7:AH:98:LEU:HB3    | 1.90        | 0.53     |
| 23:DB:2146:C:H4'   | 23:DB:2148:G:C1'   | 2.39        | 0.53     |
| 23:DB:2846:G:H2'   | 23:DB:2847:U:C6    | 2.43        | 0.53     |
| 23:DB:2845:U:O2'   | 23:DB:2846:G:H5'   | 2.09        | 0.53     |
| 26:BD:170:VAL:O    | 26:BD:170:VAL:HG23 | 2.09        | 0.53     |
| 1:CA:255:G:H2'     | 1:CA:256:U:H6      | 1.73        | 0.53     |
| 33:D1:47:ILE:H     | 33:D1:47:ILE:HD12  | 1.73        | 0.53     |
| 3:CD:129:VAL:HG12  | 3:CD:131:ILE:H     | 1.74        | 0.53     |
| 23:DB:705:A:N6     | 23:DB:726:G:O2'    | 2.42        | 0.53     |
| 1:CA:393:A:O2'     | 1:CA:394:G:H5'     | 2.08        | 0.53     |
| 1:CA:677:U:H2'     | 1:CA:678:U:C6      | 2.44        | 0.53     |
| 37:BL:110:VAL:HG23 | 37:BL:126:ARG:O    | 2.09        | 0.53     |
| 50:DT:12:ARG:HH11  | 50:DT:12:ARG:HB3   | 1.74        | 0.53     |
| 23:DB:2196:C:H2'   | 23:DB:2197:U:C6    | 2.44        | 0.53     |
| 16:CQ:30:HIS:CG    | 16:CQ:33:TYR:HB2   | 2.43        | 0.53     |
| 23:BB:4:U:H2'      | 23:BB:5:A:C8       | 2.44        | 0.53     |
| 43:BO:110:ALA:O    | 43:BO:115:LEU:HB2  | 2.09        | 0.53     |
| 1:AA:452:A:H2'     | 1:AA:453:G:O4'     | 2.09        | 0.53     |
| 23:BB:1097:U:C2'   | 23:BB:1098:A:H5'   | 2.38        | 0.53     |
| 23:BB:2553:G:H2'   | 23:BB:2554:U:O4'   | 2.09        | 0.53     |
| 23:DB:806:C:O2'    | 23:DB:807:U:H5'    | 2.08        | 0.53     |
| 23:BB:2543:G:H2'   | 23:BB:2544:G:C8    | 2.44        | 0.53     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 48:BG:154:GLU:C   | 48:BG:156:TYR:H    | 2.12        | 0.53     |
| 24:BI:52:LEU:HD21 | 24:BI:81:LYS:HZ2   | 1.74        | 0.53     |
| 29:DE:47:LYS:HA   | 29:DE:51:GLU:OE2   | 2.09        | 0.53     |
| 1:AA:1477:U:H2'   | 1:AA:1478:U:C6     | 2.44        | 0.53     |
| 23:DB:1234:U:O2'  | 23:DB:1235:G:H5'   | 2.08        | 0.53     |
| 1:AA:1102:A:H2'   | 1:AA:1103:C:C6     | 2.44        | 0.53     |
| 23:BB:724:U:H2'   | 23:BB:725:G:O4'    | 2.09        | 0.53     |
| 1:CA:911:U:H2'    | 1:CA:912:C:C6      | 2.44        | 0.53     |
| 21:CU:27:VAL:O    | 21:CU:31:VAL:HG23  | 2.08        | 0.53     |
| 25:DC:261:ARG:O   | 25:DC:261:ARG:HG2  | 2.08        | 0.53     |
| 23:DB:2758:A:H2'  | 23:DB:2759:G:O4'   | 2.09        | 0.53     |
| 23:BB:1671:U:H2'  | 23:BB:1673:G:OP2   | 2.09        | 0.53     |
| 6:AG:35:LYS:O     | 6:AG:39:GLU:HG3    | 2.08        | 0.53     |
| 23:BB:598:U:H2'   | 23:BB:599:A:H8     | 1.74        | 0.53     |
| 23:BB:533:G:H2'   | 23:BB:534:U:C6     | 2.43        | 0.52     |
| 23:BB:1021:A:H61  | 23:BB:1142:A:H61   | 1.55        | 0.52     |
| 20:CB:210:THR:HA  | 20:CB:213:LEU:HB2  | 1.91        | 0.52     |
| 35:DV:1:MET:O     | 35:DV:62:THR:HG23  | 2.08        | 0.52     |
| 25:BC:128:THR:OG1 | 25:BC:190:THR:HG22 | 2.09        | 0.52     |
| 47:BF:177:ARG:HA  | 47:BF:177:ARG:NE   | 2.24        | 0.52     |
| 7:CH:77:VAL:HG11  | 7:CH:124:ILE:HG21  | 1.91        | 0.52     |
| 44:BQ:56:PHE:HA   | 44:BQ:59:LEU:HB3   | 1.90        | 0.52     |
| 25:BC:66:PHE:HB2  | 25:BC:150:GLY:O    | 2.08        | 0.52     |
| 37:BL:56:PRO:O    | 37:BL:59:ARG:HB2   | 2.07        | 0.52     |
| 21:AU:19:LYS:HB2  | 21:AU:20:ARG:HE    | 1.74        | 0.52     |
| 1:CA:1227:A:H5''  | 12:CM:113:LYS:HD2  | 1.91        | 0.52     |
| 18:CS:20:LYS:NZ   | 18:CS:27:LYS:HD2   | 2.24        | 0.52     |
| 12:AM:14:ALA:HB1  | 12:AM:33:LEU:HD21  | 1.90        | 0.52     |
| 15:AP:66:THR:O    | 15:AP:67:ILE:HB    | 2.09        | 0.52     |
| 15:AP:52:LEU:HD21 | 15:AP:75:ILE:HG12  | 1.91        | 0.52     |
| 23:DB:2868:A:H2'  | 23:DB:2869:G:H8    | 1.74        | 0.52     |
| 48:DG:152:ARG:NH2 | 48:DG:162:ARG:HA   | 2.24        | 0.52     |
| 23:BB:1188:U:O2'  | 23:BB:1189:A:H5'   | 2.09        | 0.52     |
| 1:CA:309:A:O2'    | 1:CA:310:G:H5'     | 2.10        | 0.52     |
| 40:BH:73:ASN:ND2  | 40:BH:73:ASN:N     | 2.58        | 0.52     |
| 49:DR:16:GLU:HG2  | 49:DR:101:ILE:HG13 | 1.91        | 0.52     |
| 28:BP:3:ILE:HD13  | 28:BP:3:ILE:C      | 2.30        | 0.52     |
| 23:BB:863:A:H2'   | 23:BB:864:G:H8     | 1.74        | 0.52     |
| 28:DP:52:ARG:HB2  | 28:DP:55:HIS:O     | 2.09        | 0.52     |
| 23:BB:1654:A:H2'  | 23:BB:1655:A:H8    | 1.75        | 0.52     |
| 23:BB:1784:A:H4'  | 23:BB:1785:A:O5'   | 2.08        | 0.52     |
| 48:DG:174:LYS:HZ2 | 48:DG:176:LYS:HG2  | 1.73        | 0.52     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:BK:89:ASN:C    | 27:BK:89:ASN:HD22  | 2.13        | 0.52     |
| 23:BB:559:G:H21   | 44:BQ:51:GLN:HE22  | 1.57        | 0.52     |
| 1:AA:1162:C:H2'   | 1:AA:1163:A:C8     | 2.44        | 0.52     |
| 5:CF:54:LEU:N     | 5:CF:54:LEU:HD13   | 2.24        | 0.52     |
| 23:BB:2098:U:H2'  | 23:BB:2099:U:O4'   | 2.08        | 0.52     |
| 6:AG:59:GLU:O     | 6:AG:63:VAL:HG23   | 2.09        | 0.52     |
| 19:AT:38:ILE:HD13 | 19:AT:38:ILE:O     | 2.09        | 0.52     |
| 23:DB:184:C:H2'   | 23:DB:185:G:C8     | 2.43        | 0.52     |
| 1:CA:389:A:H2'    | 1:CA:389:A:N3      | 2.23        | 0.52     |
| 23:DB:1562:U:H2'  | 23:DB:1563:U:C6    | 2.43        | 0.52     |
| 23:DB:861:A:H2'   | 23:DB:862:G:O4'    | 2.09        | 0.52     |
| 1:AA:833:G:O2'    | 1:AA:834:U:H5'     | 2.09        | 0.52     |
| 23:DB:1537:G:H5'' | 23:DB:1537:G:N3    | 2.25        | 0.52     |
| 25:DC:61:TYR:HA   | 25:DC:85:ASN:ND2   | 2.24        | 0.52     |
| 23:DB:2728:U:H2'  | 23:DB:2729:G:C8    | 2.44        | 0.52     |
| 17:CR:63:TYR:CD2  | 17:CR:63:TYR:N     | 2.76        | 0.52     |
| 24:BI:49:GLU:CG   | 24:BI:54:ILE:HD11  | 2.39        | 0.52     |
| 23:DB:347:A:H2'   | 23:DB:348:A:C8     | 2.44        | 0.52     |
| 1:AA:820:U:H4'    | 1:AA:821:G:OP2     | 2.09        | 0.52     |
| 23:DB:406:G:O2'   | 23:DB:407:G:H5'    | 2.09        | 0.52     |
| 26:BD:141:ARG:O   | 26:BD:142:VAL:HG13 | 2.09        | 0.52     |
| 1:CA:162:A:H2'    | 1:CA:163:C:O4'     | 2.08        | 0.52     |
| 45:DS:10:ALA:HB3  | 45:DS:101:SER:OG   | 2.08        | 0.52     |
| 43:DO:105:ALA:C   | 43:DO:107:ALA:H    | 2.11        | 0.52     |
| 6:CG:70:PRO:O     | 6:CG:95:ARG:HG3    | 2.09        | 0.52     |
| 26:DD:97:SER:HB3  | 26:DD:99:GLU:HG3   | 1.91        | 0.52     |
| 23:BB:2600:A:O2'  | 23:BB:2601:C:H5'   | 2.09        | 0.52     |
| 23:DB:2213:U:C2'  | 23:DB:2213:U:O2    | 2.58        | 0.52     |
| 1:AA:250:A:H1'    | 1:AA:252:U:C5      | 2.44        | 0.52     |
| 1:AA:157:U:O2'    | 1:AA:158:G:H5'     | 2.09        | 0.52     |
| 26:DD:176:ASP:HB2 | 26:DD:190:LYS:HG2  | 1.90        | 0.52     |
| 4:AE:87:VAL:HG23  | 4:AE:91:SER:O      | 2.09        | 0.52     |
| 23:BB:854:C:O2'   | 23:BB:855:G:H5'    | 2.09        | 0.52     |
| 47:DF:32:LYS:HA   | 47:DF:95:MET:SD    | 2.50        | 0.52     |
| 53:B6:41:LEU:HD21 | 53:B6:88:LEU:HD13  | 1.90        | 0.52     |
| 48:DG:26:LYS:HA   | 48:DG:32:LEU:H     | 1.74        | 0.52     |
| 44:BQ:83:LYS:NZ   | 44:BQ:87:VAL:HA    | 2.24        | 0.52     |
| 1:AA:410:G:H2'    | 1:AA:429:U:C5      | 2.44        | 0.52     |
| 9:AJ:53:ILE:HG23  | 9:AJ:54:SER:H      | 1.75        | 0.52     |
| 13:AN:20:PHE:HB3  | 13:AN:24:ALA:HB2   | 1.91        | 0.52     |
| 18:AS:42:ASN:H    | 18:AS:42:ASN:HD22  | 1.57        | 0.52     |
| 46:DU:47:PRO:CD   | 46:DU:55:GLY:HA3   | 2.38        | 0.52     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:135:U:H2'    | 23:DB:136:G:C8     | 2.45        | 0.52     |
| 17:AR:33:THR:C     | 17:AR:35:SER:H     | 2.13        | 0.52     |
| 1:AA:1472:U:H2'    | 1:AA:1473:G:C8     | 2.44        | 0.52     |
| 3:CD:113:ALA:O     | 3:CD:116:LEU:HB2   | 2.10        | 0.52     |
| 23:DB:783:A:H8     | 23:DB:784:G:H4'    | 1.74        | 0.52     |
| 20:CB:68:PHE:HA    | 20:CB:161:PHE:O    | 2.09        | 0.52     |
| 20:CB:57:ASN:HA    | 20:CB:60:ALA:HB3   | 1.91        | 0.52     |
| 57:BB:3457:HOH:O   | 37:BL:99:ASN:HB3   | 2.09        | 0.52     |
| 20:CB:101:THR:HG22 | 20:CB:174:GLU:OE1  | 2.09        | 0.52     |
| 1:AA:253:A:H2'     | 1:AA:254:G:C8      | 2.44        | 0.52     |
| 1:AA:255:G:H2'     | 1:AA:256:U:H6      | 1.73        | 0.52     |
| 23:BB:275:C:C2'    | 23:BB:276:U:H5'    | 2.39        | 0.52     |
| 20:AB:68:PHE:CD1   | 20:AB:83:ALA:HB2   | 2.45        | 0.52     |
| 50:DT:69:ARG:HG3   | 50:DT:70:HIS:N     | 2.24        | 0.52     |
| 23:DB:1947:C:H2'   | 23:DB:1948:G:C8    | 2.44        | 0.52     |
| 23:BB:1220:G:H2'   | 23:BB:1221:C:H6    | 1.73        | 0.52     |
| 23:BB:1063:G:H1'   | 24:BI:134:SER:O    | 2.10        | 0.52     |
| 1:AA:505:G:H2'     | 1:AA:506:G:H8      | 1.73        | 0.52     |
| 33:D1:40:PRO:O     | 33:D1:43:ARG:HG2   | 2.08        | 0.52     |
| 33:B1:18:HIS:CD2   | 33:B1:40:PRO:HD2   | 2.45        | 0.52     |
| 22:BA:93:C:O2'     | 22:BA:94:A:H5'     | 2.09        | 0.52     |
| 53:B6:178:LYS:O    | 53:B6:182:GLU:HG3  | 2.10        | 0.52     |
| 22:DA:90:C:OP1     | 38:DM:16:ARG:HB2   | 2.09        | 0.52     |
| 12:CM:43:LYS:HB2   | 12:CM:46:GLU:CG    | 2.39        | 0.52     |
| 31:D0:25:THR:O     | 31:D0:26:SER:HB3   | 2.09        | 0.52     |
| 23:DB:1011:G:O2'   | 23:DB:1013:C:H5''  | 2.08        | 0.52     |
| 23:DB:950:G:H2'    | 23:DB:951:C:H6     | 1.73        | 0.52     |
| 1:CA:1096:C:H2'    | 1:CA:1097:C:H6     | 1.73        | 0.52     |
| 23:BB:1253:A:H4'   | 23:BB:1254:A:OP2   | 2.08        | 0.52     |
| 1:CA:405:U:O4      | 3:CD:1:ALA:HA      | 2.09        | 0.52     |
| 1:AA:811:C:H4'     | 1:AA:900:A:N6      | 2.24        | 0.52     |
| 23:DB:1036:G:O2'   | 23:DB:1037:G:H5'   | 2.10        | 0.52     |
| 23:DB:771:G:O2'    | 23:DB:772:C:H5'    | 2.09        | 0.52     |
| 23:BB:2204:G:O2'   | 23:BB:2205:A:H5'   | 2.09        | 0.52     |
| 23:DB:1159:U:H2'   | 23:DB:1160:G:H8    | 1.73        | 0.52     |
| 23:DB:1747:U:H2'   | 23:DB:1748:C:H6    | 1.74        | 0.52     |
| 6:CG:49:LEU:HD12   | 6:CG:124:SER:OG    | 2.10        | 0.52     |
| 23:BB:1747:U:H2'   | 23:BB:1748:C:H6    | 1.74        | 0.52     |
| 29:BE:1:MET:HB3    | 29:BE:14:VAL:O     | 2.09        | 0.52     |
| 1:AA:317:U:H2'     | 1:AA:318:G:H8      | 1.74        | 0.52     |
| 23:BB:2213:U:C2'   | 23:BB:2213:U:O2    | 2.57        | 0.52     |
| 28:DP:113:LEU:O    | 28:DP:113:LEU:HD23 | 2.09        | 0.52     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1084:G:H2'    | 1:AA:1085:U:C6     | 2.45        | 0.52     |
| 24:DI:92:PRO:O     | 24:DI:93:ASN:HB2   | 2.09        | 0.52     |
| 52:BW:22:VAL:O     | 52:BW:23:LYS:HG3   | 2.10        | 0.52     |
| 23:DB:1826:G:H2'   | 23:DB:1827:U:C6    | 2.44        | 0.52     |
| 40:BH:83:LYS:HB2   | 40:BH:92:GLY:N     | 2.24        | 0.52     |
| 1:CA:1287:A:H2'    | 1:CA:1288:A:C8     | 2.44        | 0.52     |
| 41:DJ:44:TYR:O     | 41:DJ:45:THR:HB    | 2.09        | 0.52     |
| 44:DQ:91:ARG:HB2   | 49:DR:11:GLN:NE2   | 2.25        | 0.52     |
| 30:DY:11:SER:HA    | 30:DY:31:ILE:HG22  | 1.91        | 0.52     |
| 26:DD:107:VAL:HG12 | 26:DD:109:VAL:HG23 | 1.90        | 0.52     |
| 35:BV:72:VAL:HB    | 35:BV:92:VAL:O     | 2.09        | 0.52     |
| 47:DF:43:ILE:HG23  | 47:DF:44:ALA:N     | 2.15        | 0.52     |
| 23:BB:670:A:H4'    | 23:BB:671:C:C5'    | 2.32        | 0.52     |
| 23:BB:1060:U:O2    | 23:BB:1088:A:C8    | 2.63        | 0.52     |
| 45:BS:15:GLN:HA    | 45:BS:18:ARG:CG    | 2.39        | 0.52     |
| 12:AM:42:VAL:HB    | 12:AM:47:LEU:HD21  | 1.91        | 0.52     |
| 18:AS:66:VAL:HG23  | 18:AS:67:GLY:H     | 1.74        | 0.52     |
| 23:BB:1174:U:HO2'  | 23:BB:1176:U:H5    | 1.54        | 0.52     |
| 13:CN:20:PHE:HB3   | 13:CN:24:ALA:HB2   | 1.91        | 0.52     |
| 35:DV:26:PHE:CE2   | 35:DV:44:HIS:HA    | 2.44        | 0.52     |
| 25:BC:209:ALA:HA   | 25:BC:212:TRP:CE2  | 2.45        | 0.52     |
| 40:BH:4:ILE:HD12   | 40:BH:4:ILE:H      | 1.74        | 0.52     |
| 26:DD:149:ASN:O    | 26:DD:152:PRO:HD2  | 2.08        | 0.52     |
| 23:BB:1427:A:H5''  | 23:BB:1559:U:O2    | 2.10        | 0.52     |
| 27:DK:75:SER:HB2   | 28:DP:73:PHE:HA    | 1.91        | 0.52     |
| 1:AA:308:C:H2'     | 1:AA:309:A:C8      | 2.43        | 0.52     |
| 1:AA:1533:C:C3'    | 1:AA:1534:A:H5''   | 2.39        | 0.52     |
| 1:AA:869:G:H5'     | 1:AA:872:A:O4'     | 2.10        | 0.52     |
| 23:BB:96:C:H4'     | 39:BX:41:HIS:CE1   | 2.44        | 0.52     |
| 23:DB:1353:A:H2'   | 23:DB:1354:A:H8    | 1.74        | 0.52     |
| 1:AA:1142:G:C2     | 1:AA:1143:G:H1'    | 2.45        | 0.52     |
| 1:CA:213:G:H5''    | 1:CA:214:C:H5      | 1.74        | 0.52     |
| 52:BW:46:ALA:HB2   | 52:BW:78:PHE:CD1   | 2.44        | 0.52     |
| 1:CA:1064:G:OP1    | 1:CA:1386:G:H4'    | 2.09        | 0.52     |
| 23:DB:1939:U:O2    | 23:DB:1967:C:H4'   | 2.09        | 0.52     |
| 23:DB:1347:A:H2'   | 23:DB:1348:C:O4'   | 2.10        | 0.52     |
| 4:CE:32:PHE:CE2    | 4:CE:55:VAL:HG22   | 2.45        | 0.52     |
| 12:AM:63:VAL:CG1   | 12:AM:67:ASP:HB2   | 2.40        | 0.52     |
| 1:AA:513:C:H2'     | 1:AA:514:C:H6      | 1.74        | 0.52     |
| 22:DA:49:C:H2'     | 22:DA:50:A:H8      | 1.75        | 0.52     |
| 37:DL:129:LYS:HA   | 37:DL:132:ARG:HG2  | 1.91        | 0.52     |
| 5:AF:85:ILE:HG22   | 5:AF:86:ARG:N      | 2.24        | 0.52     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 17:CR:21:ASP:OD1  | 17:CR:23:LYS:HD2   | 2.10        | 0.52     |
| 23:BB:2303:G:H1'  | 47:BF:122:ASP:OD1  | 2.09        | 0.52     |
| 23:BB:1201:U:H2'  | 23:BB:1202:G:H8    | 1.75        | 0.52     |
| 44:BQ:35:PHE:O    | 44:BQ:39:ILE:HG12  | 2.09        | 0.52     |
| 16:AQ:28:VAL:HG12 | 16:AQ:37:ILE:O     | 2.10        | 0.52     |
| 36:D2:22:MET:SD   | 36:D2:28:ARG:HG2   | 2.49        | 0.52     |
| 20:AB:93:HIS:CD2  | 20:AB:145:ASN:HB3  | 2.45        | 0.52     |
| 1:CA:898:G:N2     | 1:CA:900:A:H3'     | 2.24        | 0.52     |
| 19:CT:19:HIS:O    | 19:CT:23:ARG:HG2   | 2.08        | 0.52     |
| 17:CR:44:THR:C    | 17:CR:46:THR:H     | 2.13        | 0.52     |
| 23:BB:1753:G:N2   | 23:BB:1755:A:H3'   | 2.25        | 0.52     |
| 23:BB:1676:A:H2'  | 23:BB:1677:A:O4'   | 2.10        | 0.52     |
| 23:DB:1099:G:H4'  | 24:DI:4:VAL:CG1    | 2.39        | 0.52     |
| 24:DI:2:LYS:NZ    | 24:DI:2:LYS:HB3    | 2.25        | 0.52     |
| 48:BG:8:VAL:HG11  | 48:BG:49:LEU:CB    | 2.37        | 0.52     |
| 48:BG:84:LYS:HB2  | 48:BG:132:LEU:H    | 1.74        | 0.52     |
| 23:DB:947:A:H2'   | 23:DB:948:C:C6     | 2.44        | 0.52     |
| 53:B6:64:ARG:HA   | 53:B6:103:ILE:HB   | 1.90        | 0.52     |
| 40:BH:100:ALA:CB  | 40:BH:112:LYS:HA   | 2.32        | 0.52     |
| 8:CI:67:LYS:HZ3   | 8:CI:67:LYS:HB2    | 1.74        | 0.52     |
| 44:DQ:56:PHE:HA   | 44:DQ:59:LEU:HB3   | 1.92        | 0.52     |
| 25:BC:76:VAL:CG1  | 25:BC:114:GLN:HG2  | 2.33        | 0.52     |
| 26:DD:51:THR:HG22 | 26:DD:52:THR:N     | 2.24        | 0.52     |
| 43:DO:51:ALA:HB3  | 43:DO:78:VAL:CG2   | 2.39        | 0.52     |
| 50:BT:43:ILE:O    | 50:BT:47:VAL:HG23  | 2.09        | 0.52     |
| 50:BT:47:VAL:HG13 | 50:BT:51:PHE:CD1   | 2.44        | 0.52     |
| 53:B6:126:ARG:HA  | 53:B6:129:ILE:HD12 | 1.92        | 0.52     |
| 1:AA:411:A:H62    | 1:AA:413:G:N2      | 1.98        | 0.52     |
| 47:BF:142:TYR:CD1 | 47:BF:142:TYR:N    | 2.76        | 0.52     |
| 29:BE:131:THR:HB  | 29:BE:164:LEU:HG   | 1.90        | 0.52     |
| 42:DN:76:VAL:HA   | 42:DN:79:LEU:HD12  | 1.90        | 0.52     |
| 1:AA:1060:U:H2'   | 1:AA:1061:G:C8     | 2.44        | 0.52     |
| 47:DF:141:ASP:O   | 47:DF:145:VAL:HG13 | 2.10        | 0.52     |
| 35:BV:26:PHE:HE2  | 35:BV:44:HIS:HA    | 1.75        | 0.52     |
| 1:CA:1318:A:H4'   | 18:CS:9:PHE:CE1    | 2.45        | 0.52     |
| 27:BK:43:ILE:CG2  | 27:BK:54:LYS:HA    | 2.40        | 0.52     |
| 40:BH:14:SER:HB2  | 40:BH:17:ASP:CB    | 2.36        | 0.52     |
| 23:BB:279:A:C2    | 23:BB:362:A:H4'    | 2.45        | 0.52     |
| 53:B6:180:GLU:HA  | 53:B6:183:ILE:HG22 | 1.92        | 0.52     |
| 23:BB:1549:A:H2'  | 23:BB:1550:C:C6    | 2.44        | 0.52     |
| 20:CB:127:LYS:HD2 | 20:CB:127:LYS:O    | 2.09        | 0.52     |
| 51:BZ:28:ARG:HG2  | 51:BZ:28:ARG:O     | 2.09        | 0.52     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 31:B0:31:LYS:N     | 31:B0:31:LYS:HD2  | 2.23        | 0.52     |
| 1:AA:36:C:O3'      | 11:AL:119:LYS:HA  | 2.09        | 0.52     |
| 23:DB:857:G:H2'    | 23:DB:858:G:H5'   | 1.91        | 0.52     |
| 46:BU:78:LYS:CD    | 46:BU:79:ALA:H    | 2.22        | 0.52     |
| 23:BB:275:C:H2'    | 23:BB:276:U:O4'   | 2.09        | 0.52     |
| 23:DB:1387:A:H2'   | 23:DB:1388:G:C8   | 2.43        | 0.52     |
| 23:DB:2138:G:H2'   | 23:DB:2139:U:C6   | 2.44        | 0.52     |
| 19:AT:42:ASP:HA    | 19:AT:43:LYS:NZ   | 2.25        | 0.52     |
| 1:CA:284:C:H2'     | 1:CA:285:C:C6     | 2.45        | 0.52     |
| 43:BO:68:LYS:HA    | 43:BO:102:ARG:HG2 | 1.92        | 0.52     |
| 23:BB:2030:A:H4'   | 23:BB:2031:A:H5'  | 1.89        | 0.52     |
| 23:DB:2801:G:H2'   | 23:DB:2802:G:H8   | 1.73        | 0.52     |
| 53:B6:12:SER:O     | 53:B6:16:LYS:HD2  | 2.09        | 0.52     |
| 47:BF:119:LYS:HA   | 47:BF:121:PHE:CE1 | 2.44        | 0.52     |
| 1:AA:731:G:H5'     | 1:AA:766:A:H4'    | 1.90        | 0.52     |
| 1:CA:607:A:H2'     | 1:CA:608:A:H8     | 1.73        | 0.52     |
| 23:DB:1010:A:N3    | 23:DB:1153:C:H1'  | 2.24        | 0.52     |
| 1:CA:89:U:H2'      | 1:CA:90:C:H6      | 1.75        | 0.52     |
| 23:DB:1774:C:O2    | 23:DB:1774:C:H2'  | 2.10        | 0.52     |
| 43:BO:94:ARG:O     | 43:BO:97:PHE:HB2  | 2.10        | 0.52     |
| 23:DB:1994:C:O2'   | 23:DB:1995:U:H5'  | 2.09        | 0.52     |
| 23:DB:627:A:H4'    | 23:DB:628:G:OP1   | 2.09        | 0.52     |
| 23:DB:732:C:O2'    | 23:DB:733:G:H5'   | 2.09        | 0.52     |
| 23:DB:292:U:O2'    | 23:DB:293:U:H5'   | 2.09        | 0.52     |
| 50:DT:36:LYS:O     | 50:DT:36:LYS:HD3  | 2.10        | 0.52     |
| 1:AA:993:G:N2      | 1:AA:996:A:N6     | 2.56        | 0.52     |
| 25:BC:134:ILE:HG13 | 25:BC:134:ILE:O   | 2.08        | 0.52     |
| 23:DB:1820:U:OP1   | 25:DC:176:ARG:HD2 | 2.10        | 0.52     |
| 48:DG:51:PHE:CD2   | 48:DG:68:ARG:HG2  | 2.44        | 0.52     |
| 37:DL:141:LYS:NZ   | 37:DL:143:GLU:HA  | 2.24        | 0.52     |
| 48:DG:122:ALA:HB2  | 48:DG:132:LEU:HB3 | 1.92        | 0.52     |
| 22:DA:43:C:H1'     | 47:DF:91:ARG:NH2  | 2.25        | 0.52     |
| 8:CI:24:ASN:HD21   | 8:CI:26:LYS:HG3   | 1.74        | 0.52     |
| 44:DQ:57:ARG:HA    | 44:DQ:60:TRP:CE3  | 2.44        | 0.52     |
| 41:DJ:56:VAL:HG12  | 41:DJ:57:LEU:H    | 1.75        | 0.52     |
| 43:DO:35:ILE:HG22  | 43:DO:53:THR:HG23 | 1.90        | 0.52     |
| 34:D3:50:SER:C     | 34:D3:52:GLY:H    | 2.13        | 0.52     |
| 3:CD:157:ALA:O     | 3:CD:160:LEU:HD22 | 2.09        | 0.52     |
| 42:DN:79:LEU:HA    | 42:DN:83:LEU:CD1  | 2.39        | 0.52     |
| 47:BF:149:ARG:HA   | 47:BF:149:ARG:NH1 | 2.23        | 0.52     |
| 47:DF:111:ARG:O    | 47:DF:112:ASP:HB2 | 2.09        | 0.52     |
| 1:CA:1317:C:H3'    | 1:CA:1318:A:H8    | 1.75        | 0.52     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 18:AS:20:LYS:NZ   | 18:AS:27:LYS:HD2   | 2.24        | 0.52     |
| 23:DB:2789:C:O2   | 23:DB:2892:G:H5''  | 2.10        | 0.52     |
| 24:DI:24:GLY:HA2  | 24:DI:34:ILE:HD12  | 1.90        | 0.52     |
| 6:CG:114:SER:O    | 6:CG:118:ARG:HG3   | 2.10        | 0.52     |
| 46:BU:81:ARG:HB2  | 46:BU:96:LYS:CG    | 2.39        | 0.52     |
| 46:BU:12:VAL:HG22 | 46:BU:69:VAL:CG1   | 2.37        | 0.52     |
| 13:CN:27:LYS:HA   | 13:CN:31:SER:HB2   | 1.91        | 0.52     |
| 45:BS:36:LEU:N    | 45:BS:36:LEU:HD22  | 2.24        | 0.52     |
| 20:AB:15:PHE:HA   | 20:AB:42:LEU:HD21  | 1.91        | 0.52     |
| 26:DD:114:LYS:HE3 | 26:DD:116:LYS:NZ   | 2.25        | 0.52     |
| 30:BY:2:LYS:HE3   | 30:BY:58:GLU:HB3   | 1.91        | 0.52     |
| 3:CD:154:VAL:O    | 3:CD:158:LEU:HD12  | 2.09        | 0.52     |
| 42:DN:51:LEU:HD11 | 42:DN:69:ARG:HG3   | 1.91        | 0.52     |
| 49:BR:40:MET:O    | 49:BR:41:ILE:HD13  | 2.10        | 0.52     |
| 29:BE:176:ASP:OD1 | 29:BE:178:VAL:HG12 | 2.10        | 0.52     |
| 20:AB:144:GLU:O   | 20:AB:148:GLY:HA3  | 2.09        | 0.52     |
| 23:DB:276:U:O2    | 23:DB:362:A:N1     | 2.43        | 0.52     |
| 23:DB:278:A:H3'   | 23:DB:278:A:OP2    | 2.08        | 0.52     |
| 51:DZ:28:ARG:O    | 51:DZ:28:ARG:HG2   | 2.10        | 0.52     |
| 19:AT:66:ILE:HG22 | 19:AT:67:HIS:N     | 2.24        | 0.52     |
| 4:CE:80:LEU:HA    | 4:CE:146:MET:HE1   | 1.90        | 0.52     |
| 1:AA:238:A:C2'    | 1:AA:239:U:H5''    | 2.39        | 0.52     |
| 1:AA:635:A:H2'    | 1:AA:636:U:H6      | 1.74        | 0.52     |
| 23:DB:151:C:H2'   | 23:DB:152:A:C8     | 2.44        | 0.52     |
| 30:BY:40:THR:HB   | 30:BY:43:ILE:HG22  | 1.91        | 0.52     |
| 50:DT:54:GLU:CB   | 50:DT:88:LYS:HB2   | 2.39        | 0.52     |
| 3:AD:2:ARG:HG3    | 3:AD:114:ARG:NH1   | 2.24        | 0.52     |
| 23:DB:1593:A:H2'  | 23:DB:1594:U:H6    | 1.73        | 0.52     |
| 23:BB:72:U:H1'    | 39:BX:51:ALA:CB    | 2.39        | 0.52     |
| 1:CA:777:A:H2'    | 1:CA:778:G:C8      | 2.45        | 0.52     |
| 23:DB:934:U:H2'   | 23:DB:935:C:H6     | 1.73        | 0.52     |
| 23:BB:414:C:H2'   | 23:BB:415:A:H8     | 1.73        | 0.52     |
| 23:DB:962:G:H21   | 23:DB:2250:G:H22   | 1.57        | 0.52     |
| 23:BB:1317:G:H2'  | 23:BB:1318:U:O4'   | 2.10        | 0.52     |
| 37:BL:23:ILE:HD12 | 37:BL:23:ILE:N     | 2.24        | 0.52     |
| 23:DB:7:G:H4'     | 41:DJ:15:TRP:CH2   | 2.43        | 0.52     |
| 23:DB:2746:U:H5'' | 48:DG:137:LYS:HG3  | 1.92        | 0.52     |
| 23:BB:2814:A:H2'  | 23:BB:2815:C:C6    | 2.45        | 0.52     |
| 50:BT:61:LEU:HD12 | 50:BT:62:VAL:O     | 2.09        | 0.52     |
| 22:DA:50:A:OP1    | 43:DO:68:LYS:HB2   | 2.10        | 0.52     |
| 23:BB:1637:A:H2'  | 23:BB:1638:C:C6    | 2.44        | 0.52     |
| 41:DJ:109:LEU:CD1 | 41:DJ:119:PHE:HB2  | 2.39        | 0.52     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 29:BE:18:THR:HA   | 29:BE:106:LYS:HD3  | 1.91        | 0.52     |
| 1:CA:731:G:H5'    | 1:CA:766:A:H4'     | 1.91        | 0.52     |
| 23:DB:1577:C:H2'  | 23:DB:1578:U:O4'   | 2.10        | 0.52     |
| 23:BB:600:G:H2'   | 23:BB:601:C:C6     | 2.45        | 0.52     |
| 24:BI:23:VAL:HG23 | 24:BI:24:GLY:N     | 2.25        | 0.52     |
| 49:BR:20:VAL:HG12 | 49:BR:21:ARG:H     | 1.75        | 0.52     |
| 23:DB:82:U:H2'    | 23:DB:83:A:O4'     | 2.10        | 0.52     |
| 23:DB:132:G:H2'   | 23:DB:133:U:C6     | 2.44        | 0.52     |
| 1:AA:384:G:H2'    | 1:AA:385:C:C6      | 2.44        | 0.52     |
| 23:DB:336:C:O2'   | 23:DB:337:C:H5'    | 2.09        | 0.52     |
| 9:AJ:40:ILE:HD12  | 9:AJ:73:LEU:HD12   | 1.91        | 0.52     |
| 6:CG:45:ALA:HB3   | 6:CG:119:LEU:HD23  | 1.91        | 0.52     |
| 23:BB:1532:A:H2'  | 23:BB:1532:A:N3    | 2.25        | 0.52     |
| 7:AH:34:ALA:O     | 7:AH:38:VAL:HG23   | 2.10        | 0.52     |
| 23:BB:1870:C:H5"  | 23:BB:1871:A:C6    | 2.45        | 0.52     |
| 12:CM:58:GLU:O    | 12:CM:61:LYS:HG2   | 2.09        | 0.52     |
| 25:BC:222:THR:HA  | 25:BC:231:HIS:O    | 2.10        | 0.52     |
| 23:DB:2033:A:O2'  | 23:DB:2035:G:OP2   | 2.26        | 0.52     |
| 20:AB:69:VAL:HB   | 20:AB:162:VAL:HB   | 1.91        | 0.52     |
| 40:BH:68:ARG:HG3  | 40:BH:138:VAL:O    | 2.10        | 0.52     |
| 53:B6:67:VAL:HG12 | 53:B6:99:LEU:O     | 2.08        | 0.52     |
| 53:B6:83:ILE:HG23 | 53:B6:90:LEU:HD12  | 1.91        | 0.52     |
| 25:BC:116:GLN:O   | 25:BC:127:ASN:HA   | 2.10        | 0.52     |
| 1:AA:1014:A:N3    | 1:AA:1219:A:H1'    | 2.24        | 0.52     |
| 22:DA:28:C:N4     | 22:DA:56:G:H1      | 2.05        | 0.52     |
| 25:BC:107:LYS:O   | 25:BC:109:LEU:HD22 | 2.10        | 0.52     |
| 47:BF:107:VAL:N   | 47:BF:108:PRO:CD   | 2.73        | 0.52     |
| 42:DN:87:PHE:C    | 42:DN:89:SER:H     | 2.13        | 0.52     |
| 47:BF:37:MET:HE1  | 47:BF:149:ARG:HD2  | 1.91        | 0.52     |
| 20:AB:45:THR:HG22 | 20:AB:49:PHE:CZ    | 2.44        | 0.52     |
| 12:AM:10:ASP:O    | 12:AM:11:HIS:HB2   | 2.09        | 0.52     |
| 12:AM:14:ALA:HB2  | 12:AM:42:VAL:HG23  | 1.91        | 0.52     |
| 18:AS:15:LEU:O    | 18:AS:18:VAL:HG12  | 2.09        | 0.52     |
| 18:AS:42:ASN:N    | 18:AS:42:ASN:HD22  | 2.08        | 0.52     |
| 45:DS:70:LYS:HD3  | 45:DS:110:ARG:O    | 2.10        | 0.52     |
| 9:CJ:59:LYS:HB2   | 9:CJ:62:ARG:NH2    | 2.25        | 0.52     |
| 23:DB:2105:U:H2'  | 23:DB:2106:U:O4'   | 2.10        | 0.52     |
| 29:DE:134:LEU:CD2 | 29:DE:161:ALA:HB2  | 2.40        | 0.52     |
| 29:DE:134:LEU:O   | 29:DE:138:LEU:HG   | 2.09        | 0.52     |
| 17:CR:33:THR:C    | 17:CR:35:SER:H     | 2.12        | 0.52     |
| 44:BQ:111:LYS:HZ3 | 49:BR:50:GLY:HA2   | 1.75        | 0.52     |
| 49:BR:16:GLU:HG2  | 49:BR:101:ILE:HG13 | 1.91        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 48:DG:30:GLY:N    | 48:DG:78:VAL:HA   | 2.24        | 0.52     |
| 40:DH:64:ALA:O    | 40:DH:68:ARG:HG2  | 2.10        | 0.52     |
| 48:BG:30:GLY:H    | 48:BG:78:VAL:HA   | 1.74        | 0.52     |
| 1:AA:674:G:H2'    | 1:AA:675:A:C8     | 2.41        | 0.52     |
| 46:BU:35:VAL:HB   | 46:BU:38:ILE:CB   | 2.40        | 0.52     |
| 35:DV:29:ILE:HD13 | 35:DV:31:TYR:CE2  | 2.44        | 0.52     |
| 23:BB:2344:U:H4'  | 23:BB:2345:G:OP1  | 2.09        | 0.52     |
| 23:BB:151:C:H2'   | 23:BB:152:A:C8    | 2.44        | 0.52     |
| 23:DB:642:U:O2    | 23:DB:644:A:H3'   | 2.10        | 0.52     |
| 1:CA:1521:C:O2'   | 1:CA:1522:U:H5'   | 2.10        | 0.52     |
| 23:BB:704:G:H1'   | 23:BB:727:A:N6    | 2.24        | 0.52     |
| 3:CD:84:ASN:ND2   | 3:CD:86:GLY:H     | 2.08        | 0.52     |
| 37:DL:47:ARG:HG3  | 37:DL:48:ARG:N    | 2.24        | 0.52     |
| 39:BX:9:LYS:NZ    | 39:BX:60:LYS:HE3  | 2.25        | 0.52     |
| 1:AA:377:G:H2'    | 1:AA:378:G:H8     | 1.75        | 0.52     |
| 52:BW:77:LYS:O    | 52:BW:78:PHE:HB2  | 2.09        | 0.52     |
| 3:CD:10:LEU:HB3   | 3:CD:62:ARG:HD3   | 1.92        | 0.52     |
| 23:DB:272:A:H2'   | 23:DB:273:G:H8    | 1.74        | 0.52     |
| 23:BB:573:U:N3    | 23:BB:2031:A:OP1  | 2.38        | 0.52     |
| 1:AA:1464:U:H2'   | 1:AA:1465:A:C8    | 2.45        | 0.52     |
| 23:DB:222:A:H61   | 23:DB:232:G:H1'   | 1.73        | 0.52     |
| 23:BB:1477:A:H2'  | 23:BB:1478:G:O4'  | 2.09        | 0.52     |
| 3:AD:149:LYS:HB2  | 3:AD:177:MET:HG3  | 1.92        | 0.52     |
| 1:CA:696:A:H2'    | 1:CA:697:U:H6     | 1.73        | 0.52     |
| 48:DG:154:GLU:OE2 | 48:DG:156:TYR:HB2 | 2.09        | 0.52     |
| 23:BB:1994:C:O2'  | 23:BB:1995:U:H5'  | 2.10        | 0.52     |
| 23:DB:1230:A:H2'  | 23:DB:1231:U:C6   | 2.45        | 0.52     |
| 1:CA:640:A:O2'    | 1:CA:641:U:H5'    | 2.09        | 0.52     |
| 23:BB:1835:G:H2'  | 23:BB:1836:C:C6   | 2.44        | 0.52     |
| 23:BB:2520:C:O2'  | 23:BB:2521:C:H5'  | 2.10        | 0.52     |
| 23:BB:2436:G:O2'  | 23:BB:2437:G:H5'  | 2.10        | 0.52     |
| 6:CG:29:LEU:O     | 6:CG:29:LEU:HD23  | 2.10        | 0.52     |
| 23:BB:1732:C:H2'  | 23:BB:1732:C:OP1  | 2.10        | 0.52     |
| 6:AG:29:LEU:HD23  | 6:AG:29:LEU:O     | 2.10        | 0.52     |
| 38:BM:78:LEU:O    | 38:BM:80:VAL:HG12 | 2.10        | 0.52     |
| 1:CA:1234:C:H1'   | 1:CA:1364:U:O2    | 2.10        | 0.52     |
| 23:DB:1099:G:C5'  | 24:DI:4:VAL:HG12  | 2.40        | 0.52     |
| 52:BW:32:ALA:C    | 52:BW:34:SER:H    | 2.12        | 0.52     |
| 23:DB:2354:C:H4'  | 52:DW:31:LEU:CD2  | 2.39        | 0.52     |
| 47:BF:64:PRO:HA   | 47:BF:88:VAL:HG21 | 1.90        | 0.52     |
| 37:BL:121:THR:HA  | 37:BL:141:LYS:HB3 | 1.91        | 0.52     |
| 47:DF:33:ILE:O    | 47:DF:90:LEU:N    | 2.42        | 0.52     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 49:DR:6:GLN:HE22   | 49:DR:10:LYS:H     | 1.55        | 0.52     |
| 20:CB:187:ASP:H    | 20:CB:190:SER:HB2  | 1.75        | 0.52     |
| 50:BT:1:MET:CG     | 50:BT:2:ILE:H      | 2.23        | 0.52     |
| 35:BV:1:MET:O      | 35:BV:62:THR:HG23  | 2.09        | 0.52     |
| 23:DB:2548:U:H1'   | 27:DK:23:LYS:HZ3   | 1.71        | 0.52     |
| 3:AD:26:ALA:HA     | 3:AD:30:LYS:CE     | 2.40        | 0.52     |
| 29:BE:155:GLU:O    | 29:BE:159:LEU:HB2  | 2.08        | 0.52     |
| 18:CS:51:HIS:HB2   | 18:CS:56:HIS:CE1   | 2.45        | 0.52     |
| 23:DB:372:G:O2'    | 51:DZ:54:LYS:HE2   | 2.10        | 0.52     |
| 25:DC:209:ALA:HA   | 25:DC:212:TRP:CE2  | 2.45        | 0.52     |
| 45:DS:36:LEU:HD22  | 45:DS:36:LEU:H     | 1.75        | 0.52     |
| 23:BB:1125:G:H4'   | 32:B4:37:GLN:NE2   | 2.25        | 0.52     |
| 10:CK:92:ARG:HH21  | 21:CU:24:LYS:HG2   | 1.74        | 0.52     |
| 53:B6:133:ARG:NH1  | 53:B6:162:GLN:HE22 | 2.07        | 0.52     |
| 32:D4:15:LYS:O     | 32:D4:15:LYS:HE2   | 2.10        | 0.52     |
| 23:DB:1123:C:O2'   | 23:DB:1124:G:H5'   | 2.10        | 0.52     |
| 48:DG:166:GLU:CG   | 48:DG:168:VAL:HG23 | 2.39        | 0.52     |
| 29:DE:149:ILE:HG23 | 29:DE:188:MET:CA   | 2.40        | 0.52     |
| 23:BB:969:G:H2'    | 23:BB:970:U:H6     | 1.74        | 0.52     |
| 1:CA:1332:A:H2'    | 1:CA:1333:A:H8     | 1.73        | 0.52     |
| 49:DR:3:ALA:O      | 49:DR:4:VAL:HG13   | 2.09        | 0.52     |
| 37:DL:95:LEU:HB2   | 37:DL:101:ILE:CG1  | 2.40        | 0.52     |
| 1:AA:841:C:H2'     | 1:AA:843:U:OP2     | 2.10        | 0.52     |
| 1:AA:86:G:C2       | 1:AA:87:C:N4       | 2.77        | 0.52     |
| 23:BB:125:A:H5'    | 36:B2:19:ARG:CG    | 2.40        | 0.52     |
| 20:AB:107:ARG:HA   | 20:AB:110:ILE:HD12 | 1.92        | 0.52     |
| 40:DH:49:ALA:HB3   | 40:DH:50:ARG:NH2   | 2.24        | 0.52     |
| 47:DF:162:ASP:O    | 47:DF:166:ARG:HD2  | 2.10        | 0.52     |
| 1:CA:1000:A:H2'    | 1:CA:1001:C:C6     | 2.45        | 0.52     |
| 20:AB:27:LYS:HB3   | 20:AB:28:PRO:HD3   | 1.91        | 0.52     |
| 46:DU:70:ALA:HB1   | 46:DU:79:ALA:HB3   | 1.90        | 0.52     |
| 4:CE:84:VAL:CG1    | 4:CE:146:MET:HB3   | 2.40        | 0.52     |
| 35:BV:31:TYR:HB3   | 35:BV:37:PRO:HG3   | 1.91        | 0.52     |
| 23:DB:126:A:OP2    | 36:D2:19:ARG:HB2   | 2.08        | 0.52     |
| 1:CA:502:A:H2'     | 1:CA:503:C:C6      | 2.44        | 0.52     |
| 1:AA:1522:U:O2'    | 1:AA:1523:G:H5'    | 2.09        | 0.52     |
| 1:AA:1512:U:H2'    | 1:AA:1513:A:C8     | 2.45        | 0.52     |
| 23:BB:2002:G:OP1   | 42:BN:13:ASN:HA    | 2.10        | 0.52     |
| 1:AA:1142:G:H3'    | 1:AA:1143:G:H8     | 1.74        | 0.52     |
| 1:CA:1141:C:H2'    | 1:CA:1142:G:C8     | 2.43        | 0.52     |
| 23:DB:1317:G:H2'   | 23:DB:1318:U:O4'   | 2.10        | 0.52     |
| 23:BB:1562:U:H2'   | 23:BB:1563:U:C6    | 2.45        | 0.52     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 53:D6:113:ASP:HA   | 53:D6:116:ARG:HD3  | 1.90        | 0.52     |
| 23:BB:1351:C:H4'   | 23:BB:1572:A:O4'   | 2.10        | 0.52     |
| 23:DB:1599:U:H2'   | 23:DB:1600:C:H6    | 1.75        | 0.52     |
| 23:DB:2814:A:H2'   | 23:DB:2815:C:C6    | 2.45        | 0.52     |
| 23:DB:1253:A:H4'   | 23:DB:1254:A:OP2   | 2.09        | 0.52     |
| 23:DB:2439:A:N7    | 23:DB:2586:U:H4'   | 2.25        | 0.52     |
| 5:AF:86:ARG:HH11   | 17:AR:64:LEU:HD12  | 1.73        | 0.52     |
| 29:DE:47:LYS:HB3   | 29:DE:51:GLU:HB2   | 1.90        | 0.52     |
| 11:CL:122:LYS:HG3  | 11:CL:123:ALA:H    | 1.74        | 0.52     |
| 23:DB:69:C:O2'     | 23:DB:70:G:H5'     | 2.10        | 0.52     |
| 24:DI:102:ARG:HG3  | 24:DI:141:ASP:HB2  | 1.92        | 0.52     |
| 23:DB:686:U:H1'    | 36:D2:6:GLN:O      | 2.10        | 0.52     |
| 1:AA:1069:C:O2'    | 1:AA:1192:C:H1'    | 2.09        | 0.52     |
| 23:BB:1714:U:H3'   | 23:BB:1715:G:H5'   | 1.92        | 0.52     |
| 36:B2:13:ASN:O     | 36:B2:17:GLY:N     | 2.43        | 0.52     |
| 37:BL:92:LEU:HD23  | 37:BL:92:LEU:H     | 1.74        | 0.52     |
| 23:DB:1479:G:O2'   | 23:DB:1480:C:H5'   | 2.10        | 0.52     |
| 23:BB:1414:C:H2'   | 23:BB:1415:U:H6    | 1.75        | 0.52     |
| 23:BB:920:A:H2'    | 23:BB:921:C:O4'    | 2.09        | 0.52     |
| 44:DQ:34:ALA:O     | 44:DQ:38:VAL:HG23  | 2.09        | 0.52     |
| 10:CK:70:ALA:C     | 10:CK:72:ALA:H     | 2.12        | 0.52     |
| 47:DF:64:PRO:HA    | 47:DF:88:VAL:HG21  | 1.92        | 0.52     |
| 23:DB:996:A:H4'    | 44:DQ:91:ARG:HH11  | 1.73        | 0.52     |
| 12:AM:13:HIS:HB3   | 12:AM:40:GLU:O     | 2.09        | 0.52     |
| 23:DB:2358:A:H61   | 37:DL:54:GLN:HE22  | 1.58        | 0.52     |
| 12:CM:13:HIS:HB3   | 12:CM:40:GLU:O     | 2.09        | 0.52     |
| 48:BG:15:ASP:OD2   | 48:BG:17:LYS:HB2   | 2.09        | 0.52     |
| 29:BE:153:LEU:HG   | 29:BE:154:ASP:H    | 1.75        | 0.52     |
| 47:DF:169:LEU:HD22 | 47:DF:174:PHE:CE1  | 2.44        | 0.52     |
| 35:BV:23:ALA:O     | 35:BV:24:ASN:HB2   | 2.10        | 0.52     |
| 18:AS:51:HIS:HB2   | 18:AS:56:HIS:CE1   | 2.44        | 0.52     |
| 11:AL:49:ARG:HD2   | 11:AL:49:ARG:N     | 2.24        | 0.52     |
| 25:DC:15:VAL:HG22  | 25:DC:204:LEU:O    | 2.10        | 0.52     |
| 45:DS:55:ILE:HD12  | 45:DS:69:LEU:HD23  | 1.91        | 0.52     |
| 48:BG:145:ALA:HA   | 48:BG:148:ARG:CG   | 2.39        | 0.52     |
| 20:AB:64:GLY:O     | 20:AB:66:ILE:HG12  | 2.09        | 0.52     |
| 42:DN:28:LEU:HD23  | 42:DN:113:ILE:HG23 | 1.90        | 0.52     |
| 37:DL:93:ASN:O     | 37:DL:95:LEU:N     | 2.38        | 0.52     |
| 23:DB:2897:U:H2'   | 23:DB:2898:U:H6    | 1.73        | 0.52     |
| 34:B3:22:LYS:HB2   | 34:B3:48:MET:SD    | 2.50        | 0.52     |
| 27:BK:58:LEU:N     | 27:BK:58:LEU:HD23  | 2.24        | 0.52     |
| 24:DI:100:ILE:O    | 24:DI:139:VAL:HA   | 2.10        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 5:AF:4:TYR:O      | 5:AF:63:ASN:HA    | 2.10        | 0.52     |
| 51:BZ:17:ASN:HD22 | 51:BZ:25:THR:HB   | 1.75        | 0.52     |
| 23:BB:1655:A:H2'  | 23:BB:1656:C:O4'  | 2.09        | 0.52     |
| 26:BD:124:ARG:HA  | 26:BD:165:MET:HE3 | 1.90        | 0.52     |
| 27:BK:60:ALA:HA   | 27:BK:87:LEU:CD2  | 2.39        | 0.52     |
| 23:DB:713:G:O2'   | 23:DB:714:U:H5'   | 2.10        | 0.52     |
| 29:BE:48:THR:C    | 29:BE:50:ALA:H    | 2.12        | 0.52     |
| 39:BX:18:LEU:HA   | 39:BX:21:LEU:HD12 | 1.91        | 0.52     |
| 1:AA:621:A:H2'    | 1:AA:622:A:H8     | 1.74        | 0.52     |
| 23:DB:2026:U:H2'  | 23:DB:2027:G:H8   | 1.75        | 0.52     |
| 2:AC:82:ASP:O     | 2:AC:86:LEU:HG    | 2.10        | 0.52     |
| 1:AA:392:C:H2'    | 1:AA:393:A:H8     | 1.75        | 0.52     |
| 52:DW:77:LYS:O    | 52:DW:78:PHE:HB2  | 2.10        | 0.52     |
| 1:CA:1142:G:C2    | 1:CA:1143:G:H1'   | 2.44        | 0.52     |
| 9:CJ:80:THR:HG21  | 9:CJ:82:LYS:NZ    | 2.25        | 0.52     |
| 48:DG:38:ASP:CG   | 48:DG:39:ALA:H    | 2.13        | 0.52     |
| 23:DB:2286:G:H5'  | 23:DB:2286:G:C8   | 2.45        | 0.52     |
| 50:DT:45:ALA:O    | 50:DT:48:GLN:HB2  | 2.10        | 0.52     |
| 1:CA:590:U:H2'    | 1:CA:591:U:C6     | 2.45        | 0.52     |
| 24:DI:99:LYS:HD3  | 24:DI:99:LYS:N    | 2.24        | 0.52     |
| 23:BB:81:G:H2'    | 23:BB:82:U:O4'    | 2.10        | 0.52     |
| 23:DB:175:G:O2'   | 23:DB:176:A:H5'   | 2.10        | 0.52     |
| 23:BB:1252:G:N2   | 44:BQ:32:ARG:HB3  | 2.24        | 0.52     |
| 24:BI:23:VAL:HG23 | 24:BI:24:GLY:H    | 1.74        | 0.52     |
| 22:DA:91:C:H2'    | 22:DA:92:C:C6     | 2.45        | 0.52     |
| 7:AH:118:ALA:HB3  | 7:AH:120:LEU:HD22 | 1.92        | 0.52     |
| 47:DF:56:LEU:HD22 | 47:DF:59:ILE:HD12 | 1.92        | 0.52     |
| 3:CD:145:ARG:NH2  | 3:CD:147:LYS:HE2  | 2.24        | 0.52     |
| 1:CA:1366:C:H2'   | 1:CA:1367:C:H6    | 1.75        | 0.52     |
| 25:DC:226:PRO:HA  | 25:DC:232:GLY:HA3 | 1.92        | 0.52     |
| 6:AG:12:LEU:HD22  | 6:AG:13:PRO:HD2   | 1.90        | 0.52     |
| 23:BB:1577:C:H2'  | 23:BB:1578:U:C6   | 2.45        | 0.52     |
| 23:BB:406:G:O2'   | 23:BB:407:G:H5'   | 2.10        | 0.52     |
| 23:DB:2226:C:H2'  | 23:DB:2227:A:H8   | 1.74        | 0.52     |
| 1:CA:223:A:H2'    | 1:CA:224:U:C6     | 2.45        | 0.52     |
| 1:CA:227:G:H2'    | 1:CA:228:A:C8     | 2.45        | 0.52     |
| 23:BB:2639:A:H2'  | 23:BB:2640:G:O4'  | 2.10        | 0.52     |
| 25:DC:141:HIS:HB3 | 25:DC:190:THR:HG1 | 1.74        | 0.52     |
| 23:DB:533:G:H2'   | 23:DB:534:U:C6    | 2.45        | 0.52     |
| 47:BF:31:GLU:O    | 47:BF:32:LYS:HD3  | 2.10        | 0.52     |
| 37:BL:124:GLY:H   | 37:BL:143:GLU:HG3 | 1.75        | 0.52     |
| 37:BL:125:LEU:H   | 37:BL:143:GLU:HG3 | 1.74        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 27:BK:35:VAL:CG2  | 27:BK:36:GLY:H    | 2.07        | 0.52     |
| 1:CA:1250:A:H4'   | 8:CI:69:GLY:N     | 2.24        | 0.52     |
| 8:AI:67:LYS:NZ    | 8:AI:67:LYS:HB2   | 2.22        | 0.52     |
| 51:DZ:38:PHE:CE2  | 51:DZ:51:VAL:HG21 | 2.45        | 0.52     |
| 23:BB:141:G:C6    | 50:BT:2:ILE:HD12  | 2.44        | 0.52     |
| 1:AA:1296:C:H4'   | 1:AA:1302:C:N4    | 2.11        | 0.52     |
| 50:BT:54:GLU:CB   | 50:BT:88:LYS:HB2  | 2.40        | 0.52     |
| 1:CA:410:G:P      | 3:CD:25:ARG:HE    | 2.33        | 0.52     |
| 1:CA:410:G:H2'    | 1:CA:429:U:C5     | 2.45        | 0.52     |
| 53:B6:126:ARG:O   | 53:B6:130:ARG:HG2 | 2.10        | 0.52     |
| 1:CA:1060:U:H2'   | 1:CA:1061:G:C8    | 2.45        | 0.52     |
| 40:DH:8:LYS:O     | 40:DH:13:GLY:HA3  | 2.10        | 0.52     |
| 1:CA:764:C:O2'    | 1:CA:765:G:H5'    | 2.10        | 0.52     |
| 23:DB:165:A:H2'   | 23:DB:166:U:C6    | 2.44        | 0.52     |
| 10:CK:22:ILE:HD13 | 10:CK:95:THR:HG21 | 1.91        | 0.52     |
| 23:BB:978:G:O2'   | 23:BB:979:A:H5'   | 2.10        | 0.52     |
| 1:AA:1250:A:H4'   | 8:AI:69:GLY:N     | 2.25        | 0.52     |
| 35:DV:51:GLN:NE2  | 35:DV:79:ARG:HH22 | 2.07        | 0.52     |
| 5:CF:6:ILE:HD11   | 5:CF:8:PHE:CD2    | 2.45        | 0.52     |
| 44:BQ:86:SER:O    | 44:BQ:88:GLU:N    | 2.42        | 0.52     |
| 23:DB:1441:G:H2'  | 23:DB:1442:U:C6   | 2.45        | 0.52     |
| 20:CB:68:PHE:CD1  | 20:CB:83:ALA:HB2  | 2.44        | 0.52     |
| 48:BG:30:GLY:N    | 48:BG:78:VAL:HA   | 2.25        | 0.52     |
| 53:D6:110:ARG:NH1 | 53:D6:110:ARG:HB3 | 2.21        | 0.52     |
| 29:DE:153:LEU:HG  | 29:DE:154:ASP:H   | 1.75        | 0.52     |
| 26:BD:114:LYS:HE3 | 26:BD:116:LYS:NZ  | 2.25        | 0.52     |
| 3:AD:94:GLU:HA    | 3:AD:99:ASN:ND2   | 2.24        | 0.52     |
| 27:DK:60:ALA:HA   | 27:DK:87:LEU:CD2  | 2.39        | 0.52     |
| 6:AG:50:ALA:HB2   | 6:AG:57:GLU:HG3   | 1.90        | 0.52     |
| 39:BX:17:GLU:HB3  | 39:BX:53:VAL:CG1  | 2.39        | 0.52     |
| 37:BL:47:ARG:HH21 | 37:BL:47:ARG:CB   | 2.23        | 0.52     |
| 23:BB:1824:G:O2'  | 23:BB:1825:U:H5'  | 2.10        | 0.52     |
| 23:DB:364:C:H2'   | 23:DB:365:U:C6    | 2.44        | 0.52     |
| 23:BB:75:G:H4'    | 39:BX:48:ARG:NH2  | 2.25        | 0.52     |
| 4:CE:110:MET:SD   | 4:CE:126:ALA:HB2  | 2.50        | 0.52     |
| 1:AA:1516:G:H2'   | 1:AA:1518:A:OP2   | 2.09        | 0.52     |
| 26:BD:121:THR:C   | 26:BD:123:LYS:H   | 2.14        | 0.52     |
| 23:DB:2671:G:H2'  | 23:DB:2672:U:H6   | 1.74        | 0.52     |
| 23:BB:2859:G:H2'  | 23:BB:2860:A:C8   | 2.43        | 0.52     |
| 23:DB:1220:G:H2'  | 23:DB:1221:C:H6   | 1.75        | 0.52     |
| 35:BV:16:ALA:HA   | 35:BV:19:ARG:HE   | 1.74        | 0.52     |
| 23:DB:2784:U:O2'  | 23:DB:2785:C:H5'  | 2.09        | 0.52     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:1152:A:H2'   | 1:CA:1153:G:H8     | 1.75        | 0.52     |
| 27:BK:107:LEU:C   | 27:BK:109:SER:H    | 2.13        | 0.52     |
| 23:BB:236:C:O2'   | 23:BB:237:C:H5'    | 2.10        | 0.52     |
| 25:BC:181:ARG:HD3 | 25:BC:182:LYS:H    | 1.74        | 0.52     |
| 5:CF:85:ILE:HG22  | 5:CF:86:ARG:H      | 1.75        | 0.52     |
| 23:DB:1714:U:H3'  | 23:DB:1715:G:H5'   | 1.91        | 0.52     |
| 1:CA:810:C:O2'    | 1:CA:811:C:H5'     | 2.10        | 0.52     |
| 23:BB:732:C:O2'   | 23:BB:733:G:H5'    | 2.10        | 0.52     |
| 11:AL:34:THR:HG21 | 11:AL:53:ARG:HH21  | 1.75        | 0.52     |
| 37:BL:41:ARG:HH21 | 37:BL:41:ARG:HG2   | 1.75        | 0.52     |
| 51:DZ:30:LEU:HD23 | 51:DZ:30:LEU:N     | 2.25        | 0.52     |
| 50:BT:36:LYS:O    | 50:BT:36:LYS:HD3   | 2.09        | 0.52     |
| 23:DB:1825:U:H2'  | 23:DB:1826:G:C8    | 2.45        | 0.52     |
| 37:BL:141:LYS:NZ  | 37:BL:143:GLU:HA   | 2.24        | 0.52     |
| 16:CQ:45:VAL:HG12 | 16:CQ:46:HIS:N     | 2.25        | 0.52     |
| 23:DB:920:A:H2'   | 23:DB:921:C:O4'    | 2.09        | 0.52     |
| 23:DB:2734:A:C2'  | 23:DB:2735:G:H5'   | 2.40        | 0.52     |
| 1:CA:1219:A:H2'   | 1:CA:1220:G:C8     | 2.45        | 0.52     |
| 44:BQ:94:LEU:HG   | 49:BR:11:GLN:HE21  | 1.75        | 0.52     |
| 51:BZ:30:LEU:N    | 51:BZ:30:LEU:HD23  | 2.25        | 0.52     |
| 53:B6:10:THR:HG22 | 53:B6:14:MET:HE3   | 1.92        | 0.52     |
| 23:BB:1059:G:N2   | 24:BI:130:GLY:HA3  | 2.25        | 0.52     |
| 2:CC:84:GLU:OE2   | 2:CC:87:ARG:HD3    | 2.10        | 0.52     |
| 1:CA:1316:G:H22   | 1:CA:1318:A:H3'    | 1.73        | 0.52     |
| 45:BS:47:VAL:HG12 | 45:BS:103:ILE:CG2  | 2.40        | 0.52     |
| 18:AS:29:PRO:HA   | 18:AS:47:THR:O     | 2.10        | 0.52     |
| 41:DJ:81:ILE:HG23 | 41:DJ:82:GLY:N     | 2.18        | 0.52     |
| 23:DB:135:U:H2'   | 23:DB:136:G:H8     | 1.74        | 0.52     |
| 9:AJ:59:LYS:HB2   | 9:AJ:62:ARG:NH2    | 2.24        | 0.52     |
| 16:AQ:59:GLU:O    | 16:AQ:74:LEU:HD22  | 2.10        | 0.52     |
| 45:DS:36:LEU:HD22 | 45:DS:36:LEU:N     | 2.25        | 0.52     |
| 15:AP:72:ALA:HA   | 15:AP:75:ILE:HD12  | 1.92        | 0.52     |
| 35:DV:23:ALA:O    | 35:DV:24:ASN:HB2   | 2.10        | 0.52     |
| 20:CB:40:ILE:HG21 | 20:CB:200:PRO:O    | 2.09        | 0.52     |
| 20:CB:15:PHE:HA   | 20:CB:42:LEU:HD11  | 1.90        | 0.52     |
| 1:AA:312:C:H2'    | 1:AA:313:A:C8      | 2.45        | 0.52     |
| 38:DM:18:ARG:C    | 38:DM:38:ARG:HH22  | 2.13        | 0.52     |
| 23:BB:1724:G:H2'  | 23:BB:1725:U:C6    | 2.45        | 0.52     |
| 23:BB:1445:G:H2'  | 23:BB:1446:C:C6    | 2.44        | 0.52     |
| 38:BM:2:LEU:CD2   | 38:BM:46:ILE:HD11  | 2.39        | 0.52     |
| 20:AB:99:MET:HA   | 20:AB:106:VAL:HG21 | 1.92        | 0.52     |
| 37:BL:95:LEU:HD13 | 37:BL:101:ILE:HG13 | 1.92        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:582:A:H2'   | 23:DB:583:G:C8    | 2.45        | 0.52     |
| 23:DB:358:U:H2'   | 23:DB:359:G:C8    | 2.45        | 0.52     |
| 38:DM:4:PRO:HG3   | 38:DM:68:PHE:HE2  | 1.74        | 0.52     |
| 23:DB:2339:C:H2'  | 23:DB:2340:A:C8   | 2.45        | 0.52     |
| 1:AA:1514:G:H2'   | 1:AA:1515:G:H8    | 1.74        | 0.52     |
| 7:CH:94:VAL:HG21  | 7:CH:100:ILE:O    | 2.10        | 0.52     |
| 1:AA:215:C:H2'    | 1:AA:216:U:H6     | 1.73        | 0.52     |
| 23:DB:547:A:C6    | 23:DB:548:G:H1'   | 2.45        | 0.52     |
| 23:BB:1561:C:H2'  | 23:BB:1562:U:C6   | 2.45        | 0.52     |
| 20:AB:18:GLN:HB2  | 20:AB:188:THR:OG1 | 2.10        | 0.52     |
| 23:BB:1236:G:H1'  | 23:BB:1237:A:C8   | 2.44        | 0.52     |
| 34:D3:41:ARG:HG3  | 34:D3:44:ARG:NH2  | 2.25        | 0.52     |
| 43:DO:28:VAL:O    | 43:DO:28:VAL:HG13 | 2.10        | 0.52     |
| 44:BQ:40:LYS:HD2  | 44:BQ:44:TYR:CE1  | 2.44        | 0.52     |
| 23:DB:2648:G:H2'  | 23:DB:2649:C:C6   | 2.45        | 0.52     |
| 23:DB:1859:U:H2'  | 23:DB:1860:G:H8   | 1.75        | 0.52     |
| 37:DL:136:GLU:HA  | 37:DL:140:GLY:H   | 1.74        | 0.52     |
| 23:BB:1465:G:H2'  | 23:BB:1466:U:C6   | 2.45        | 0.52     |
| 17:AR:31:TYR:CG   | 17:AR:54:LEU:HD11 | 2.44        | 0.52     |
| 34:B3:15:LYS:HA   | 34:B3:21:PHE:HA   | 1.92        | 0.52     |
| 1:AA:724:G:O2'    | 1:AA:725:G:H5'    | 2.10        | 0.52     |
| 1:AA:642:A:H2'    | 1:AA:643:C:H6     | 1.75        | 0.52     |
| 23:BB:167:A:H2'   | 23:BB:168:G:O4'   | 2.10        | 0.52     |
| 23:DB:1319:C:O2'  | 23:DB:1320:C:H5'  | 2.09        | 0.52     |
| 42:DN:54:LEU:CD1  | 42:DN:62:ASN:HB3  | 2.40        | 0.52     |
| 23:DB:1613:G:H2'  | 23:DB:1617:C:H42  | 1.74        | 0.52     |
| 23:BB:41:C:H2'    | 23:BB:42:A:O4'    | 2.09        | 0.52     |
| 23:BB:925:A:O2'   | 23:BB:926:G:H5'   | 2.09        | 0.52     |
| 23:DB:2100:G:H3'  | 23:DB:2101:A:H8   | 1.75        | 0.52     |
| 1:CA:363:A:P      | 11:CL:57:THR:HG21 | 2.50        | 0.52     |
| 50:BT:67:VAL:HG23 | 50:BT:75:GLY:O    | 2.10        | 0.52     |
| 23:BB:1767:G:O2'  | 23:BB:1768:C:H5'  | 2.09        | 0.52     |
| 1:AA:614:C:O2'    | 1:AA:615:G:H5'    | 2.10        | 0.52     |
| 49:BR:14:VAL:HG21 | 49:BR:98:ILE:HG12 | 1.92        | 0.52     |
| 45:DS:72:THR:CG2  | 45:DS:108:SER:HB3 | 2.40        | 0.52     |
| 14:CO:35:GLN:O    | 14:CO:39:LEU:HD13 | 2.09        | 0.52     |
| 24:DI:2:LYS:C     | 24:DI:3:LYS:HD2   | 2.31        | 0.51     |
| 23:DB:1098:A:C4   | 24:DI:3:LYS:O     | 2.63        | 0.51     |
| 26:BD:104:VAL:HA  | 26:BD:106:LYS:HZ3 | 1.75        | 0.51     |
| 44:DQ:91:ARG:HB2  | 44:DQ:94:LEU:HD23 | 1.92        | 0.51     |
| 8:AI:66:VAL:HG11  | 8:AI:78:ILE:HD11  | 1.93        | 0.51     |
| 26:DD:106:LYS:HB3 | 26:DD:206:ALA:CB  | 2.39        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:DD:32:ASN:HA   | 26:DD:51:THR:O    | 2.09        | 0.51     |
| 47:DF:43:ILE:HG13 | 47:DF:44:ALA:N    | 2.26        | 0.51     |
| 47:DF:46:LYS:O    | 47:DF:49:LEU:HB3  | 2.09        | 0.51     |
| 23:DB:1652:A:OP1  | 42:DN:8:ARG:HD3   | 2.10        | 0.51     |
| 41:BJ:44:TYR:O    | 41:BJ:45:THR:HB   | 2.10        | 0.51     |
| 48:BG:34:ARG:NH1  | 48:BG:34:ARG:HG2  | 2.24        | 0.51     |
| 3:CD:29:THR:HG22  | 3:CD:30:LYS:N     | 2.24        | 0.51     |
| 3:AD:29:THR:HG22  | 3:AD:30:LYS:N     | 2.25        | 0.51     |
| 24:DI:79:LEU:HD12 | 24:DI:135:MET:SD  | 2.50        | 0.51     |
| 45:BS:13:SER:OG   | 45:BS:16:LYS:HB2  | 2.11        | 0.51     |
| 23:DB:589:U:H2'   | 23:DB:590:A:C8    | 2.45        | 0.51     |
| 42:DN:34:ILE:O    | 42:DN:112:TYR:HA  | 2.09        | 0.51     |
| 29:DE:69:ARG:O    | 29:DE:70:SER:CB   | 2.56        | 0.51     |
| 1:AA:1239:A:H4'   | 1:AA:1240:U:H5'   | 1.92        | 0.51     |
| 23:BB:125:A:H3'   | 23:BB:126:A:H5'   | 1.91        | 0.51     |
| 1:CA:1239:A:H4'   | 1:CA:1240:U:H5'   | 1.92        | 0.51     |
| 23:DB:360:U:H2'   | 23:DB:361:G:C8    | 2.45        | 0.51     |
| 23:BB:2590:A:H2'  | 23:BB:2591:C:H6   | 1.76        | 0.51     |
| 23:DB:1150:C:O2'  | 23:DB:1151:A:H5'  | 2.10        | 0.51     |
| 49:BR:68:ARG:NH2  | 49:BR:90:ARG:HB2  | 2.25        | 0.51     |
| 23:DB:1724:G:H2'  | 23:DB:1725:U:C6   | 2.46        | 0.51     |
| 22:BA:13:G:H1'    | 22:BA:69:G:N2     | 2.25        | 0.51     |
| 1:CA:737:C:H2'    | 1:CA:738:C:C6     | 2.44        | 0.51     |
| 20:AB:68:PHE:HA   | 20:AB:161:PHE:O   | 2.10        | 0.51     |
| 1:AA:1523:G:O2'   | 1:AA:1524:C:H5'   | 2.10        | 0.51     |
| 19:CT:78:LEU:O    | 19:CT:82:ILE:HG23 | 2.09        | 0.51     |
| 9:CJ:10:LEU:HD11  | 9:CJ:25:ILE:HD12  | 1.90        | 0.51     |
| 2:CC:78:LYS:HG3   | 2:CC:81:GLU:HB2   | 1.92        | 0.51     |
| 11:CL:107:LYS:H   | 11:CL:107:LYS:HZ2 | 1.57        | 0.51     |
| 20:CB:25:LYS:HD3  | 20:CB:193:ASP:OD1 | 2.10        | 0.51     |
| 23:DB:877:A:O2'   | 23:DB:878:A:H5'   | 2.10        | 0.51     |
| 23:BB:955:U:OP1   | 38:BM:86:LYS:HE3  | 2.10        | 0.51     |
| 2:AC:131:ARG:HG2  | 2:AC:131:ARG:NH1  | 2.25        | 0.51     |
| 23:DB:2253:G:H22  | 53:D6:152:ASP:CG  | 2.13        | 0.51     |
| 23:DB:2604:U:O2'  | 23:DB:2605:U:H5'  | 2.11        | 0.51     |
| 23:DB:864:G:O2'   | 23:DB:865:C:H5'   | 2.11        | 0.51     |
| 23:DB:2728:U:H2'  | 23:DB:2729:G:H8   | 1.75        | 0.51     |
| 1:CA:852:G:H2'    | 1:CA:853:C:H6     | 1.73        | 0.51     |
| 26:DD:40:LEU:HD12 | 26:DD:41:ALA:N    | 2.24        | 0.51     |
| 23:BB:1526:C:O2'  | 23:BB:1527:G:H5'  | 2.10        | 0.51     |
| 48:DG:173:ALA:HB3 | 48:DG:175:LYS:NZ  | 2.25        | 0.51     |
| 10:AK:35:ASP:OD1  | 10:AK:37:GLN:HB2  | 2.09        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:925:A:O2'   | 23:DB:926:G:H5'    | 2.10        | 0.51     |
| 23:DB:1332:G:N3   | 23:DB:1332:G:H2'   | 2.24        | 0.51     |
| 23:BB:464:U:H2'   | 23:BB:465:G:O4'    | 2.10        | 0.51     |
| 1:CA:558:G:C8     | 1:CA:559:A:H2'     | 2.46        | 0.51     |
| 18:AS:79:TYR:CE1  | 18:AS:80:ARG:HG3   | 2.45        | 0.51     |
| 1:AA:1243:C:H2'   | 1:AA:1244:G:H8     | 1.75        | 0.51     |
| 21:CU:46:ARG:O    | 21:CU:49:ALA:HB3   | 2.10        | 0.51     |
| 20:AB:69:VAL:O    | 20:AB:163:ILE:HG22 | 2.10        | 0.51     |
| 23:DB:2365:G:H4'  | 52:DW:59:PHE:CE1   | 2.45        | 0.51     |
| 40:BH:78:VAL:HG21 | 40:BH:142:VAL:CG1  | 2.36        | 0.51     |
| 26:DD:4:LEU:HD12  | 26:DD:32:ASN:HB2   | 1.92        | 0.51     |
| 35:BV:63:ILE:HD12 | 35:BV:63:ILE:N     | 2.23        | 0.51     |
| 23:DB:2359:C:O2'  | 23:DB:2360:G:H5'   | 2.10        | 0.51     |
| 1:CA:1014:A:C2    | 1:CA:1219:A:H1'    | 2.46        | 0.51     |
| 46:DU:82:VAL:HG13 | 46:DU:93:ARG:HB3   | 1.91        | 0.51     |
| 47:BF:46:LYS:O    | 47:BF:49:LEU:HB3   | 2.10        | 0.51     |
| 47:BF:174:PHE:HB3 | 47:BF:176:PHE:CD1  | 2.45        | 0.51     |
| 3:AD:173:ASP:CB   | 3:AD:178:GLU:HB2   | 2.36        | 0.51     |
| 29:BE:29:HIS:CD2  | 37:BL:8:PRO:HA     | 2.44        | 0.51     |
| 23:DB:1287:A:H3'  | 23:DB:1288:G:H21   | 1.74        | 0.51     |
| 23:BB:2734:A:N6   | 23:BB:2770:G:H1'   | 2.24        | 0.51     |
| 45:BS:36:LEU:H    | 45:BS:36:LEU:CD2   | 2.22        | 0.51     |
| 42:BN:28:LEU:HD23 | 42:BN:113:ILE:HG23 | 1.92        | 0.51     |
| 23:BB:2895:G:H2'  | 23:BB:2896:C:H6    | 1.75        | 0.51     |
| 20:AB:95:TRP:CH2  | 20:AB:100:LEU:HB2  | 2.42        | 0.51     |
| 38:DM:31:PHE:HB3  | 38:DM:130:PHE:CZ   | 2.46        | 0.51     |
| 37:BL:95:LEU:HA   | 37:BL:98:ALA:HB3   | 1.90        | 0.51     |
| 23:DB:560:C:H2'   | 23:DB:561:G:O4'    | 2.10        | 0.51     |
| 23:DB:1007:C:O3'  | 41:DJ:110:PRO:HB3  | 2.09        | 0.51     |
| 26:BD:168:GLU:O   | 26:BD:170:VAL:HG22 | 2.09        | 0.51     |
| 23:DB:99:U:O2     | 23:DB:99:U:H5'     | 2.09        | 0.51     |
| 8:CI:123:ARG:HB3  | 8:CI:123:ARG:CZ    | 2.39        | 0.51     |
| 27:BK:88:ASN:C    | 27:BK:88:ASN:ND2   | 2.61        | 0.51     |
| 1:CA:237:G:H2'    | 1:CA:238:A:C8      | 2.45        | 0.51     |
| 1:CA:337:G:H2'    | 1:CA:338:A:H8      | 1.71        | 0.51     |
| 23:BB:642:U:O2    | 23:BB:644:A:H3'    | 2.09        | 0.51     |
| 23:BB:1809:A:H2'  | 23:BB:1810:A:C8    | 2.45        | 0.51     |
| 23:BB:946:C:H2'   | 23:BB:947:A:C8     | 2.45        | 0.51     |
| 23:BB:1826:G:H2'  | 23:BB:1827:U:C6    | 2.45        | 0.51     |
| 23:BB:1827:U:C2'  | 23:BB:1828:G:H5'   | 2.41        | 0.51     |
| 23:DB:1485:U:H2'  | 23:DB:1486:U:H6    | 1.74        | 0.51     |
| 1:CA:833:G:H2'    | 1:CA:834:U:C6      | 2.45        | 0.51     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:1998:A:H2'   | 23:BB:1999:C:H6    | 1.75        | 0.51     |
| 1:CA:1086:U:H2'    | 1:CA:1087:G:H8     | 1.74        | 0.51     |
| 1:AA:67:C:H4'      | 1:AA:172:A:C4'     | 2.40        | 0.51     |
| 2:AC:46:LEU:HB3    | 2:AC:49:ALA:CB     | 2.39        | 0.51     |
| 1:CA:1471:U:O2'    | 1:CA:1472:U:H5'    | 2.10        | 0.51     |
| 1:AA:369:G:O2'     | 1:AA:370:C:H5'     | 2.10        | 0.51     |
| 26:DD:133:THR:HG23 | 26:DD:134:HIS:CD2  | 2.45        | 0.51     |
| 23:BB:2339:C:H2'   | 23:BB:2340:A:C8    | 2.46        | 0.51     |
| 16:AQ:30:HIS:CG    | 16:AQ:33:TYR:HB2   | 2.45        | 0.51     |
| 33:D1:18:HIS:CD2   | 33:D1:40:PRO:HD2   | 2.45        | 0.51     |
| 37:BL:136:GLU:HA   | 37:BL:140:GLY:H    | 1.74        | 0.51     |
| 23:DB:2260:C:O2'   | 23:DB:2261:C:H5'   | 2.09        | 0.51     |
| 22:DA:49:C:H2'     | 22:DA:50:A:C8      | 2.46        | 0.51     |
| 43:DO:68:LYS:HA    | 43:DO:102:ARG:HG2  | 1.90        | 0.51     |
| 23:DB:127:A:C8     | 36:D2:46:LYS:HE2   | 2.46        | 0.51     |
| 23:DB:2889:C:O2'   | 23:DB:2890:G:H5'   | 2.10        | 0.51     |
| 1:CA:546:A:P       | 3:CD:68:GLU:HB3    | 2.51        | 0.51     |
| 23:DB:1234:U:H2'   | 23:DB:1235:G:O4'   | 2.11        | 0.51     |
| 23:BB:1577:C:H2'   | 23:BB:1578:U:O4'   | 2.10        | 0.51     |
| 1:AA:1105:A:H2'    | 1:AA:1106:G:H8     | 1.75        | 0.51     |
| 23:BB:189:G:H2'    | 23:BB:205:G:H22    | 1.75        | 0.51     |
| 1:CA:724:G:O2'     | 1:CA:725:G:H5'     | 2.10        | 0.51     |
| 23:DB:1425:G:H2'   | 23:DB:1426:G:C8    | 2.45        | 0.51     |
| 1:CA:106:C:H2'     | 1:CA:107:G:H8      | 1.74        | 0.51     |
| 42:BN:2:ARG:HA     | 42:BN:5:LYS:HD3    | 1.92        | 0.51     |
| 1:CA:1310:G:O2'    | 1:CA:1311:A:H5'    | 2.10        | 0.51     |
| 23:BB:2329:U:H2'   | 23:BB:2330:G:C8    | 2.46        | 0.51     |
| 52:DW:36:ILE:HB    | 52:DW:39:GLN:NE2   | 2.24        | 0.51     |
| 52:DW:43:LYS:HB3   | 52:DW:58:LEU:CD1   | 2.40        | 0.51     |
| 10:AK:70:ALA:C     | 10:AK:72:ALA:H     | 2.13        | 0.51     |
| 23:DB:945:A:H3'    | 23:DB:946:C:H5''   | 1.91        | 0.51     |
| 47:BF:32:LYS:HA    | 47:BF:95:MET:SD    | 2.50        | 0.51     |
| 48:DG:85:LYS:HA    | 48:DG:131:VAL:HG12 | 1.92        | 0.51     |
| 16:CQ:59:GLU:O     | 16:CQ:74:LEU:HD22  | 2.10        | 0.51     |
| 16:CQ:60:ILE:HD13  | 16:CQ:60:ILE:H     | 1.76        | 0.51     |
| 40:BH:78:VAL:H     | 40:BH:143:ILE:HD11 | 1.75        | 0.51     |
| 8:CI:113:LYS:HA    | 8:CI:120:ALA:HB2   | 1.92        | 0.51     |
| 23:DB:2358:A:H2'   | 23:DB:2359:C:C6    | 2.46        | 0.51     |
| 44:BQ:57:ARG:HA    | 44:BQ:60:TRP:CE3   | 2.45        | 0.51     |
| 22:BA:28:C:N4      | 22:BA:56:G:H1      | 2.05        | 0.51     |
| 12:CM:10:ASP:O     | 12:CM:11:HIS:HB2   | 2.10        | 0.51     |
| 47:BF:7:TYR:OH     | 47:BF:29:ARG:HG3   | 2.10        | 0.51     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 40:DH:126:GLY:N    | 40:DH:146:VAL:HB  | 2.26        | 0.51     |
| 21:AU:19:LYS:HD3   | 21:AU:20:ARG:HH21 | 1.75        | 0.51     |
| 18:CS:69:LYS:O     | 18:CS:72:GLU:HG2  | 2.11        | 0.51     |
| 11:AL:86:VAL:HG11  | 11:AL:89:LEU:HD23 | 1.92        | 0.51     |
| 50:DT:43:ILE:O     | 50:DT:46:ALA:HB3  | 2.11        | 0.51     |
| 25:DC:204:LEU:HD23 | 25:DC:209:ALA:CB  | 2.40        | 0.51     |
| 23:BB:1180:U:O2'   | 23:BB:1181:U:H5'  | 2.10        | 0.51     |
| 20:AB:65:LYS:HA    | 20:AB:89:PHE:HE1  | 1.76        | 0.51     |
| 20:CB:27:LYS:HB3   | 20:CB:28:PRO:HD3  | 1.91        | 0.51     |
| 3:AD:154:VAL:O     | 3:AD:158:LEU:HD12 | 2.10        | 0.51     |
| 23:BB:363:G:H2'    | 23:BB:364:C:C6    | 2.46        | 0.51     |
| 40:DH:73:ASN:CG    | 40:DH:140:ALA:HB1 | 2.31        | 0.51     |
| 10:AK:23:HIS:O     | 10:AK:29:THR:HA   | 2.10        | 0.51     |
| 1:AA:320:A:H2'     | 1:AA:321:A:H8     | 1.74        | 0.51     |
| 7:CH:49:LYS:O      | 7:CH:59:GLU:N     | 2.43        | 0.51     |
| 11:CL:52:CYS:SG    | 11:CL:66:ILE:HD11 | 2.50        | 0.51     |
| 22:BA:101:A:H2'    | 22:BA:102:G:O4'   | 2.11        | 0.51     |
| 23:BB:2773:C:H5''  | 26:BD:169:ARG:HB2 | 1.91        | 0.51     |
| 14:AO:85:LEU:N     | 14:AO:85:LEU:HD12 | 2.24        | 0.51     |
| 24:DI:85:ILE:HD12  | 24:DI:87:SER:O    | 2.10        | 0.51     |
| 2:AC:139:ASN:O     | 2:AC:143:LEU:HD23 | 2.11        | 0.51     |
| 1:AA:1048:G:H4'    | 13:AN:2:LYS:HZ1   | 1.73        | 0.51     |
| 35:DV:29:ILE:HG13  | 35:DV:88:HIS:CE1  | 2.41        | 0.51     |
| 1:AA:239:U:C5'     | 1:AA:239:U:H6     | 2.24        | 0.51     |
| 29:DE:173:THR:C    | 29:DE:175:ILE:H   | 2.13        | 0.51     |
| 45:BS:42:LYS:O     | 45:BS:45:VAL:HG22 | 2.10        | 0.51     |
| 1:CA:1461:G:O2'    | 1:CA:1462:C:H5'   | 2.11        | 0.51     |
| 23:DB:1177:G:H2'   | 23:DB:1178:C:C6   | 2.45        | 0.51     |
| 50:DT:54:GLU:HG3   | 50:DT:89:GLU:H    | 1.75        | 0.51     |
| 46:BU:32:LYS:HA    | 46:BU:65:GLN:HA   | 1.92        | 0.51     |
| 1:AA:1007:U:H2'    | 1:AA:1008:U:H6    | 1.74        | 0.51     |
| 11:CL:109:ARG:HH21 | 11:CL:112:ALA:HB3 | 1.75        | 0.51     |
| 17:CR:19:GLU:HG3   | 17:CR:54:LEU:HD12 | 1.92        | 0.51     |
| 23:BB:909:A:H2'    | 23:BB:912:C:C5    | 2.45        | 0.51     |
| 23:BB:1319:C:O2'   | 23:BB:1320:C:H5'  | 2.09        | 0.51     |
| 23:DB:755:U:H2'    | 23:DB:756:A:C8    | 2.46        | 0.51     |
| 23:DB:2356:U:C5'   | 52:DW:16:GLU:HG3  | 2.40        | 0.51     |
| 50:BT:62:VAL:HG12  | 50:BT:63:VAL:N    | 2.26        | 0.51     |
| 1:CA:83:C:H1'      | 1:CA:84:U:C6      | 2.45        | 0.51     |
| 5:AF:15:SER:HA     | 5:AF:18:VAL:HG23  | 1.91        | 0.51     |
| 5:CF:7:VAL:HG11    | 17:CR:64:LEU:HD21 | 1.92        | 0.51     |
| 1:AA:560:A:H5'     | 1:AA:566:G:N2     | 2.25        | 0.51     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:878:A:H5''    | 7:AH:80:PRO:HG2    | 1.91        | 0.51     |
| 1:AA:31:G:N7       | 1:AA:306:A:H1'     | 2.26        | 0.51     |
| 1:CA:49:U:O2'      | 1:CA:50:A:H2'      | 2.10        | 0.51     |
| 23:BB:477:A:H2'    | 23:BB:478:A:C8     | 2.45        | 0.51     |
| 23:DB:1083:U:H2'   | 23:DB:1085:A:OP2   | 2.10        | 0.51     |
| 1:CA:930:C:H2'     | 1:CA:931:C:H6      | 1.76        | 0.51     |
| 1:CA:190:A:O5'     | 1:CA:190:A:H8      | 1.93        | 0.51     |
| 1:CA:131:A:H2'     | 1:CA:132:C:C6      | 2.45        | 0.51     |
| 1:CA:882:C:O2'     | 1:CA:883:C:H5'     | 2.10        | 0.51     |
| 24:DI:1:ALA:CB     | 24:DI:2:LYS:HD2    | 2.40        | 0.51     |
| 25:DC:91:ALA:HB3   | 25:DC:105:ALA:HB2  | 1.92        | 0.51     |
| 47:DF:177:ARG:HA   | 47:DF:177:ARG:NE   | 2.26        | 0.51     |
| 20:CB:14:HIS:CD2   | 20:CB:202:ASN:H    | 2.29        | 0.51     |
| 13:AN:9:GLU:OE2    | 13:AN:60:ARG:HG2   | 2.10        | 0.51     |
| 23:DB:672:C:O2'    | 23:DB:673:C:H5'    | 2.11        | 0.51     |
| 30:DY:40:THR:HB    | 30:DY:43:ILE:HG22  | 1.92        | 0.51     |
| 23:DB:2674:G:H4'   | 27:DK:30:ARG:HG3   | 1.91        | 0.51     |
| 1:CA:1219:A:H2'    | 1:CA:1220:G:H8     | 1.75        | 0.51     |
| 44:BQ:96:ASP:C     | 44:BQ:98:ALA:N     | 2.64        | 0.51     |
| 3:CD:164:ARG:HG2   | 3:CD:164:ARG:HH11  | 1.75        | 0.51     |
| 29:BE:158:PHE:HA   | 29:BE:169:VAL:CG2  | 2.41        | 0.51     |
| 47:DF:131:VAL:HG22 | 47:DF:151:LEU:O    | 2.10        | 0.51     |
| 18:AS:28:LYS:HB2   | 18:AS:29:PRO:HD2   | 1.93        | 0.51     |
| 10:AK:22:ILE:HD13  | 10:AK:95:THR:HG21  | 1.91        | 0.51     |
| 23:DB:165:A:H2'    | 23:DB:166:U:H6     | 1.76        | 0.51     |
| 23:DB:587:C:N3     | 37:DL:33:ARG:NH2   | 2.58        | 0.51     |
| 8:AI:36:GLN:N      | 8:AI:36:GLN:HE21   | 2.09        | 0.51     |
| 29:BE:149:ILE:HG23 | 29:BE:188:MET:CA   | 2.40        | 0.51     |
| 1:CA:719:C:H1'     | 17:CR:37:LYS:HB2   | 1.92        | 0.51     |
| 26:DD:168:GLU:O    | 26:DD:170:VAL:HG13 | 2.09        | 0.51     |
| 23:BB:873:C:H2'    | 23:BB:874:G:C8     | 2.44        | 0.51     |
| 24:BI:17:ALA:O     | 24:BI:18:ASN:CB    | 2.59        | 0.51     |
| 38:DM:19:GLY:N     | 38:DM:38:ARG:NH2   | 2.58        | 0.51     |
| 23:DB:969:G:H2'    | 23:DB:970:U:C6     | 2.45        | 0.51     |
| 26:BD:148:GLN:HG3  | 26:BD:152:PRO:CG   | 2.41        | 0.51     |
| 20:CB:70:GLY:HA3   | 20:CB:79:VAL:HG21  | 1.92        | 0.51     |
| 45:BS:81:SER:HB3   | 45:BS:99:ARG:HB3   | 1.93        | 0.51     |
| 43:DO:2:ASP:OD2    | 43:DO:4:LYS:HB3    | 2.10        | 0.51     |
| 1:CA:552:U:H2'     | 1:CA:553:A:C8      | 2.46        | 0.51     |
| 11:AL:79:ILE:HD12  | 11:AL:96:THR:HG22  | 1.93        | 0.51     |
| 23:BB:152:A:H2'    | 23:BB:153:U:H6     | 1.71        | 0.51     |
| 28:BP:52:ARG:HG2   | 28:BP:52:ARG:NH1   | 2.25        | 0.51     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2135:A:O2'   | 23:DB:2136:G:H5'   | 2.11        | 0.51     |
| 23:BB:2457:U:O2'   | 23:BB:2458:G:H5'   | 2.10        | 0.51     |
| 23:DB:2776:A:H4'   | 23:DB:2777:G:C5'   | 2.40        | 0.51     |
| 1:AA:1179:A:H2'    | 1:AA:1180:A:O4'    | 2.11        | 0.51     |
| 23:BB:1063:G:H4'   | 24:BI:135:MET:CB   | 2.40        | 0.51     |
| 1:AA:539:A:H2'     | 1:AA:540:G:H8      | 1.75        | 0.51     |
| 51:DZ:63:GLY:O     | 51:DZ:67:VAL:HG23  | 2.09        | 0.51     |
| 37:DL:23:ILE:HD12  | 37:DL:23:ILE:N     | 2.25        | 0.51     |
| 23:DB:1220:G:H2'   | 23:DB:1221:C:C6    | 2.46        | 0.51     |
| 26:DD:121:THR:C    | 26:DD:123:LYS:H    | 2.14        | 0.51     |
| 25:DC:42:ARG:HD2   | 25:DC:48:ILE:HG12  | 1.91        | 0.51     |
| 1:CA:1283:U:O2'    | 1:CA:1284:C:H5'    | 2.11        | 0.51     |
| 23:BB:82:U:H2'     | 23:BB:83:A:O4'     | 2.10        | 0.51     |
| 23:DB:2226:C:H2'   | 23:DB:2227:A:C8    | 2.46        | 0.51     |
| 1:CA:614:C:O2'     | 1:CA:615:G:H5'     | 2.10        | 0.51     |
| 1:AA:852:G:H2'     | 1:AA:853:C:C6      | 2.46        | 0.51     |
| 1:CA:645:G:O2'     | 1:CA:646:G:H5'     | 2.11        | 0.51     |
| 10:AK:63:GLN:HG3   | 10:AK:98:ALA:HB2   | 1.93        | 0.51     |
| 23:BB:1833:C:O2'   | 23:BB:1834:U:H5'   | 2.10        | 0.51     |
| 40:DH:1:MET:HB3    | 40:DH:21:VAL:O     | 2.10        | 0.51     |
| 43:DO:81:ARG:HD3   | 43:DO:81:ARG:H     | 1.75        | 0.51     |
| 23:DB:2329:U:H2'   | 23:DB:2330:G:C8    | 2.46        | 0.51     |
| 48:BG:106:LEU:O    | 48:BG:108:PHE:HD1  | 1.94        | 0.51     |
| 47:BF:33:ILE:O     | 47:BF:90:LEU:N     | 2.43        | 0.51     |
| 37:DL:124:GLY:N    | 37:DL:143:GLU:CG   | 2.72        | 0.51     |
| 26:BD:107:VAL:HG12 | 26:BD:109:VAL:HG23 | 1.91        | 0.51     |
| 8:CI:19:PHE:HB2    | 8:CI:63:TYR:HB3    | 1.91        | 0.51     |
| 41:BJ:59:ALA:C     | 41:BJ:61:LYS:H     | 2.13        | 0.51     |
| 44:DQ:93:ILE:O     | 44:DQ:96:ASP:HB3   | 2.10        | 0.51     |
| 1:AA:1013:G:H2'    | 1:AA:1015:G:OP2    | 2.11        | 0.51     |
| 41:DJ:18:VAL:CG1   | 41:DJ:54:ILE:HD11  | 2.40        | 0.51     |
| 1:CA:1220:G:H21    | 18:CS:53:GLY:HA2   | 1.75        | 0.51     |
| 48:BG:25:ILE:O     | 48:BG:32:LEU:HA    | 2.10        | 0.51     |
| 51:BZ:38:PHE:CE2   | 51:BZ:51:VAL:HG21  | 2.44        | 0.51     |
| 51:BZ:45:ARG:HE    | 51:BZ:47:VAL:CG1   | 2.23        | 0.51     |
| 47:BF:133:GLU:HA   | 47:BF:150:GLY:CA   | 2.40        | 0.51     |
| 40:DH:125:THR:HG22 | 40:DH:146:VAL:HG12 | 1.92        | 0.51     |
| 4:CE:17:VAL:HG23   | 4:CE:33:THR:O      | 2.11        | 0.51     |
| 46:DU:27:VAL:CG2   | 46:DU:33:VAL:HG12  | 2.36        | 0.51     |
| 27:BK:7:MET:SD     | 27:BK:20:MET:HB2   | 2.51        | 0.51     |
| 20:AB:15:PHE:HD1   | 20:AB:16:GLY:N     | 2.08        | 0.51     |
| 1:AA:312:C:H2'     | 1:AA:313:A:H8      | 1.76        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 40:BH:73:ASN:ND2  | 40:BH:74:ALA:N    | 2.58        | 0.51     |
| 20:CB:64:GLY:O    | 20:CB:66:ILE:HG12 | 2.09        | 0.51     |
| 23:BB:1551:A:H2'  | 23:BB:1552:A:O4'  | 2.11        | 0.51     |
| 2:CC:183:TYR:HE1  | 2:CC:198:LYS:HB3  | 1.75        | 0.51     |
| 1:CA:1102:A:H2'   | 1:CA:1103:C:C6    | 2.46        | 0.51     |
| 5:AF:6:ILE:HD11   | 5:AF:8:PHE:CD2    | 2.45        | 0.51     |
| 14:CO:85:LEU:N    | 14:CO:85:LEU:HD12 | 2.25        | 0.51     |
| 1:CA:1048:G:H5''  | 13:CN:2:LYS:HD2   | 1.93        | 0.51     |
| 16:CQ:16:MET:HB3  | 16:CQ:19:SER:HB2  | 1.91        | 0.51     |
| 4:CE:84:VAL:HG11  | 4:CE:146:MET:HB3  | 1.93        | 0.51     |
| 49:BR:31:GLU:O    | 49:BR:63:VAL:HG22 | 2.11        | 0.51     |
| 1:CA:1161:C:O2'   | 1:CA:1162:C:H5'   | 2.11        | 0.51     |
| 3:CD:96:ARG:O     | 3:CD:100:VAL:HG23 | 2.10        | 0.51     |
| 39:DX:18:LEU:HD12 | 39:DX:22:LEU:HD22 | 1.92        | 0.51     |
| 23:DB:150:U:H2'   | 23:DB:151:C:C6    | 2.45        | 0.51     |
| 25:DC:86:ARG:HB3  | 25:DC:86:ARG:CZ   | 2.41        | 0.51     |
| 23:BB:2846:G:H2'  | 23:BB:2847:U:C6   | 2.46        | 0.51     |
| 39:BX:56:LEU:O    | 39:BX:57:LEU:HB3  | 2.11        | 0.51     |
| 1:AA:734:G:O2'    | 17:AR:59:LYS:HD3  | 2.11        | 0.51     |
| 6:CG:134:VAL:HB   | 6:CG:137:ARG:NH2  | 2.26        | 0.51     |
| 23:DB:1805:A:N3   | 25:DC:49:THR:CG2  | 2.74        | 0.51     |
| 19:CT:42:ASP:HA   | 19:CT:43:LYS:NZ   | 2.25        | 0.51     |
| 11:CL:106:VAL:CG2 | 11:CL:116:TYR:HB3 | 2.41        | 0.51     |
| 23:DB:2002:G:OP1  | 42:DN:13:ASN:HA   | 2.10        | 0.51     |
| 27:BK:2:ILE:HG23  | 27:BK:33:ALA:O    | 2.11        | 0.51     |
| 23:DB:2217:G:O2'  | 23:DB:2218:G:H5'  | 2.11        | 0.51     |
| 23:BB:1405:U:H2'  | 23:BB:1406:U:C6   | 2.46        | 0.51     |
| 22:BA:50:A:OP1    | 43:BO:68:LYS:HB2  | 2.11        | 0.51     |
| 53:D6:14:MET:CE   | 53:D6:165:THR:HA  | 2.40        | 0.51     |
| 23:BB:2671:G:H2'  | 23:BB:2672:U:H6   | 1.75        | 0.51     |
| 23:BB:1513:U:H2'  | 23:BB:1514:G:C8   | 2.45        | 0.51     |
| 23:BB:1349:C:H2'  | 23:BB:1350:C:H6   | 1.75        | 0.51     |
| 23:DB:528:A:C2    | 23:DB:2042:A:H2'  | 2.45        | 0.51     |
| 31:B0:25:THR:O    | 31:B0:26:SER:HB3  | 2.09        | 0.51     |
| 22:BA:87:U:H2'    | 22:BA:88:C:H5''   | 1.93        | 0.51     |
| 23:DB:1045:C:H4'  | 23:DB:1046:A:H5'' | 1.91        | 0.51     |
| 23:DB:2835:A:H61  | 23:DB:2878:U:H2'  | 1.74        | 0.51     |
| 1:CA:448:A:H2'    | 1:CA:449:G:C8     | 2.46        | 0.51     |
| 25:DC:259:ASN:C   | 25:DC:261:ARG:H   | 2.13        | 0.51     |
| 23:BB:1714:U:H3'  | 23:BB:1715:G:C5'  | 2.39        | 0.51     |
| 23:DB:2600:A:O2'  | 23:DB:2601:C:H5'  | 2.10        | 0.51     |
| 1:CA:1244:G:H2'   | 1:CA:1245:C:C6    | 2.46        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 14:CO:50:HIS:O    | 14:CO:53:ARG:HB3   | 2.10        | 0.51     |
| 23:DB:1965:C:H5'  | 23:DB:1966:A:H2'   | 1.93        | 0.51     |
| 16:CQ:28:VAL:HG12 | 16:CQ:37:ILE:O     | 2.11        | 0.51     |
| 23:DB:1050:A:H2'  | 23:DB:1051:G:O4'   | 2.11        | 0.51     |
| 1:CA:31:G:N7      | 1:CA:306:A:H1'     | 2.26        | 0.51     |
| 23:DB:1009:A:P    | 41:DJ:39:LYS:HZ2   | 2.33        | 0.51     |
| 1:AA:790:A:H2'    | 1:AA:791:G:C8      | 2.46        | 0.51     |
| 23:BB:1495:A:H2'  | 23:BB:1496:A:C8    | 2.46        | 0.51     |
| 23:BB:1499:C:H2'  | 23:BB:1500:G:H8    | 1.75        | 0.51     |
| 37:DL:41:ARG:HG2  | 37:DL:41:ARG:HH21  | 1.75        | 0.51     |
| 17:AR:21:ASP:OD1  | 17:AR:23:LYS:HD2   | 2.10        | 0.51     |
| 9:AJ:10:LEU:HD11  | 9:AJ:25:ILE:HD12   | 1.92        | 0.51     |
| 23:DB:103:A:H3'   | 23:DB:104:A:H8     | 1.75        | 0.51     |
| 52:BW:66:VAL:HA   | 52:BW:81:ILE:HG22  | 1.93        | 0.51     |
| 23:DB:2331:G:O2'  | 23:DB:2332:C:H5'   | 2.11        | 0.51     |
| 23:DB:2366:A:H2'  | 23:DB:2367:G:O4'   | 2.10        | 0.51     |
| 23:DB:852:U:H2'   | 23:DB:853:C:C6     | 2.45        | 0.51     |
| 52:DW:49:ASN:HB2  | 52:DW:61:LYS:N     | 2.24        | 0.51     |
| 22:BA:83:G:OP1    | 30:BY:16:LEU:HD21  | 2.11        | 0.51     |
| 24:DI:116:MET:HE1 | 24:DI:128:ILE:HG13 | 1.93        | 0.51     |
| 23:BB:626:A:H2'   | 37:BL:78:ARG:NH1   | 2.26        | 0.51     |
| 47:DF:110:ILE:CG2 | 47:DF:113:PHE:HB3  | 2.40        | 0.51     |
| 43:DO:26:LEU:HD13 | 43:DO:39:VAL:HG23  | 1.92        | 0.51     |
| 23:BB:587:C:N3    | 37:BL:33:ARG:NH2   | 2.59        | 0.51     |
| 11:CL:49:ARG:N    | 11:CL:49:ARG:HD2   | 2.26        | 0.51     |
| 23:DB:873:C:H4'   | 38:DM:64:TRP:NE1   | 2.24        | 0.51     |
| 23:BB:2038:G:H2'  | 23:BB:2039:U:C6    | 2.46        | 0.51     |
| 31:B0:32:THR:OG1  | 31:B0:50:GLY:HA2   | 2.11        | 0.51     |
| 2:AC:149:LYS:HB2  | 2:AC:168:ARG:HG3   | 1.93        | 0.51     |
| 23:BB:45:G:H5'    | 23:BB:46:G:OP1     | 2.10        | 0.51     |
| 27:BK:42:THR:O    | 27:BK:44:LYS:HG2   | 2.11        | 0.51     |
| 28:DP:4:ILE:O     | 28:DP:6:GLN:N      | 2.42        | 0.51     |
| 34:D3:15:LYS:HA   | 34:D3:21:PHE:HA    | 1.91        | 0.51     |
| 4:AE:80:LEU:HA    | 4:AE:146:MET:HE1   | 1.90        | 0.51     |
| 23:DB:191:A:H2'   | 23:DB:192:C:H6     | 1.73        | 0.51     |
| 41:DJ:114:LEU:O   | 41:DJ:117:ALA:HB3  | 2.11        | 0.51     |
| 23:BB:1779:U:C5   | 23:BB:1784:A:N7    | 2.78        | 0.51     |
| 41:BJ:93:ILE:O    | 41:BJ:97:PRO:HG3   | 2.10        | 0.51     |
| 23:BB:132:G:H2'   | 23:BB:133:U:C6     | 2.46        | 0.51     |
| 29:BE:46:GLN:HB3  | 29:BE:86:ALA:HA    | 1.92        | 0.51     |
| 6:CG:41:ILE:HG21  | 6:CG:115:MET:CG    | 2.41        | 0.51     |
| 39:BX:18:LEU:HD12 | 39:BX:22:LEU:HD22  | 1.93        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 33:D1:3:GLY:C     | 33:D1:5:ARG:H      | 2.13        | 0.51     |
| 20:AB:87:ASP:HB2  | 20:AB:224:ARG:CZ   | 2.40        | 0.51     |
| 23:DB:1351:C:H2'  | 23:DB:1352:U:O4'   | 2.11        | 0.51     |
| 23:DB:1403:A:O2'  | 23:DB:1404:C:H5'   | 2.10        | 0.51     |
| 2:CC:86:LEU:O     | 2:CC:90:VAL:HG23   | 2.11        | 0.51     |
| 20:CB:18:GLN:HB2  | 20:CB:188:THR:OG1  | 2.11        | 0.51     |
| 25:BC:242:HIS:O   | 25:BC:244:VAL:HG13 | 2.10        | 0.51     |
| 3:CD:11:SER:HA    | 3:CD:18:LEU:CD2    | 2.41        | 0.51     |
| 22:DA:6:G:H2'     | 22:DA:7:G:H8       | 1.76        | 0.51     |
| 23:DB:2455:G:O2'  | 23:DB:2456:C:H5'   | 2.11        | 0.51     |
| 23:DB:5:A:H2'     | 23:DB:6:A:H8       | 1.76        | 0.51     |
| 23:DB:753:A:H2'   | 23:DB:754:U:H6     | 1.73        | 0.51     |
| 23:BB:1683:U:H2'  | 23:BB:1684:G:C8    | 2.46        | 0.51     |
| 1:AA:1041:G:O2'   | 1:AA:1042:A:H5'    | 2.11        | 0.51     |
| 29:DE:98:LYS:HG2  | 29:DE:99:LYS:N     | 2.25        | 0.51     |
| 1:CA:358:U:H2'    | 1:CA:359:G:H8      | 1.76        | 0.51     |
| 4:CE:87:VAL:HG22  | 4:CE:88:HIS:N      | 2.25        | 0.51     |
| 5:AF:85:ILE:HG22  | 5:AF:86:ARG:H      | 1.75        | 0.51     |
| 25:BC:259:ASN:C   | 25:BC:261:ARG:H    | 2.14        | 0.51     |
| 53:D6:150:SER:O   | 53:D6:154:THR:HG23 | 2.10        | 0.51     |
| 23:DB:81:G:H2'    | 23:DB:82:U:O4'     | 2.10        | 0.51     |
| 23:BB:1339:G:N2   | 23:BB:1603:A:H1'   | 2.26        | 0.51     |
| 23:BB:2104:C:H2'  | 23:BB:2105:U:H6    | 1.76        | 0.51     |
| 40:BH:62:LEU:N    | 40:BH:62:LEU:HD12  | 2.25        | 0.51     |
| 20:CB:10:LYS:O    | 20:CB:13:VAL:HG23  | 2.10        | 0.51     |
| 23:BB:2594:C:O2'  | 23:BB:2595:G:H5'   | 2.11        | 0.51     |
| 23:DB:538:A:H2'   | 23:DB:539:G:O4'    | 2.11        | 0.51     |
| 2:AC:113:LYS:HE3  | 2:AC:117:ASP:OD1   | 2.11        | 0.51     |
| 26:BD:46:ARG:HH12 | 26:BD:88:GLU:HG3   | 1.75        | 0.51     |
| 1:AA:885:G:O2'    | 1:AA:886:G:H5'     | 2.11        | 0.51     |
| 51:BZ:18:ARG:HA   | 51:BZ:23:ASN:O     | 2.10        | 0.51     |
| 23:DB:2221:G:O2'  | 23:DB:2222:C:H5'   | 2.11        | 0.51     |
| 23:BB:1234:U:O2'  | 23:BB:1235:G:H5'   | 2.11        | 0.51     |
| 23:BB:242:G:H5''  | 34:B3:63:TYR:CE2   | 2.45        | 0.51     |
| 23:BB:217:A:H2'   | 23:BB:218:A:O4'    | 2.11        | 0.51     |
| 23:BB:857:G:H2'   | 23:BB:858:G:H5'    | 1.91        | 0.51     |
| 48:BG:122:ALA:HB2 | 48:BG:132:LEU:HB3  | 1.92        | 0.51     |
| 21:AU:46:ARG:O    | 21:AU:49:ALA:HB3   | 2.10        | 0.51     |
| 48:DG:84:LYS:HB2  | 48:DG:132:LEU:H    | 1.76        | 0.51     |
| 8:AI:64:ILE:HD12  | 8:AI:64:ILE:N      | 2.25        | 0.51     |
| 1:AA:1014:A:C2    | 1:AA:1219:A:H1'    | 2.45        | 0.51     |
| 48:DG:25:ILE:O    | 48:DG:32:LEU:HA    | 2.11        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:673:C:H2'   | 23:DB:674:G:H5'    | 1.91        | 0.51     |
| 1:CA:598:U:H2'    | 1:CA:599:C:C6      | 2.45        | 0.51     |
| 50:BT:54:GLU:HG3  | 50:BT:89:GLU:H     | 1.75        | 0.51     |
| 51:BZ:6:GLN:HE21  | 51:BZ:50:ARG:H     | 1.57        | 0.51     |
| 30:BY:16:LEU:H    | 30:BY:16:LEU:CD2   | 2.13        | 0.51     |
| 33:B1:8:ILE:HD12  | 33:B1:51:ALA:HA    | 1.92        | 0.51     |
| 47:BF:40:GLY:HA2  | 47:BF:84:ILE:CG2   | 2.40        | 0.51     |
| 12:CM:56:ARG:O    | 12:CM:59:VAL:HG12  | 2.11        | 0.51     |
| 47:BF:148:VAL:O   | 47:BF:149:ARG:HG2  | 2.10        | 0.51     |
| 49:DR:20:VAL:HG12 | 49:DR:21:ARG:H     | 1.76        | 0.51     |
| 47:DF:107:VAL:N   | 47:DF:108:PRO:CD   | 2.74        | 0.51     |
| 18:CS:28:LYS:HB2  | 18:CS:29:PRO:HD2   | 1.93        | 0.51     |
| 38:DM:96:ILE:HD11 | 38:DM:126:ILE:HG12 | 1.93        | 0.51     |
| 25:DC:15:VAL:HA   | 25:DC:203:VAL:HG12 | 1.92        | 0.51     |
| 53:D6:15:GLN:HA   | 53:D6:168:PHE:HE2  | 1.75        | 0.51     |
| 16:AQ:74:LEU:HD22 | 16:AQ:75:VAL:N     | 2.26        | 0.51     |
| 45:DS:36:LEU:H    | 45:DS:36:LEU:CD2   | 2.23        | 0.51     |
| 23:DB:160:A:H2'   | 23:DB:161:A:C8     | 2.46        | 0.51     |
| 32:B4:5:ALA:HA    | 32:B4:37:GLN:HE21  | 1.76        | 0.51     |
| 2:AC:140:ALA:HB3  | 2:AC:148:ILE:HD12  | 1.93        | 0.51     |
| 23:DB:2037:A:H2'  | 23:DB:2038:G:H8    | 1.75        | 0.51     |
| 23:BB:1197:G:O2'  | 23:BB:1198:U:H5'   | 2.11        | 0.51     |
| 22:BA:32:U:H4'    | 22:BA:52:A:H62     | 1.76        | 0.51     |
| 22:DA:32:U:C4'    | 22:DA:52:A:H62     | 2.23        | 0.51     |
| 23:BB:2147:A:H5'  | 23:BB:2148:G:C4'   | 2.40        | 0.51     |
| 23:BB:2898:U:H2'  | 23:BB:2899:A:H8    | 1.73        | 0.51     |
| 1:CA:1392:G:H2'   | 1:CA:1393:U:C6     | 2.45        | 0.51     |
| 23:DB:1198:U:H2'  | 23:DB:1199:U:C6    | 2.46        | 0.51     |
| 1:AA:279:A:C5'    | 1:AA:280:C:H3'     | 2.40        | 0.51     |
| 25:BC:43:ASN:ND2  | 25:BC:44:ASN:N     | 2.55        | 0.51     |
| 23:DB:279:A:H2'   | 23:DB:280:U:H5'    | 1.91        | 0.51     |
| 41:BJ:72:LYS:CB   | 41:BJ:89:PHE:H     | 2.24        | 0.51     |
| 1:AA:1086:U:H2'   | 1:AA:1087:G:H8     | 1.75        | 0.51     |
| 46:BU:70:ALA:HB1  | 46:BU:79:ALA:HB3   | 1.91        | 0.51     |
| 23:BB:2843:G:O2'  | 23:BB:2844:G:H5'   | 2.11        | 0.51     |
| 23:DB:1241:A:H2'  | 23:DB:1242:U:C5'   | 2.41        | 0.51     |
| 8:AI:7:GLY:HA3    | 8:AI:81:GLY:O      | 2.11        | 0.51     |
| 28:BP:31:VAL:CG1  | 28:BP:38:ARG:HG3   | 2.41        | 0.51     |
| 23:DB:2457:U:C2'  | 23:DB:2458:G:H5'   | 2.41        | 0.51     |
| 3:AD:10:LEU:HB3   | 3:AD:62:ARG:HD3    | 1.91        | 0.51     |
| 23:BB:636:G:H3'   | 37:BL:128:THR:HG21 | 1.93        | 0.51     |
| 10:CK:77:GLY:O    | 10:CK:79:LYS:HE3   | 2.11        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 43:BO:66:GLY:HA2  | 43:BO:102:ARG:NE  | 2.25        | 0.51     |
| 1:CA:1170:A:H2'   | 1:CA:1171:A:O4'   | 2.10        | 0.51     |
| 23:BB:1599:U:H2'  | 23:BB:1600:C:H6   | 1.76        | 0.51     |
| 23:DB:1856:U:H2'  | 23:DB:1857:G:H5'  | 1.91        | 0.51     |
| 23:BB:1292:G:H2'  | 23:BB:1293:C:C6   | 2.45        | 0.51     |
| 23:DB:951:C:O2'   | 23:DB:952:G:H5'   | 2.10        | 0.51     |
| 27:BK:109:SER:HB2 | 27:BK:111:LYS:HG2 | 1.93        | 0.51     |
| 23:BB:2359:C:O2'  | 23:BB:2360:G:H5'  | 2.11        | 0.51     |
| 42:BN:54:LEU:HD11 | 42:BN:62:ASN:HB3  | 1.92        | 0.51     |
| 41:BJ:88:THR:HG22 | 41:BJ:91:GLU:HG3  | 1.92        | 0.51     |
| 1:CA:1198:G:H2'   | 1:CA:1199:U:C6    | 2.46        | 0.51     |
| 1:AA:777:A:H2'    | 1:AA:778:G:H8     | 1.75        | 0.51     |
| 49:BR:74:ILE:HB   | 49:BR:87:GLN:O    | 2.11        | 0.51     |
| 6:CG:86:VAL:HG13  | 6:CG:151:ALA:O    | 2.11        | 0.51     |
| 23:DB:640:C:H2'   | 23:DB:641:U:C6    | 2.46        | 0.51     |
| 37:DL:92:LEU:HD23 | 37:DL:92:LEU:H    | 1.75        | 0.51     |
| 23:DB:195:A:H61   | 23:DB:198:C:H3'   | 1.76        | 0.51     |
| 14:AO:62:GLN:O    | 14:AO:66:LEU:HD23 | 2.11        | 0.51     |
| 47:DF:10:GLU:O    | 47:DF:13:LYS:HG3  | 2.11        | 0.51     |
| 23:DB:2880:C:C1'  | 42:DN:91:ALA:HB3  | 2.41        | 0.51     |
| 1:CA:885:G:O2'    | 1:CA:886:G:H5'    | 2.11        | 0.51     |
| 23:BB:1669:A:O3'  | 23:BB:2549:G:H5'  | 2.10        | 0.51     |
| 3:AD:145:ARG:HB3  | 3:AD:147:LYS:HD2  | 1.93        | 0.51     |
| 49:DR:34:GLU:OE1  | 49:DR:60:LYS:HE2  | 2.11        | 0.51     |
| 23:BB:2366:A:H2'  | 23:BB:2367:G:O4'  | 2.11        | 0.51     |
| 44:BQ:30:VAL:CG1  | 44:BQ:31:TYR:N    | 2.65        | 0.51     |
| 5:CF:3:HIS:CD2    | 5:CF:3:HIS:N      | 2.77        | 0.51     |
| 8:CI:22:PRO:HA    | 8:CI:60:LEU:HB3   | 1.93        | 0.51     |
| 53:B6:81:LYS:O    | 53:B6:84:ARG:HG2  | 2.10        | 0.51     |
| 44:DQ:59:LEU:HD13 | 44:DQ:60:TRP:N    | 2.25        | 0.51     |
| 20:CB:69:VAL:HG12 | 20:CB:168:GLU:HG3 | 1.92        | 0.51     |
| 38:DM:17:ASN:ND2  | 38:DM:95:LEU:HG   | 2.14        | 0.51     |
| 2:AC:84:GLU:OE2   | 2:AC:87:ARG:HD3   | 2.10        | 0.51     |
| 50:BT:41:ALA:C    | 50:BT:43:ILE:H    | 2.12        | 0.51     |
| 13:AN:63:CYS:HB3  | 13:AN:67:GLY:N    | 2.26        | 0.51     |
| 33:B1:49:LYS:HG3  | 33:B1:50:GLU:N    | 2.20        | 0.51     |
| 47:BF:12:VAL:O    | 47:BF:16:MET:HG2  | 2.10        | 0.51     |
| 47:BF:137:PHE:O   | 47:BF:139:GLU:N   | 2.43        | 0.51     |
| 42:BN:106:ASP:C   | 42:BN:108:ALA:H   | 2.13        | 0.51     |
| 42:BN:108:ALA:O   | 42:BN:110:MET:HE3 | 2.10        | 0.51     |
| 1:AA:1399:C:H1'   | 57:AA:1973:HOH:O  | 2.11        | 0.51     |
| 4:AE:136:VAL:HG13 | 4:AE:137:ARG:N    | 2.25        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 35:BV:51:GLN:NE2  | 35:BV:79:ARG:HH22  | 2.09        | 0.51     |
| 1:CA:764:C:N4     | 1:CA:812:G:N1      | 2.59        | 0.51     |
| 23:BB:673:C:C4'   | 29:BE:77:ILE:HD11  | 2.40        | 0.51     |
| 50:DT:41:ALA:C    | 50:DT:43:ILE:H     | 2.13        | 0.51     |
| 23:DB:1789:A:H2'  | 23:DB:1790:C:C6    | 2.46        | 0.51     |
| 23:DB:2471:A:O2'  | 23:DB:2472:G:C8    | 2.55        | 0.51     |
| 23:BB:663:G:OP1   | 37:BL:17:LYS:HG2   | 2.11        | 0.51     |
| 23:BB:165:A:H2'   | 23:BB:166:U:C6     | 2.46        | 0.51     |
| 23:BB:2547:A:H5'  | 23:BB:2566:A:C2    | 2.46        | 0.51     |
| 23:BB:2674:G:H4'  | 27:BK:30:ARG:HG3   | 1.92        | 0.51     |
| 20:AB:38:HIS:O    | 20:AB:39:ILE:HD13  | 2.11        | 0.51     |
| 27:DK:105:ARG:HD2 | 27:DK:122:VAL:CG1  | 2.40        | 0.51     |
| 3:AD:113:ALA:O    | 3:AD:116:LEU:HB2   | 2.11        | 0.51     |
| 23:DB:1793:C:H2'  | 23:DB:1794:A:H8    | 1.76        | 0.51     |
| 23:DB:1445:G:H2'  | 23:DB:1446:C:C6    | 2.46        | 0.51     |
| 4:AE:84:VAL:CG1   | 4:AE:146:MET:HB3   | 2.41        | 0.51     |
| 20:CB:99:MET:HA   | 20:CB:106:VAL:HG21 | 1.92        | 0.51     |
| 14:CO:16:GLY:HA2  | 14:CO:27:VAL:HG22  | 1.92        | 0.51     |
| 1:AA:1096:C:H2'   | 1:AA:1097:C:H6     | 1.76        | 0.51     |
| 1:CA:238:A:C2'    | 1:CA:239:U:H5''    | 2.39        | 0.51     |
| 23:BB:1007:C:O3'  | 41:BJ:110:PRO:HB3  | 2.11        | 0.51     |
| 23:BB:263:G:H2'   | 23:BB:264:C:O4'    | 2.11        | 0.51     |
| 6:CG:58:LEU:HA    | 6:CG:61:PHE:HB3    | 1.93        | 0.51     |
| 38:BM:40:ARG:HB2  | 38:BM:93:VAL:HG22  | 1.92        | 0.51     |
| 30:BY:7:THR:HG23  | 30:BY:34:THR:OG1   | 2.11        | 0.51     |
| 37:DL:47:ARG:CB   | 37:DL:47:ARG:HH21  | 2.23        | 0.51     |
| 43:DO:52:SER:OG   | 43:DO:54:VAL:HG12  | 2.11        | 0.51     |
| 23:DB:2093:G:O2'  | 23:DB:2094:A:H5'   | 2.11        | 0.51     |
| 10:CK:51:PHE:CZ   | 10:CK:61:ALA:HA    | 2.46        | 0.51     |
| 23:BB:2605:U:H2'  | 23:BB:2606:C:C5    | 2.46        | 0.51     |
| 23:DB:863:A:H2'   | 23:DB:864:G:H8     | 1.75        | 0.51     |
| 40:DH:135:HIS:CG  | 40:DH:136:SER:H    | 2.28        | 0.51     |
| 1:AA:425:G:H2'    | 1:AA:426:U:C6      | 2.46        | 0.51     |
| 1:CA:129:A:H1'    | 1:CA:130:A:C8      | 2.46        | 0.51     |
| 29:BE:98:LYS:HG2  | 29:BE:99:LYS:N     | 2.25        | 0.51     |
| 53:B6:4:LYS:HA    | 53:B6:7:TYR:CD2    | 2.46        | 0.51     |
| 22:DA:91:C:H2'    | 22:DA:92:C:H6      | 1.76        | 0.51     |
| 23:BB:1773:A:N7   | 23:BB:1829:A:H1'   | 2.26        | 0.51     |
| 6:AG:119:LEU:O    | 6:AG:123:LEU:HG    | 2.11        | 0.51     |
| 23:BB:538:A:H2'   | 23:BB:539:G:O4'    | 2.10        | 0.51     |
| 1:CA:66:A:H4'     | 1:CA:173:U:C4      | 2.46        | 0.51     |
| 1:AA:1491:G:H3'   | 55:AA:1661:PAR:O31 | 2.11        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 8:CI:11:ARG:HA    | 8:CI:105:ARG:NH1   | 2.26        | 0.51     |
| 23:BB:1842:G:H2'  | 23:BB:1843:C:C6    | 2.46        | 0.51     |
| 27:DK:25:LEU:HD13 | 27:DK:38:ILE:HG22  | 1.93        | 0.51     |
| 24:DI:10:LEU:HD12 | 24:DI:10:LEU:O     | 2.10        | 0.51     |
| 53:B6:71:TRP:CE3  | 53:B6:71:TRP:HA    | 2.45        | 0.51     |
| 6:CG:121:ASN:HD22 | 6:CG:121:ASN:N     | 2.07        | 0.51     |
| 53:D6:137:LEU:O   | 53:D6:140:LEU:HB3  | 2.11        | 0.51     |
| 1:AA:358:U:H2'    | 1:AA:359:G:C8      | 2.45        | 0.51     |
| 1:CA:233:C:O2'    | 1:CA:234:C:H5'     | 2.11        | 0.51     |
| 23:DB:1767:G:O2'  | 23:DB:1768:C:H5'   | 2.11        | 0.51     |
| 23:BB:2355:G:H4'  | 52:BW:20:LEU:CD1   | 2.41        | 0.51     |
| 23:BB:853:C:H2'   | 23:BB:854:C:H6     | 1.75        | 0.51     |
| 52:BW:43:LYS:HB3  | 52:BW:58:LEU:CD1   | 2.40        | 0.51     |
| 23:DB:569:U:H2'   | 23:DB:570:G:O4'    | 2.11        | 0.51     |
| 48:DG:9:VAL:HA    | 48:DG:48:THR:CG2   | 2.41        | 0.51     |
| 26:BD:104:VAL:O   | 26:BD:177:VAL:HG21 | 2.10        | 0.51     |
| 53:D6:70:SER:HB3  | 53:D6:76:LEU:HD21  | 1.92        | 0.51     |
| 23:DB:917:A:C2    | 23:DB:918:A:H1'    | 2.45        | 0.51     |
| 53:B6:104:PRO:HB2 | 53:B6:105:PRO:CD   | 2.40        | 0.51     |
| 40:BH:128:HIS:NE2 | 40:BH:130:VAL:HG13 | 2.26        | 0.51     |
| 8:CI:19:PHE:O     | 8:CI:62:LEU:HA     | 2.10        | 0.51     |
| 44:DQ:91:ARG:HH21 | 44:DQ:94:LEU:HD21  | 1.75        | 0.51     |
| 8:AI:79:ARG:NH2   | 8:AI:102:PHE:HA    | 2.26        | 0.51     |
| 26:DD:104:VAL:O   | 26:DD:177:VAL:HG21 | 2.11        | 0.51     |
| 47:DF:79:ARG:HE   | 47:DF:79:ARG:N     | 2.09        | 0.51     |
| 46:BU:82:VAL:HG13 | 46:BU:93:ARG:HB3   | 1.91        | 0.51     |
| 53:B6:14:MET:SD   | 53:B6:129:ILE:HG23 | 2.51        | 0.51     |
| 46:DU:81:ARG:HB2  | 46:DU:96:LYS:CG    | 2.41        | 0.51     |
| 47:BF:141:ASP:HB2 | 47:BF:144:LYS:HB2  | 1.92        | 0.51     |
| 42:BN:102:PHE:N   | 42:BN:109:PRO:HA   | 2.24        | 0.51     |
| 18:CS:28:LYS:H    | 18:CS:28:LYS:HD2   | 1.76        | 0.51     |
| 45:BS:13:SER:OG   | 45:BS:14:ALA:N     | 2.40        | 0.51     |
| 13:AN:30:ILE:CG2  | 13:AN:41:TRP:HB2   | 2.40        | 0.51     |
| 10:AK:88:PRO:HD3  | 21:AU:28:LEU:CD1   | 2.41        | 0.51     |
| 50:DT:23:ALA:C    | 50:DT:25:GLU:H     | 2.15        | 0.51     |
| 45:DS:26:GLY:O    | 45:DS:28:LYS:N     | 2.44        | 0.51     |
| 23:BB:2789:C:O2   | 23:BB:2892:G:H5''  | 2.10        | 0.51     |
| 23:DB:973:A:H1'   | 23:DB:1188:U:C5    | 2.46        | 0.51     |
| 40:BH:5:LEU:HD13  | 40:BH:13:GLY:CA    | 2.38        | 0.51     |
| 23:DB:26:G:H1'    | 23:DB:514:A:N6     | 2.26        | 0.51     |
| 22:DA:103:U:O2'   | 22:DA:104:A:H5'    | 2.11        | 0.51     |
| 48:BG:148:ARG:HB2 | 48:BG:152:ARG:HH21 | 1.74        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 40:BH:4:ILE:HG22  | 40:BH:17:ASP:H     | 1.75        | 0.51     |
| 20:CB:16:GLY:HA2  | 20:CB:40:ILE:CG1   | 2.41        | 0.51     |
| 1:CA:1237:C:H3'   | 1:CA:1238:A:H5'    | 1.92        | 0.51     |
| 1:AA:437:U:H4'    | 3:AD:153:ARG:NH1   | 2.26        | 0.51     |
| 23:BB:1439:A:N7   | 23:BB:1440:U:C2    | 2.79        | 0.51     |
| 1:AA:1343:G:H2'   | 1:AA:1344:C:H6     | 1.76        | 0.51     |
| 23:BB:91:A:H1'    | 23:BB:92:U:C6      | 2.46        | 0.51     |
| 9:AJ:76:ILE:O     | 9:AJ:76:ILE:HD12   | 2.11        | 0.51     |
| 41:BJ:89:PHE:CE1  | 41:BJ:93:ILE:HD13  | 2.46        | 0.51     |
| 1:CA:1162:C:H2'   | 1:CA:1163:A:C8     | 2.46        | 0.51     |
| 6:CG:47:GLU:OE1   | 6:CG:57:GLU:HG2    | 2.11        | 0.51     |
| 1:AA:635:A:H2'    | 1:AA:636:U:C6      | 2.46        | 0.51     |
| 29:DE:48:THR:C    | 29:DE:50:ALA:H     | 2.14        | 0.51     |
| 1:CA:833:G:H2'    | 1:CA:834:U:H6      | 1.75        | 0.51     |
| 23:DB:2461:A:N1   | 23:DB:2490:G:N2    | 2.59        | 0.51     |
| 20:CB:22:TRP:HA   | 20:CB:188:THR:HB   | 1.92        | 0.51     |
| 41:BJ:124:VAL:O   | 41:BJ:125:TYR:HB2  | 2.10        | 0.51     |
| 1:AA:399:G:H2'    | 1:AA:400:C:H6      | 1.76        | 0.51     |
| 23:DB:909:A:H2'   | 23:DB:912:C:C5     | 2.46        | 0.51     |
| 23:BB:740:C:O2'   | 23:BB:741:U:H5'    | 2.10        | 0.51     |
| 1:CA:1277:C:O2'   | 1:CA:1279:G:H1'    | 2.11        | 0.51     |
| 1:CA:97:G:H2'     | 1:CA:98:A:O4'      | 2.09        | 0.51     |
| 1:CA:89:U:H2'     | 1:CA:90:C:O4'      | 2.11        | 0.51     |
| 49:BR:14:VAL:HG22 | 49:BR:15:SER:N     | 2.25        | 0.51     |
| 1:CA:930:C:H2'    | 1:CA:931:C:C6      | 2.46        | 0.51     |
| 23:BB:1704:C:O2'  | 23:BB:1705:A:H5'   | 2.11        | 0.51     |
| 23:BB:702:U:H2'   | 23:BB:703:U:C6     | 2.46        | 0.51     |
| 23:BB:1083:U:H2'  | 23:BB:1085:A:OP2   | 2.11        | 0.51     |
| 11:CL:34:THR:HG21 | 11:CL:53:ARG:HH21  | 1.76        | 0.51     |
| 29:BE:11:ALA:O    | 29:BE:12:LEU:HD22  | 2.11        | 0.51     |
| 23:BB:2226:C:H2'  | 23:BB:2227:A:H8    | 1.75        | 0.51     |
| 28:BP:113:LEU:O   | 28:BP:113:LEU:HD23 | 2.11        | 0.51     |
| 19:AT:68:LYS:HE2  | 19:AT:68:LYS:HA    | 1.91        | 0.51     |
| 23:DB:840:C:H2'   | 23:DB:841:G:H8     | 1.75        | 0.51     |
| 23:BB:856:G:C1'   | 52:BW:23:LYS:HB3   | 2.40        | 0.51     |
| 40:BH:94:ILE:HG23 | 40:BH:99:ILE:HD11  | 1.92        | 0.51     |
| 44:DQ:83:LYS:HZ1  | 44:DQ:87:VAL:HA    | 1.75        | 0.51     |
| 51:DZ:45:ARG:HE   | 51:DZ:47:VAL:CG1   | 2.24        | 0.51     |
| 41:DJ:128:ASN:C   | 41:DJ:129:GLU:HG3  | 2.31        | 0.51     |
| 2:AC:63:ILE:HD12  | 2:AC:98:ALA:CB     | 2.31        | 0.51     |
| 1:AA:598:U:H2'    | 1:AA:599:C:C6      | 2.46        | 0.51     |
| 1:AA:599:C:H5''   | 7:AH:86:LYS:O      | 2.10        | 0.51     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 38:BM:17:ASN:ND2  | 38:BM:95:LEU:HG    | 2.16        | 0.51     |
| 44:BQ:59:LEU:O    | 44:BQ:62:ALA:HB3   | 2.10        | 0.51     |
| 44:BQ:63:ARG:HH22 | 44:BQ:96:ASP:CA    | 2.24        | 0.51     |
| 46:DU:90:LYS:HB3  | 46:DU:92:VAL:HG23  | 1.93        | 0.51     |
| 23:BB:76:C:O2'    | 23:BB:77:G:H5'     | 2.11        | 0.51     |
| 24:DI:76:ALA:HA   | 24:DI:135:MET:SD   | 2.51        | 0.51     |
| 24:DI:54:ILE:C    | 24:DI:54:ILE:HD13  | 2.31        | 0.51     |
| 12:CM:14:ALA:HB2  | 12:CM:42:VAL:HG23  | 1.93        | 0.51     |
| 42:DN:106:ASP:C   | 42:DN:108:ALA:H    | 2.13        | 0.51     |
| 42:DN:108:ALA:O   | 42:DN:110:MET:HE3  | 2.11        | 0.51     |
| 11:CL:41:PRO:HB3  | 11:CL:49:ARG:NH1   | 2.26        | 0.51     |
| 38:DM:32:GLY:HA2  | 38:DM:117:PHE:CZ   | 2.46        | 0.51     |
| 23:DB:663:G:OP1   | 37:DL:17:LYS:HG2   | 2.11        | 0.51     |
| 49:BR:78:ARG:HG3  | 49:BR:78:ARG:HH21  | 1.76        | 0.51     |
| 26:DD:29:VAL:O    | 26:DD:185:ASN:HB3  | 2.10        | 0.51     |
| 1:AA:1472:U:H2'   | 1:AA:1473:G:H8     | 1.76        | 0.51     |
| 26:DD:138:LEU:N   | 26:DD:138:LEU:HD22 | 2.26        | 0.51     |
| 20:AB:57:ASN:HA   | 20:AB:60:ALA:HB3   | 1.92        | 0.51     |
| 23:BB:2147:A:H5'  | 23:BB:2148:G:O4'   | 2.11        | 0.51     |
| 1:CA:465:A:H5'    | 1:CA:465:A:N3      | 2.25        | 0.51     |
| 20:CB:107:ARG:HA  | 20:CB:110:ILE:HD12 | 1.92        | 0.51     |
| 28:BP:4:ILE:O     | 28:BP:6:GLN:N      | 2.41        | 0.51     |
| 1:AA:256:U:H3'    | 1:AA:257:G:H8      | 1.75        | 0.51     |
| 1:CA:236:A:H2'    | 1:CA:237:G:H8      | 1.76        | 0.51     |
| 42:BN:49:GLU:HA   | 42:BN:94:TYR:HD2   | 1.76        | 0.51     |
| 23:BB:2356:U:C5'  | 52:BW:16:GLU:HG3   | 2.39        | 0.51     |
| 3:CD:169:TRP:NE1  | 3:CD:170:LEU:HD23  | 2.25        | 0.51     |
| 1:CA:857:C:H2'    | 1:CA:858:G:O4'     | 2.11        | 0.51     |
| 6:CG:59:GLU:O     | 6:CG:63:VAL:HG23   | 2.10        | 0.51     |
| 1:CA:801:U:O2'    | 1:CA:802:A:H5'     | 2.11        | 0.51     |
| 1:CA:803:G:H2'    | 1:CA:804:U:C6      | 2.46        | 0.51     |
| 23:DB:1372:U:O2'  | 23:DB:1373:A:H5'   | 2.11        | 0.51     |
| 35:BV:53:LYS:HA   | 35:BV:53:LYS:HZ3   | 1.75        | 0.51     |
| 1:AA:405:U:O4     | 3:AD:1:ALA:HA      | 2.11        | 0.51     |
| 23:DB:1351:C:H2'  | 23:DB:1352:U:C1'   | 2.41        | 0.51     |
| 9:CJ:92:LEU:HD22  | 9:CJ:92:LEU:N      | 2.25        | 0.51     |
| 23:DB:1999:C:O2'  | 23:DB:2000:C:H5'   | 2.11        | 0.51     |
| 1:CA:1386:G:O2'   | 1:CA:1387:G:H5'    | 2.10        | 0.51     |
| 1:CA:1387:G:H2'   | 1:CA:1388:C:H6     | 1.76        | 0.51     |
| 40:DH:131:SER:HA  | 40:DH:141:LYS:HA   | 1.93        | 0.51     |
| 41:DJ:124:VAL:O   | 41:DJ:125:TYR:HB2  | 2.11        | 0.51     |
| 23:BB:1868:C:H2'  | 23:BB:1869:G:O4'   | 2.11        | 0.51     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:692:U:C2      | 1:AA:694:A:H5''    | 2.45        | 0.51     |
| 48:BG:174:LYS:HZ2  | 48:BG:176:LYS:HG2  | 1.76        | 0.51     |
| 23:BB:951:C:O2'    | 23:BB:952:G:H5'    | 2.11        | 0.51     |
| 23:BB:615:U:O4     | 29:BE:39:ALA:HB2   | 2.11        | 0.51     |
| 3:AD:145:ARG:NH2   | 3:AD:147:LYS:HE2   | 2.26        | 0.51     |
| 23:BB:2756:U:H1'   | 23:BB:2757:A:H5''  | 1.93        | 0.51     |
| 1:CA:1069:C:O2'    | 1:CA:1192:C:H1'    | 2.10        | 0.51     |
| 7:CH:118:ALA:HB3   | 7:CH:120:LEU:HD22  | 1.92        | 0.51     |
| 23:DB:657:U:H2'    | 23:DB:658:U:C6     | 2.46        | 0.51     |
| 23:DB:1732:C:OP1   | 23:DB:1732:C:H2'   | 2.11        | 0.51     |
| 9:AJ:26:VAL:HG12   | 9:AJ:30:LYS:HE2    | 1.92        | 0.51     |
| 50:DT:5:GLU:CA     | 50:DT:8:LEU:HB2    | 2.22        | 0.50     |
| 25:BC:129:LEU:HB3  | 25:BC:134:ILE:HG22 | 1.92        | 0.50     |
| 25:BC:183:VAL:HG22 | 25:BC:184:GLU:H    | 1.76        | 0.50     |
| 6:AG:144:ALA:O     | 6:AG:145:GLU:HB3   | 2.11        | 0.50     |
| 48:DG:42:VAL:HG23  | 48:DG:50:THR:O     | 2.11        | 0.50     |
| 53:D6:84:ARG:CZ    | 53:D6:92:PRO:HG2   | 2.41        | 0.50     |
| 23:DB:2365:G:O2'   | 52:DW:59:PHE:HE1   | 1.94        | 0.50     |
| 53:B6:72:ASP:HB3   | 53:B6:75:ALA:CB    | 2.41        | 0.50     |
| 40:BH:90:LEU:HD13  | 40:BH:124:THR:O    | 2.12        | 0.50     |
| 41:BJ:128:ASN:C    | 41:BJ:129:GLU:HG3  | 2.32        | 0.50     |
| 41:DJ:4:PHE:HB3    | 41:DJ:44:TYR:CE1   | 2.46        | 0.50     |
| 44:DQ:59:LEU:O     | 44:DQ:62:ALA:HB3   | 2.10        | 0.50     |
| 35:BV:2:PHE:HD2    | 35:BV:59:GLU:OE1   | 1.94        | 0.50     |
| 48:DG:22:VAL:HG13  | 48:DG:36:LEU:HD13  | 1.93        | 0.50     |
| 23:DB:2393:U:C5'   | 37:DL:62:PRO:HG3   | 2.35        | 0.50     |
| 1:CA:1014:A:N3     | 1:CA:1219:A:H1'    | 2.26        | 0.50     |
| 48:BG:26:LYS:HA    | 48:BG:32:LEU:H     | 1.74        | 0.50     |
| 42:BN:83:LEU:HD12  | 42:BN:84:GLY:N     | 2.27        | 0.50     |
| 23:DB:1060:U:O2    | 23:DB:1088:A:C8    | 2.63        | 0.50     |
| 12:CM:44:ILE:HD12  | 12:CM:45:SER:H     | 1.76        | 0.50     |
| 12:CM:42:VAL:HB    | 12:CM:47:LEU:HD21  | 1.93        | 0.50     |
| 1:CA:946:A:H2'     | 1:CA:947:G:H8      | 1.72        | 0.50     |
| 12:CM:100:ARG:HH11 | 12:CM:103:THR:HB   | 1.76        | 0.50     |
| 10:AK:34:THR:HB    | 10:AK:40:ALA:CA    | 2.38        | 0.50     |
| 39:DX:7:ARG:HH11   | 39:DX:7:ARG:HB2    | 1.75        | 0.50     |
| 1:AA:719:C:H1'     | 17:AR:37:LYS:HB2   | 1.94        | 0.50     |
| 26:DD:168:GLU:O    | 26:DD:170:VAL:HG22 | 2.10        | 0.50     |
| 22:DA:33:G:O2'     | 22:DA:34:A:H5'     | 2.10        | 0.50     |
| 49:BR:40:MET:HG3   | 49:BR:48:LYS:HA    | 1.92        | 0.50     |
| 49:BR:39:LEU:CB    | 49:BR:49:ILE:HG12  | 2.41        | 0.50     |
| 1:AA:1392:G:H2'    | 1:AA:1393:U:C6     | 2.45        | 0.50     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:87:C:H2'      | 1:AA:88:U:H4'      | 1.92        | 0.50     |
| 24:DI:126:ARG:HB3  | 24:DI:126:ARG:NH1  | 2.25        | 0.50     |
| 1:CA:617:G:H4'     | 15:CP:46:LYS:HE2   | 1.93        | 0.50     |
| 35:BV:9:ARG:HH21   | 35:BV:12:GLN:HA    | 1.73        | 0.50     |
| 23:DB:1683:U:H2'   | 23:DB:1684:G:C8    | 2.46        | 0.50     |
| 23:DB:1998:A:H2'   | 23:DB:1999:C:H6    | 1.76        | 0.50     |
| 23:BB:2415:G:H4'   | 37:BL:66:PHE:HB2   | 1.93        | 0.50     |
| 23:BB:569:U:H2'    | 23:BB:570:G:O4'    | 2.11        | 0.50     |
| 23:DB:2605:U:H2'   | 23:DB:2606:C:C5    | 2.46        | 0.50     |
| 33:B1:40:PRO:O     | 33:B1:43:ARG:HG2   | 2.10        | 0.50     |
| 23:BB:1400:U:H2'   | 23:BB:1401:G:C8    | 2.46        | 0.50     |
| 23:BB:528:A:C2     | 23:BB:2042:A:H2'   | 2.45        | 0.50     |
| 1:CA:992:U:H1'     | 1:CA:993:G:C2      | 2.46        | 0.50     |
| 23:DB:1952:A:C2    | 27:DK:22:ILE:HD12  | 2.45        | 0.50     |
| 6:CG:30:MET:HG2    | 6:CG:31:VAL:N      | 2.25        | 0.50     |
| 23:BB:289:G:H2'    | 23:BB:290:U:O4'    | 2.11        | 0.50     |
| 6:CG:109:LYS:HE2   | 6:CG:109:LYS:HA    | 1.92        | 0.50     |
| 23:DB:1754:A:N1    | 23:DB:2716:C:O2'   | 2.43        | 0.50     |
| 25:DC:107:LYS:O    | 25:DC:109:LEU:HD22 | 2.11        | 0.50     |
| 23:BB:15:G:O2'     | 23:BB:16:C:H5'     | 2.11        | 0.50     |
| 23:BB:533:G:H5'    | 44:BQ:23:TYR:CD2   | 2.46        | 0.50     |
| 26:BD:104:VAL:HG13 | 26:BD:106:LYS:HE2  | 1.94        | 0.50     |
| 53:D6:39:LEU:CA    | 53:D6:52:LEU:HB3   | 2.40        | 0.50     |
| 53:B6:83:ILE:HG13  | 53:B6:92:PRO:HD2   | 1.92        | 0.50     |
| 40:BH:100:ALA:HA   | 40:BH:103:VAL:CG2  | 2.42        | 0.50     |
| 1:CA:1128:C:H4'    | 1:CA:1148:U:O2     | 2.11        | 0.50     |
| 44:DQ:86:SER:O     | 44:DQ:88:GLU:N     | 2.43        | 0.50     |
| 8:AI:56:MET:SD     | 8:AI:57:VAL:N      | 2.83        | 0.50     |
| 41:DJ:58:ASN:HA    | 41:DJ:127:GLY:HA2  | 1.94        | 0.50     |
| 23:DB:2645:G:H4'   | 23:DB:2732:G:H2'   | 1.94        | 0.50     |
| 43:BO:36:TYR:HD2   | 43:BO:36:TYR:N     | 2.09        | 0.50     |
| 30:BY:8:GLN:HB3    | 30:BY:31:ILE:C     | 2.31        | 0.50     |
| 1:AA:1277:C:O2'    | 1:AA:1279:G:H1'    | 2.12        | 0.50     |
| 1:AA:1078:U:H2'    | 1:AA:1079:G:O4'    | 2.11        | 0.50     |
| 1:AA:1081:A:O2'    | 1:AA:1082:A:H5'    | 2.11        | 0.50     |
| 29:DE:105:LEU:HA   | 29:DE:108:ILE:CG2  | 2.41        | 0.50     |
| 1:CA:1225:A:H3'    | 1:CA:1226:C:H6     | 1.73        | 0.50     |
| 18:CS:66:VAL:HG23  | 18:CS:67:GLY:H     | 1.76        | 0.50     |
| 29:BE:58:LYS:HE2   | 29:BE:60:TRP:CD1   | 2.46        | 0.50     |
| 23:DB:2502:G:H5'   | 23:DB:2503:A:C5'   | 2.35        | 0.50     |
| 42:BN:32:GLU:HB3   | 42:BN:115:LEU:HG   | 1.92        | 0.50     |
| 24:DI:18:ASN:HB2   | 24:DI:38:CYS:SG    | 2.52        | 0.50     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 20:CB:15:PHE:HD1 | 20:CB:16:GLY:N     | 2.09        | 0.50     |
| 38:BM:19:GLY:CA  | 38:BM:97:GLN:HB2   | 2.39        | 0.50     |
| 7:AH:40:LYS:HA   | 7:AH:45:ILE:HG13   | 1.94        | 0.50     |
| 7:AH:58:LEU:CD2  | 7:AH:60:LEU:HB2    | 2.41        | 0.50     |
| 20:CB:216:VAL:O  | 20:CB:220:VAL:HG23 | 2.11        | 0.50     |
| 1:CA:841:C:H2'   | 1:CA:843:U:OP2     | 2.11        | 0.50     |
| 23:BB:1438:U:H2' | 23:BB:1439:A:O4'   | 2.11        | 0.50     |
| 23:BB:1441:G:H2' | 23:BB:1442:U:H6    | 1.76        | 0.50     |
| 20:AB:98:GLY:O   | 20:AB:102:ASN:N    | 2.44        | 0.50     |
| 45:DS:81:SER:HB3 | 45:DS:99:ARG:HB3   | 1.93        | 0.50     |
| 49:DR:31:GLU:O   | 49:DR:63:VAL:HG22  | 2.11        | 0.50     |
| 8:AI:123:ARG:HB3 | 8:AI:123:ARG:CZ    | 2.41        | 0.50     |
| 29:DE:158:PHE:HA | 29:DE:169:VAL:CG2  | 2.41        | 0.50     |
| 1:AA:1058:G:OP1  | 2:AC:198:LYS:HE3   | 2.10        | 0.50     |
| 28:DP:52:ARG:NH1 | 28:DP:52:ARG:HG2   | 2.25        | 0.50     |
| 26:BD:168:GLU:O  | 26:BD:170:VAL:HG13 | 2.12        | 0.50     |
| 1:AA:254:G:O2'   | 1:AA:255:G:H5'     | 2.11        | 0.50     |
| 1:CA:256:U:H3'   | 1:CA:257:G:H8      | 1.74        | 0.50     |
| 23:BB:150:U:H2'  | 23:BB:151:C:C6     | 2.45        | 0.50     |
| 49:BR:2:TYR:HB2  | 49:BR:42:ALA:N     | 2.26        | 0.50     |
| 1:AA:6:G:H3'     | 1:AA:6:G:N3        | 2.26        | 0.50     |
| 23:BB:2460:U:H2' | 23:BB:2461:A:H8    | 1.76        | 0.50     |
| 23:BB:2026:U:H2' | 23:BB:2027:G:H8    | 1.75        | 0.50     |
| 23:DB:2247:A:H2' | 23:DB:2248:C:H6    | 1.77        | 0.50     |
| 23:BB:1258:U:C4' | 29:BE:79:ARG:HD2   | 2.41        | 0.50     |
| 17:CR:31:TYR:CD1 | 17:CR:54:LEU:HD11  | 2.46        | 0.50     |
| 1:AA:1063:C:H2'  | 1:AA:1064:G:C8     | 2.46        | 0.50     |
| 10:CK:52:ARG:NH1 | 10:CK:53:GLY:H     | 2.07        | 0.50     |
| 1:AA:284:C:H2'   | 1:AA:285:C:C6      | 2.46        | 0.50     |
| 22:DA:109:A:H2'  | 22:DA:110:C:H6     | 1.75        | 0.50     |
| 23:DB:660:C:H2'  | 23:DB:661:A:C8     | 2.45        | 0.50     |
| 23:DB:41:C:H2'   | 23:DB:42:A:O4'     | 2.11        | 0.50     |
| 23:BB:1107:G:H2' | 23:BB:1108:U:H6    | 1.75        | 0.50     |
| 23:DB:1773:A:N7  | 23:DB:1829:A:H1'   | 2.26        | 0.50     |
| 1:AA:560:A:H4'   | 1:AA:561:U:H5''    | 1.92        | 0.50     |
| 1:CA:886:G:O2'   | 1:CA:887:G:H5'     | 2.11        | 0.50     |
| 23:DB:2333:A:H5' | 23:DB:2335:A:H1'   | 1.92        | 0.50     |
| 23:BB:438:G:H2'  | 23:BB:439:A:H8     | 1.76        | 0.50     |
| 1:CA:434:U:H3'   | 1:CA:435:A:H8      | 1.74        | 0.50     |
| 23:DB:963:U:O2'  | 23:DB:964:C:H5'    | 2.10        | 0.50     |
| 23:BB:1268:A:H2' | 23:BB:1269:A:O4'   | 2.10        | 0.50     |
| 51:DZ:18:ARG:HA  | 51:DZ:23:ASN:O     | 2.12        | 0.50     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:1368:G:H2'  | 23:BB:1369:G:H8   | 1.77        | 0.50     |
| 1:AA:580:C:H2'    | 1:AA:581:G:O4'    | 2.12        | 0.50     |
| 23:DB:1704:C:O2'  | 23:DB:1705:A:H5'  | 2.11        | 0.50     |
| 23:BB:1742:U:H2'  | 23:BB:1743:G:C8   | 2.46        | 0.50     |
| 23:BB:1100:C:H2'  | 23:BB:1101:U:H6   | 1.75        | 0.50     |
| 1:CA:1105:A:H2'   | 1:CA:1106:G:H8    | 1.76        | 0.50     |
| 23:DB:724:U:H2'   | 23:DB:725:G:O4'   | 2.12        | 0.50     |
| 46:BU:41:VAL:O    | 46:BU:42:LYS:HB2  | 2.11        | 0.50     |
| 41:DJ:9:GLU:H     | 41:DJ:9:GLU:CD    | 2.15        | 0.50     |
| 6:AG:49:LEU:HD12  | 6:AG:124:SER:OG   | 2.12        | 0.50     |
| 1:AA:251:G:N3     | 1:AA:266:G:O6     | 2.44        | 0.50     |
| 1:AA:532:A:C8     | 2:AC:192:TYR:HD2  | 2.29        | 0.50     |
| 40:DH:27:ARG:HH21 | 40:DH:27:ARG:HG2  | 1.76        | 0.50     |
| 23:BB:2269:G:H4'  | 52:BW:19:ARG:HH11 | 1.74        | 0.50     |
| 40:BH:111:ALA:HB3 | 40:BH:114:GLU:CG  | 2.41        | 0.50     |
| 53:D6:38:LEU:HD12 | 53:D6:66:LEU:HD23 | 1.92        | 0.50     |
| 53:D6:84:ARG:HD2  | 53:D6:92:PRO:CD   | 2.41        | 0.50     |
| 53:D6:86:SER:C    | 53:D6:88:LEU:H    | 2.15        | 0.50     |
| 53:B6:58:VAL:HG13 | 53:B6:68:VAL:HA   | 1.93        | 0.50     |
| 41:DJ:31:GLU:O    | 41:DJ:34:ARG:HB2  | 2.10        | 0.50     |
| 41:DJ:38:GLY:HA3  | 41:DJ:50:THR:O    | 2.11        | 0.50     |
| 8:AI:19:PHE:HB2   | 8:AI:63:TYR:HB3   | 1.93        | 0.50     |
| 23:DB:2734:A:N6   | 23:DB:2770:G:H1'  | 2.26        | 0.50     |
| 51:BZ:76:GLU:HG3  | 51:BZ:77:LYS:N    | 2.25        | 0.50     |
| 34:B3:36:ALA:O    | 34:B3:39:ARG:HB3  | 2.11        | 0.50     |
| 4:AE:132:PRO:O    | 4:AE:136:VAL:HG12 | 2.12        | 0.50     |
| 4:AE:89:THR:HG22  | 4:AE:90:GLY:N     | 2.26        | 0.50     |
| 1:CA:411:A:H62    | 1:CA:413:G:N2     | 1.99        | 0.50     |
| 20:CB:45:THR:HG22 | 20:CB:49:PHE:CZ   | 2.47        | 0.50     |
| 23:DB:2789:C:H3'  | 23:DB:2893:A:H62  | 1.75        | 0.50     |
| 1:CA:521:G:O2'    | 1:CA:522:C:H5'    | 2.12        | 0.50     |
| 31:B0:42:ILE:HD11 | 42:BN:98:LEU:HB3  | 1.92        | 0.50     |
| 48:DG:148:ARG:HA  | 48:DG:161:VAL:CG1 | 2.42        | 0.50     |
| 42:BN:72:ASP:OD2  | 42:BN:74:GLU:HB3  | 2.11        | 0.50     |
| 22:BA:106:G:H2'   | 22:BA:107:G:C8    | 2.46        | 0.50     |
| 42:DN:72:ASP:C    | 42:DN:74:GLU:H    | 2.14        | 0.50     |
| 38:DM:19:GLY:CA   | 38:DM:97:GLN:HB2  | 2.40        | 0.50     |
| 23:BB:126:A:O2'   | 23:BB:127:A:H5'   | 2.12        | 0.50     |
| 48:BG:30:GLY:HA3  | 48:BG:78:VAL:HG12 | 1.91        | 0.50     |
| 7:CH:11:THR:HA    | 7:CH:14:ARG:CZ    | 2.41        | 0.50     |
| 26:BD:9:VAL:HG13  | 26:BD:9:VAL:O     | 2.10        | 0.50     |
| 23:DB:1324:G:H1'  | 23:DB:1616:A:C6   | 2.47        | 0.50     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 31:B0:30:ASP:OD2   | 31:B0:31:LYS:HD2   | 2.11        | 0.50     |
| 5:AF:70:VAL:HG23   | 5:AF:71:ILE:H      | 1.76        | 0.50     |
| 23:BB:864:G:O2'    | 23:BB:865:C:H5'    | 2.12        | 0.50     |
| 43:BO:76:LYS:HG3   | 43:BO:113:ALA:CB   | 2.41        | 0.50     |
| 23:BB:132:G:O2'    | 23:BB:133:U:H5'    | 2.11        | 0.50     |
| 23:BB:1585:C:H2'   | 23:BB:1586:A:O4'   | 2.11        | 0.50     |
| 23:BB:945:A:H4'    | 23:BB:945:A:OP2    | 2.11        | 0.50     |
| 28:BP:52:ARG:HB2   | 28:BP:55:HIS:O     | 2.10        | 0.50     |
| 20:CB:19:THR:OG1   | 20:CB:20:ARG:N     | 2.45        | 0.50     |
| 20:AB:70:GLY:HA3   | 20:AB:79:VAL:HG21  | 1.94        | 0.50     |
| 19:CT:50:PHE:HD2   | 19:CT:78:LEU:HD13  | 1.76        | 0.50     |
| 25:BC:245:THR:OG1  | 25:BC:249:VAL:HG23 | 2.11        | 0.50     |
| 1:CA:376:G:H2'     | 1:CA:377:G:H8      | 1.76        | 0.50     |
| 3:CD:10:LEU:HD12   | 3:CD:20:LEU:CD1    | 2.42        | 0.50     |
| 5:CF:15:SER:HA     | 5:CF:18:VAL:HG23   | 1.93        | 0.50     |
| 1:CA:45:G:H2'      | 1:CA:46:G:C8       | 2.45        | 0.50     |
| 23:DB:2254:C:H1'   | 53:D6:151:GLU:HB2  | 1.92        | 0.50     |
| 16:AQ:28:VAL:O     | 16:AQ:36:PHE:HA    | 2.11        | 0.50     |
| 23:BB:1332:G:H2'   | 23:BB:1332:G:N3    | 2.25        | 0.50     |
| 1:AA:986:U:H2'     | 1:AA:987:G:O4'     | 2.12        | 0.50     |
| 48:DG:59:ASP:O     | 48:DG:63:GLN:HB2   | 2.11        | 0.50     |
| 23:DB:2594:C:O2'   | 23:DB:2595:G:H5'   | 2.10        | 0.50     |
| 1:CA:1289:A:H2'    | 1:CA:1290:G:H5'    | 1.93        | 0.50     |
| 26:BD:39:ASP:HB3   | 26:BD:42:ASN:HB3   | 1.92        | 0.50     |
| 23:BB:660:C:H2'    | 23:BB:661:A:H8     | 1.76        | 0.50     |
| 1:AA:1234:C:O2'    | 1:AA:1235:U:H5'    | 2.12        | 0.50     |
| 1:CA:966:G:H2'     | 1:CA:967:C:C6      | 2.46        | 0.50     |
| 23:BB:855:G:N3     | 52:BW:23:LYS:HE3   | 2.26        | 0.50     |
| 23:BB:1819:A:OP1   | 25:BC:154:ALA:HA   | 2.11        | 0.50     |
| 25:BC:183:VAL:HG22 | 25:BC:184:GLU:N    | 2.26        | 0.50     |
| 48:DG:120:ILE:HD13 | 48:DG:121:THR:N    | 2.27        | 0.50     |
| 53:D6:38:LEU:CB    | 53:D6:58:VAL:HG21  | 2.42        | 0.50     |
| 40:BH:83:LYS:HB2   | 40:BH:92:GLY:H     | 1.76        | 0.50     |
| 1:AA:946:A:H2'     | 1:AA:947:G:H8      | 1.74        | 0.50     |
| 43:BO:51:ALA:O     | 43:BO:74:VAL:HG13  | 2.12        | 0.50     |
| 1:AA:764:C:O2'     | 1:AA:765:G:H5'     | 2.10        | 0.50     |
| 1:CA:1226:C:H4'    | 1:CA:1227:A:OP1    | 2.10        | 0.50     |
| 18:AS:30:LEU:HB2   | 18:AS:48:ILE:CG2   | 2.38        | 0.50     |
| 18:AS:42:ASN:HD21  | 18:AS:43:MET:HG2   | 1.75        | 0.50     |
| 28:BP:92:ARG:O     | 28:BP:92:ARG:HG2   | 2.11        | 0.50     |
| 25:DC:18:VAL:HG11  | 25:DC:202:ARG:HD2  | 1.93        | 0.50     |
| 23:DB:2807:U:H1'   | 23:DB:2892:G:N2    | 2.27        | 0.50     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 24:BI:125:THR:O   | 24:BI:129:GLU:HG3  | 2.11        | 0.50     |
| 1:AA:1471:U:O2'   | 1:AA:1472:U:H5'    | 2.11        | 0.50     |
| 38:BM:19:GLY:N    | 38:BM:38:ARG:NH2   | 2.58        | 0.50     |
| 44:DQ:109:VAL:O   | 44:DQ:113:LYS:HG3  | 2.12        | 0.50     |
| 1:CA:314:C:O2'    | 1:CA:315:A:H5'     | 2.11        | 0.50     |
| 23:BB:279:A:N6    | 23:BB:361:G:H1'    | 2.26        | 0.50     |
| 20:AB:119:GLN:O   | 20:AB:125:PHE:HB3  | 2.11        | 0.50     |
| 45:DS:42:LYS:O    | 45:DS:45:VAL:HG22  | 2.11        | 0.50     |
| 23:DB:360:U:H2'   | 23:DB:361:G:C1'    | 2.42        | 0.50     |
| 23:BB:1777:U:O2'  | 23:BB:1778:U:H5'   | 2.11        | 0.50     |
| 1:AA:35:G:H2'     | 1:AA:36:C:H6       | 1.76        | 0.50     |
| 3:AD:84:ASN:ND2   | 3:AD:86:GLY:H      | 2.10        | 0.50     |
| 29:BE:47:LYS:HA   | 29:BE:51:GLU:OE2   | 2.11        | 0.50     |
| 23:BB:947:A:H2'   | 23:BB:948:C:C6     | 2.46        | 0.50     |
| 1:AA:192:A:O2'    | 1:AA:193:C:H5'     | 2.12        | 0.50     |
| 20:AB:19:THR:OG1  | 20:AB:20:ARG:N     | 2.45        | 0.50     |
| 23:DB:704:G:H1'   | 23:DB:727:A:N6     | 2.26        | 0.50     |
| 14:CO:5:THR:O     | 14:CO:8:THR:HB     | 2.11        | 0.50     |
| 7:CH:94:VAL:HG12  | 7:CH:99:GLY:HA3    | 1.93        | 0.50     |
| 1:AA:1225:A:N3    | 1:AA:1225:A:H2'    | 2.25        | 0.50     |
| 1:CA:215:C:H2'    | 1:CA:216:U:H6      | 1.76        | 0.50     |
| 23:DB:2218:G:O2'  | 23:DB:2219:U:H5'   | 2.12        | 0.50     |
| 23:DB:912:C:H2'   | 23:DB:913:U:C6     | 2.46        | 0.50     |
| 23:BB:139:U:H3'   | 23:BB:140:C:C5'    | 2.42        | 0.50     |
| 23:DB:416:U:H2'   | 23:DB:417:C:C6     | 2.47        | 0.50     |
| 42:DN:59:SER:O    | 42:DN:63:ARG:HB2   | 2.11        | 0.50     |
| 23:DB:4:U:H2'     | 23:DB:5:A:C8       | 2.46        | 0.50     |
| 1:CA:518:C:H2'    | 1:CA:530:G:H8      | 1.76        | 0.50     |
| 1:CA:1041:G:O2'   | 1:CA:1042:A:H5'    | 2.11        | 0.50     |
| 23:DB:1046:A:H4'  | 23:DB:1047:G:OP2   | 2.11        | 0.50     |
| 53:D6:25:LEU:HD22 | 53:D6:179:LYS:HG2  | 1.92        | 0.50     |
| 23:DB:2324:U:H3'  | 23:DB:2325:G:C5'   | 2.40        | 0.50     |
| 23:DB:1251:C:O2'  | 23:DB:1252:G:H3'   | 2.10        | 0.50     |
| 43:DO:97:PHE:HB3  | 43:DO:103:VAL:HG21 | 1.94        | 0.50     |
| 1:CA:1243:C:H2'   | 1:CA:1244:G:H8     | 1.76        | 0.50     |
| 23:BB:2226:C:H2'  | 23:BB:2227:A:C8    | 2.46        | 0.50     |
| 8:AI:11:ARG:HA    | 8:AI:105:ARG:NH1   | 2.26        | 0.50     |
| 23:BB:2008:C:H2'  | 23:BB:2009:A:H8    | 1.77        | 0.50     |
| 23:DB:697:G:H2'   | 23:DB:698:C:C6     | 2.46        | 0.50     |
| 33:B1:16:THR:OG1  | 33:B1:41:VAL:HG11  | 2.12        | 0.50     |
| 23:BB:1295:C:H2'  | 23:BB:1296:G:C8    | 2.45        | 0.50     |
| 1:CA:878:A:H5''   | 7:CH:80:PRO:HG2    | 1.92        | 0.50     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:588:U:H1'   | 29:BE:85:PHE:CG    | 2.46        | 0.50     |
| 23:DB:910:A:H2'   | 23:DB:911:A:C8     | 2.47        | 0.50     |
| 23:DB:1368:G:H2'  | 23:DB:1369:G:H8    | 1.76        | 0.50     |
| 22:DA:53:A:O2'    | 22:DA:54:G:H5'     | 2.11        | 0.50     |
| 32:D4:13:ASN:O    | 32:D4:27:CYS:HA    | 2.11        | 0.50     |
| 50:BT:5:GLU:CA    | 50:BT:8:LEU:HB2    | 2.21        | 0.50     |
| 52:BW:30:VAL:HA   | 52:BW:60:ALA:O     | 2.11        | 0.50     |
| 47:BF:90:LEU:C    | 47:BF:91:ARG:HD3   | 2.32        | 0.50     |
| 22:DA:42:C:C6     | 47:DF:65:LEU:HD13  | 2.47        | 0.50     |
| 8:CI:41:GLU:C     | 8:CI:43:ALA:H      | 2.14        | 0.50     |
| 43:DO:36:TYR:HD2  | 43:DO:36:TYR:N     | 2.10        | 0.50     |
| 39:BX:23:ARG:HA   | 39:BX:26:PHE:HB3   | 1.94        | 0.50     |
| 44:BQ:77:LYS:HA   | 44:BQ:80:ASN:HB3   | 1.93        | 0.50     |
| 48:BG:34:ARG:N    | 48:BG:34:ARG:HH11  | 1.99        | 0.50     |
| 30:BY:13:ILE:HG22 | 30:BY:14:GLY:N     | 2.25        | 0.50     |
| 24:DI:78:LEU:HD13 | 24:DI:108:ILE:HG23 | 1.94        | 0.50     |
| 45:BS:47:VAL:HG12 | 45:BS:103:ILE:HG21 | 1.93        | 0.50     |
| 23:BB:2471:A:O2'  | 23:BB:2472:G:O5'   | 2.27        | 0.50     |
| 35:DV:79:ARG:HH12 | 38:DM:134:THR:HG21 | 1.75        | 0.50     |
| 53:D6:2:THR:HB    | 53:D6:5:GLU:HG3    | 1.92        | 0.50     |
| 53:D6:4:LYS:HD3   | 53:D6:5:GLU:N      | 2.26        | 0.50     |
| 49:BR:49:ILE:HG21 | 49:BR:53:PHE:C     | 2.32        | 0.50     |
| 26:DD:36:GLN:HG2  | 26:DD:37:VAL:N     | 2.27        | 0.50     |
| 9:AJ:5:ARG:HG2    | 9:AJ:79:PRO:HD3    | 1.94        | 0.50     |
| 23:DB:1427:A:H5'' | 23:DB:1559:U:O2    | 2.11        | 0.50     |
| 4:AE:45:VAL:HG13  | 4:AE:117:ALA:HA    | 1.94        | 0.50     |
| 23:DB:2529:G:O3'  | 48:DG:174:LYS:HD2  | 2.12        | 0.50     |
| 23:BB:713:G:O2'   | 23:BB:714:U:H5'    | 2.12        | 0.50     |
| 23:DB:714:U:H1'   | 23:DB:717:C:H5     | 1.77        | 0.50     |
| 1:CA:859:G:O2'    | 1:CA:860:A:H5'     | 2.11        | 0.50     |
| 1:CA:1476:A:O2'   | 1:CA:1477:U:H5'    | 2.12        | 0.50     |
| 23:DB:727:A:OP1   | 23:DB:1431:A:O2'   | 2.28        | 0.50     |
| 23:DB:1592:C:H2'  | 23:DB:1593:A:C8    | 2.45        | 0.50     |
| 23:BB:1260:A:H2'  | 23:BB:1261:C:C6    | 2.47        | 0.50     |
| 1:AA:524:G:H2'    | 1:AA:525:C:H6      | 1.73        | 0.50     |
| 52:BW:77:LYS:HZ2  | 52:BW:77:LYS:N     | 2.09        | 0.50     |
| 1:CA:6:G:N3       | 1:CA:6:G:H3'       | 2.27        | 0.50     |
| 23:BB:7:G:H4'     | 41:BJ:15:TRP:CZ2   | 2.46        | 0.50     |
| 35:BV:14:LYS:HE3  | 35:BV:18:ARG:NH2   | 2.27        | 0.50     |
| 23:BB:1685:C:O2'  | 23:BB:1686:C:H5'   | 2.12        | 0.50     |
| 23:DB:949:G:O2'   | 23:DB:950:G:H5'    | 2.10        | 0.50     |
| 23:DB:290:U:O2'   | 23:DB:291:G:H5'    | 2.11        | 0.50     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1014:A:O2'  | 23:BB:1015:U:H5'   | 2.12        | 0.50     |
| 23:BB:807:U:H2'   | 23:BB:808:G:H8     | 1.77        | 0.50     |
| 12:CM:63:VAL:CG1  | 12:CM:67:ASP:HB2   | 2.41        | 0.50     |
| 1:CA:73:C:O2'     | 1:CA:74:A:H5'      | 2.11        | 0.50     |
| 1:AA:640:A:O2'    | 1:AA:641:U:H5'     | 2.11        | 0.50     |
| 28:DP:29:VAL:HA   | 28:DP:79:VAL:O     | 2.12        | 0.50     |
| 1:AA:1381:U:O2'   | 1:AA:1382:C:H5'    | 2.12        | 0.50     |
| 23:DB:350:G:H2'   | 23:DB:351:C:O4'    | 2.12        | 0.50     |
| 1:AA:1437:A:H2'   | 1:AA:1438:G:H8     | 1.77        | 0.50     |
| 23:BB:1754:A:N1   | 23:BB:2716:C:O2'   | 2.45        | 0.50     |
| 26:DD:39:ASP:HB3  | 26:DD:42:ASN:HB3   | 1.92        | 0.50     |
| 23:DB:208:C:H2'   | 23:DB:209:C:H6     | 1.76        | 0.50     |
| 23:BB:917:A:C2    | 23:BB:918:A:H1'    | 2.47        | 0.50     |
| 20:AB:69:VAL:HB   | 20:AB:162:VAL:CB   | 2.42        | 0.50     |
| 23:DB:2547:A:H5'' | 27:DK:29:HIS:NE2   | 2.26        | 0.50     |
| 22:BA:28:C:O2'    | 22:BA:29:A:H5'     | 2.12        | 0.50     |
| 24:BI:79:LEU:HD11 | 24:BI:131:THR:OG1  | 2.11        | 0.50     |
| 47:BF:11:VAL:HG12 | 47:BF:12:VAL:N     | 2.14        | 0.50     |
| 1:AA:521:G:O2'    | 1:AA:522:C:H5'     | 2.12        | 0.50     |
| 11:AL:41:PRO:HB3  | 11:AL:49:ARG:NH1   | 2.26        | 0.50     |
| 29:BE:60:TRP:C    | 29:BE:62:GLN:H     | 2.14        | 0.50     |
| 35:DV:77:VAL:HG23 | 35:DV:89:ILE:HG22  | 1.94        | 0.50     |
| 39:DX:23:ARG:O    | 39:DX:27:ASN:N     | 2.43        | 0.50     |
| 17:CR:38:ILE:HG23 | 17:CR:62:ARG:NH2   | 2.26        | 0.50     |
| 22:BA:32:U:H4'    | 22:BA:52:A:N6      | 2.27        | 0.50     |
| 31:D0:38:LEU:HD13 | 31:D0:41:HIS:NE2   | 2.27        | 0.50     |
| 11:CL:28:GLN:HB2  | 11:CL:80:LEU:HG    | 1.92        | 0.50     |
| 44:BQ:109:VAL:CG1 | 44:BQ:113:LYS:HE3  | 2.40        | 0.50     |
| 24:BI:29:GLN:HA   | 24:BI:29:GLN:HE21  | 1.76        | 0.50     |
| 27:BK:98:ARG:N    | 27:BK:98:ARG:HE    | 2.09        | 0.50     |
| 1:AA:82:G:C6      | 1:AA:88:U:O2       | 2.65        | 0.50     |
| 8:AI:117:LEU:HB3  | 8:AI:122:ARG:O     | 2.12        | 0.50     |
| 8:AI:123:ARG:HB3  | 8:AI:123:ARG:NH1   | 2.26        | 0.50     |
| 26:BD:138:LEU:N   | 26:BD:138:LEU:HD22 | 2.26        | 0.50     |
| 1:CA:194:C:O2'    | 1:CA:195:A:H5'     | 2.11        | 0.50     |
| 23:DB:857:G:O2'   | 23:DB:858:G:H5'    | 2.10        | 0.50     |
| 23:BB:718:A:H5'   | 23:BB:719:C:C5     | 2.46        | 0.50     |
| 23:BB:2318:G:C6   | 23:BB:2319:G:N1    | 2.80        | 0.50     |
| 23:DB:2592:G:H2'  | 23:DB:2593:U:O4'   | 2.11        | 0.50     |
| 39:DX:10:SER:HA   | 39:DX:57:LEU:HD13  | 1.93        | 0.50     |
| 23:DB:1203:U:H3'  | 23:DB:1204:A:H5''  | 1.92        | 0.50     |
| 1:CA:1523:G:O2'   | 1:CA:1524:C:H5'    | 2.12        | 0.50     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 3:CD:2:ARG:HB3    | 3:CD:114:ARG:NH2   | 2.26        | 0.50     |
| 2:AC:86:LEU:O     | 2:AC:90:VAL:HG23   | 2.11        | 0.50     |
| 23:BB:2461:A:H2'  | 23:BB:2462:C:H6    | 1.76        | 0.50     |
| 19:CT:79:THR:O    | 19:CT:82:ILE:HG12  | 2.11        | 0.50     |
| 11:CL:79:ILE:HD12 | 11:CL:96:THR:CG2   | 2.42        | 0.50     |
| 14:AO:7:ALA:O     | 14:AO:11:ILE:HG22  | 2.12        | 0.50     |
| 28:DP:25:VAL:HA   | 28:DP:85:VAL:HA    | 1.94        | 0.50     |
| 41:BJ:114:LEU:O   | 41:BJ:117:ALA:HB3  | 2.11        | 0.50     |
| 1:AA:1308:U:H3'   | 12:AM:97:ARG:NH1   | 2.27        | 0.50     |
| 23:DB:1561:C:H2'  | 23:DB:1562:U:C6    | 2.45        | 0.50     |
| 50:BT:48:GLN:NE2  | 50:BT:48:GLN:HA    | 2.27        | 0.50     |
| 23:DB:231:A:H3'   | 23:DB:232:G:H8     | 1.76        | 0.50     |
| 1:CA:1040:U:O2'   | 1:CA:1041:G:H5'    | 2.12        | 0.50     |
| 41:DJ:99:ARG:O    | 41:DJ:103:ILE:HG13 | 2.11        | 0.50     |
| 25:BC:42:ARG:HD2  | 25:BC:48:ILE:HG12  | 1.94        | 0.50     |
| 23:BB:2648:G:H2'  | 23:BB:2649:C:C6    | 2.47        | 0.50     |
| 23:BB:950:G:H2'   | 23:BB:951:C:H6     | 1.75        | 0.50     |
| 23:BB:1011:G:O2'  | 23:BB:1013:C:H5''  | 2.12        | 0.50     |
| 23:DB:598:U:H2'   | 23:DB:599:A:C8     | 2.47        | 0.50     |
| 26:DD:174:SER:O   | 26:DD:175:LEU:HB2  | 2.10        | 0.50     |
| 44:BQ:32:ARG:O    | 44:BQ:36:GLN:HG3   | 2.12        | 0.50     |
| 46:BU:13:LEU:HD12 | 46:BU:13:LEU:H     | 1.77        | 0.50     |
| 43:BO:97:PHE:HB3  | 43:BO:103:VAL:HG21 | 1.94        | 0.50     |
| 42:DN:54:LEU:HD11 | 42:DN:62:ASN:HB3   | 1.94        | 0.50     |
| 48:BG:59:ASP:O    | 48:BG:63:GLN:HB2   | 2.12        | 0.50     |
| 44:BQ:42:GLY:HA3  | 49:BR:75:VAL:HG21  | 1.93        | 0.50     |
| 44:BQ:2:ARG:HG3   | 44:BQ:3:VAL:H      | 1.76        | 0.50     |
| 23:DB:796:C:H2'   | 23:DB:797:G:C8     | 2.47        | 0.50     |
| 23:BB:2151:U:H2'  | 23:BB:2152:G:H8    | 1.77        | 0.50     |
| 1:CA:652:U:H1'    | 1:CA:653:U:C6      | 2.46        | 0.50     |
| 23:BB:841:G:O2'   | 23:BB:842:U:H5'    | 2.12        | 0.50     |
| 49:DR:84:ARG:HG3  | 49:DR:84:ARG:HH21  | 1.76        | 0.50     |
| 43:BO:81:ARG:HD3  | 43:BO:81:ARG:H     | 1.75        | 0.50     |
| 1:AA:179:A:H2'    | 1:AA:180:U:O4'     | 2.12        | 0.50     |
| 46:DU:51:LEU:O    | 46:DU:52:ASN:HB2   | 2.11        | 0.50     |
| 40:BH:25:TYR:O    | 40:BH:30:LEU:HG    | 2.11        | 0.50     |
| 40:DH:114:GLU:HG3 | 40:DH:133:GLN:O    | 2.12        | 0.50     |
| 48:BG:85:LYS:HA   | 48:BG:131:VAL:HG12 | 1.93        | 0.50     |
| 53:D6:38:LEU:HB3  | 53:D6:58:VAL:HG21  | 1.93        | 0.50     |
| 23:DB:637:A:P     | 37:DL:112:LEU:HD22 | 2.52        | 0.50     |
| 13:CN:63:CYS:HB3  | 13:CN:67:GLY:N     | 2.27        | 0.50     |
| 1:CA:981:U:C4'    | 13:CN:60:ARG:HD2   | 2.32        | 0.50     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:336:C:O2'   | 23:BB:337:C:H5'    | 2.11        | 0.50     |
| 23:BB:1240:U:O2'  | 23:BB:1241:A:H5'   | 2.11        | 0.50     |
| 42:BN:76:VAL:HA   | 42:BN:79:LEU:HD12  | 1.92        | 0.50     |
| 24:DI:57:VAL:HG23 | 24:DI:71:LYS:NZ    | 2.26        | 0.50     |
| 47:BF:79:ARG:HE   | 47:BF:79:ARG:N     | 2.08        | 0.50     |
| 1:AA:865:A:H5'    | 1:AA:1078:U:C4     | 2.45        | 0.50     |
| 1:CA:955:U:H1'    | 1:CA:1227:A:N6     | 2.27        | 0.50     |
| 11:AL:41:PRO:HB2  | 11:AL:88:ASP:HB3   | 1.94        | 0.50     |
| 40:BH:108:VAL:CG1 | 40:BH:109:GLU:H    | 2.18        | 0.50     |
| 1:AA:332:G:OP2    | 19:AT:4:LYS:HB2    | 2.12        | 0.50     |
| 13:CN:53:ASP:HA   | 13:CN:58:ARG:HD2   | 1.93        | 0.50     |
| 43:BO:49:VAL:HG11 | 43:BO:82:ALA:CA    | 2.41        | 0.50     |
| 29:DE:188:MET:HG2 | 29:DE:193:VAL:HG22 | 1.92        | 0.50     |
| 30:BY:2:LYS:CD    | 30:BY:2:LYS:H      | 2.21        | 0.50     |
| 23:DB:2073:C:C5'  | 25:DC:227:VAL:HG12 | 2.42        | 0.50     |
| 23:BB:1726:C:H2'  | 23:BB:1727:C:C6    | 2.47        | 0.50     |
| 23:DB:277:G:O2'   | 23:DB:278:A:N7     | 2.43        | 0.50     |
| 2:AC:183:TYR:HE1  | 2:AC:198:LYS:HB3   | 1.76        | 0.50     |
| 21:AU:10:PRO:CB   | 2:CC:71:ARG:HE     | 2.24        | 0.50     |
| 23:BB:1793:C:H2'  | 23:BB:1794:A:H8    | 1.77        | 0.50     |
| 41:BJ:96:ARG:CZ   | 41:BJ:99:ARG:HD2   | 2.42        | 0.50     |
| 23:DB:2590:A:H2'  | 23:DB:2591:C:H6    | 1.75        | 0.50     |
| 41:BJ:109:LEU:CD1 | 41:BJ:119:PHE:HB2  | 2.42        | 0.50     |
| 1:AA:857:C:H2'    | 1:AA:858:G:O4'     | 2.12        | 0.50     |
| 23:BB:378:C:O2'   | 23:BB:379:G:H5'    | 2.11        | 0.50     |
| 52:DW:46:ALA:HB2  | 52:DW:78:PHE:CD1   | 2.46        | 0.50     |
| 20:AB:128:LEU:CD1 | 20:AB:129:THR:H    | 2.25        | 0.50     |
| 1:CA:1063:C:H2'   | 1:CA:1064:G:C8     | 2.46        | 0.50     |
| 23:BB:1508:A:H5'  | 23:BB:1509:A:C6    | 2.47        | 0.50     |
| 43:BO:102:ARG:O   | 43:BO:106:LEU:HD23 | 2.11        | 0.50     |
| 53:B6:2:THR:HG23  | 53:B6:5:GLU:OE1    | 2.11        | 0.50     |
| 20:AB:71:THR:HG23 | 20:AB:94:ARG:H     | 1.77        | 0.50     |
| 23:BB:1536:C:H4'  | 23:BB:1537:G:C4    | 2.46        | 0.50     |
| 3:CD:149:LYS:HB2  | 3:CD:177:MET:HG3   | 1.92        | 0.50     |
| 1:CA:611:C:H2'    | 1:CA:612:C:C6      | 2.46        | 0.50     |
| 23:DB:902:C:H2'   | 23:DB:903:C:C6     | 2.47        | 0.50     |
| 23:BB:2526:G:O2'  | 32:B4:1:MET:HB2    | 2.12        | 0.50     |
| 5:CF:18:VAL:HG11  | 5:CF:58:HIS:NE2    | 2.27        | 0.50     |
| 31:B0:33:SER:OG   | 31:B0:35:GLU:HG2   | 2.11        | 0.50     |
| 23:DB:108:G:H2'   | 23:DB:109:C:H6     | 1.76        | 0.50     |
| 23:DB:77:G:H2'    | 23:DB:78:U:O4'     | 2.12        | 0.50     |
| 24:DI:5:GLN:HB2   | 24:DI:30:GLN:OE1   | 2.12        | 0.50     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 20:AB:93:HIS:HB2  | 20:AB:145:ASN:O   | 2.11        | 0.50     |
| 1:CA:1234:C:O2'   | 1:CA:1235:U:H5'   | 2.11        | 0.50     |
| 23:BB:1842:G:H2'  | 23:BB:1843:C:H6   | 1.76        | 0.50     |
| 23:BB:1295:C:H2'  | 23:BB:1296:G:H8   | 1.76        | 0.50     |
| 1:AA:652:U:H1'    | 1:AA:653:U:C6     | 2.46        | 0.50     |
| 23:DB:2436:G:O2'  | 23:DB:2437:G:H5'  | 2.12        | 0.50     |
| 31:B0:5:ASN:O     | 31:B0:7:PRO:HD3   | 2.11        | 0.50     |
| 1:AA:1407:C:O2'   | 23:BB:1912:A:N1   | 2.41        | 0.50     |
| 23:DB:458:G:N2    | 23:DB:469:G:H2'   | 2.26        | 0.50     |
| 23:BB:208:C:H2'   | 23:BB:209:C:H6    | 1.76        | 0.50     |
| 1:AA:233:C:O2'    | 1:AA:234:C:H5'    | 2.11        | 0.50     |
| 3:AD:87:GLU:OE1   | 3:AD:91:ALA:HB2   | 2.11        | 0.50     |
| 52:BW:36:ILE:HB   | 52:BW:39:GLN:NE2  | 2.26        | 0.50     |
| 8:AI:22:PRO:HA    | 8:AI:60:LEU:HB3   | 1.93        | 0.50     |
| 47:DF:74:ALA:HB1  | 47:DF:76:PHE:CD2  | 2.46        | 0.50     |
| 43:DO:36:TYR:N    | 43:DO:36:TYR:CD2  | 2.80        | 0.50     |
| 30:DY:51:SER:C    | 30:DY:53:MET:H    | 2.13        | 0.50     |
| 50:BT:39:THR:O    | 50:BT:40:LYS:HB2  | 2.12        | 0.50     |
| 30:BY:51:SER:C    | 30:BY:53:MET:H    | 2.13        | 0.50     |
| 9:CJ:53:ILE:HG23  | 9:CJ:54:SER:H     | 1.75        | 0.50     |
| 45:DS:47:VAL:HG12 | 45:DS:103:ILE:CG2 | 2.41        | 0.50     |
| 45:DS:15:GLN:HA   | 45:DS:18:ARG:CG   | 2.42        | 0.50     |
| 23:DB:1022:G:N2   | 23:DB:1142:A:N1   | 2.60        | 0.50     |
| 1:CA:1079:G:H5''  | 4:CE:49:TYR:HE2   | 1.74        | 0.50     |
| 23:BB:2869:G:H2'  | 23:BB:2870:C:C6   | 2.47        | 0.50     |
| 43:DO:49:VAL:HG11 | 43:DO:82:ALA:CA   | 2.42        | 0.50     |
| 29:DE:28:VAL:O    | 29:DE:32:VAL:HG13 | 2.11        | 0.50     |
| 23:BB:2465:C:O2'  | 23:BB:2466:C:H5'  | 2.12        | 0.50     |
| 13:AN:12:ARG:HG2  | 13:AN:53:ASP:HB3  | 1.94        | 0.50     |
| 23:BB:1199:U:H5'  | 44:BQ:4:LYS:HD3   | 1.93        | 0.50     |
| 20:CB:16:GLY:HA3  | 20:CB:39:ILE:HA   | 1.94        | 0.50     |
| 11:CL:81:ILE:HG23 | 11:CL:94:TYR:HB3  | 1.92        | 0.50     |
| 29:BE:173:THR:C   | 29:BE:175:ILE:H   | 2.15        | 0.50     |
| 26:DD:9:VAL:O     | 26:DD:9:VAL:HG13  | 2.11        | 0.50     |
| 23:BB:1439:A:N7   | 23:BB:1440:U:C6   | 2.80        | 0.50     |
| 43:BO:2:ASP:OD2   | 43:BO:4:LYS:HB3   | 2.12        | 0.50     |
| 23:BB:2821:A:OP2  | 42:BN:3:HIS:NE2   | 2.45        | 0.50     |
| 12:AM:89:ARG:HD3  | 12:AM:95:PRO:O    | 2.12        | 0.50     |
| 42:DN:24:MET:SD   | 42:DN:44:LEU:HD22 | 2.52        | 0.50     |
| 3:AD:192:ALA:C    | 3:AD:194:ILE:H    | 2.13        | 0.50     |
| 23:DB:155:A:H2'   | 23:DB:156:A:H8    | 1.77        | 0.50     |
| 23:DB:118:A:OP2   | 23:DB:119:A:H5''  | 2.11        | 0.50     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 39:DX:51:ALA:O     | 39:DX:55:THR:N     | 2.41        | 0.50     |
| 23:DB:1874:C:H2'   | 23:DB:1875:G:O4'   | 2.11        | 0.50     |
| 23:DB:702:U:H2'    | 23:DB:703:U:C6     | 2.46        | 0.50     |
| 39:BX:41:HIS:O     | 39:BX:44:LYS:HB3   | 2.12        | 0.50     |
| 19:CT:71:ALA:O     | 19:CT:74:HIS:HB2   | 2.12        | 0.50     |
| 1:CA:214:C:H2'     | 1:CA:215:C:H6      | 1.77        | 0.50     |
| 23:BB:5:A:H2'      | 23:BB:6:A:H8       | 1.73        | 0.50     |
| 22:DA:46:A:H2'     | 22:DA:47:C:O4'     | 2.12        | 0.50     |
| 23:DB:1327:A:H2'   | 23:DB:1328:A:O4'   | 2.11        | 0.50     |
| 23:BB:1350:C:H5'   | 23:BB:1351:C:OP2   | 2.12        | 0.50     |
| 1:CA:585:G:H2'     | 1:CA:586:C:H6      | 1.77        | 0.50     |
| 24:BI:124:MET:O    | 24:BI:128:ILE:HG12 | 2.12        | 0.50     |
| 23:DB:289:G:H2'    | 23:DB:290:U:H6     | 1.76        | 0.50     |
| 23:DB:600:G:H1'    | 29:DE:100:MET:HG2  | 1.94        | 0.50     |
| 29:DE:97:ASN:ND2   | 29:DE:100:MET:HG3  | 2.27        | 0.50     |
| 23:DB:1465:G:H2'   | 23:DB:1466:U:C6    | 2.47        | 0.50     |
| 23:BB:1251:C:O2'   | 23:BB:1252:G:H3'   | 2.11        | 0.50     |
| 1:AA:1234:C:H1'    | 1:AA:1364:U:O2     | 2.12        | 0.50     |
| 23:DB:796:C:H2'    | 23:DB:797:G:H8     | 1.77        | 0.50     |
| 23:DB:217:A:H2'    | 23:DB:218:A:O4'    | 2.12        | 0.50     |
| 1:CA:986:U:H2'     | 1:CA:987:G:O4'     | 2.12        | 0.50     |
| 37:DL:119:PRO:HA   | 37:DL:138:ALA:O    | 2.11        | 0.50     |
| 1:AA:742:G:H2'     | 1:AA:743:A:H8      | 1.77        | 0.50     |
| 1:CA:113:G:O4'     | 1:CA:354:G:H4'     | 2.11        | 0.50     |
| 23:DB:2639:A:H2'   | 23:DB:2640:G:O4'   | 2.11        | 0.50     |
| 44:DQ:45:ALA:O     | 44:DQ:49:ARG:N     | 2.42        | 0.50     |
| 1:AA:124:C:O2'     | 1:AA:125:U:H5'     | 2.12        | 0.50     |
| 28:DP:61:ARG:HH21  | 28:DP:61:ARG:HB3   | 1.77        | 0.50     |
| 23:DB:1711:A:O2'   | 23:DB:1712:U:H5'   | 2.12        | 0.50     |
| 23:BB:1345:C:H5'   | 23:BB:1396:U:C5    | 2.47        | 0.50     |
| 9:CJ:67:ILE:HA     | 13:CN:94:GLY:O     | 2.12        | 0.50     |
| 29:DE:88:ARG:HG3   | 29:DE:88:ARG:HH21  | 1.76        | 0.50     |
| 3:AD:43:ARG:HB3    | 3:AD:43:ARG:HH11   | 1.77        | 0.50     |
| 31:D0:5:ASN:O      | 31:D0:7:PRO:HD3    | 2.12        | 0.50     |
| 23:DB:1663:G:H3'   | 57:DB:3246:HOH:O   | 2.11        | 0.50     |
| 46:DU:13:LEU:H     | 46:DU:13:LEU:HD12  | 1.76        | 0.50     |
| 46:DU:14:THR:O     | 46:DU:18:LYS:HG2   | 2.12        | 0.50     |
| 52:BW:49:ASN:HA    | 52:BW:61:LYS:HB2   | 1.94        | 0.50     |
| 25:DC:134:ILE:HG13 | 25:DC:134:ILE:O    | 2.08        | 0.50     |
| 21:CU:40:PRO:C     | 21:CU:42:THR:H     | 2.15        | 0.50     |
| 53:D6:58:VAL:HG22  | 53:D6:68:VAL:HG13  | 1.93        | 0.50     |
| 44:DQ:57:ARG:HG2   | 44:DQ:57:ARG:NH1   | 2.25        | 0.50     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 8:AI:19:PHE:O      | 8:AI:62:LEU:HA     | 2.12        | 0.50     |
| 1:CA:1494:G:H5'    | 23:DB:1913:A:N6    | 2.27        | 0.50     |
| 23:BB:144:A:H2'    | 23:BB:145:C:C6     | 2.47        | 0.50     |
| 7:AH:100:ILE:HD11  | 7:AH:128:VAL:HB    | 1.92        | 0.50     |
| 13:CN:9:GLU:HB2    | 13:CN:62:ARG:NE    | 2.27        | 0.50     |
| 23:BB:986:C:O2'    | 23:BB:987:C:H5'    | 2.12        | 0.50     |
| 3:AD:157:ALA:O     | 3:AD:160:LEU:HD22  | 2.12        | 0.50     |
| 29:BE:134:LEU:O    | 29:BE:138:LEU:HG   | 2.12        | 0.50     |
| 45:DS:47:VAL:HG12  | 45:DS:103:ILE:HG21 | 1.94        | 0.50     |
| 47:DF:137:PHE:O    | 47:DF:139:GLU:N    | 2.44        | 0.50     |
| 35:BV:79:ARG:NH1   | 38:BM:134:THR:HG21 | 2.26        | 0.50     |
| 1:CA:1078:U:H2'    | 1:CA:1079:G:O4'    | 2.12        | 0.50     |
| 41:DJ:81:ILE:HG12  | 41:DJ:82:GLY:N     | 2.26        | 0.50     |
| 9:CJ:57:VAL:HG22   | 9:CJ:58:ASN:N      | 2.21        | 0.50     |
| 28:DP:92:ARG:HG2   | 28:DP:92:ARG:O     | 2.10        | 0.50     |
| 22:DA:106:G:H2'    | 22:DA:107:G:C8     | 2.47        | 0.50     |
| 23:BB:969:G:H2'    | 23:BB:970:U:C6     | 2.47        | 0.50     |
| 38:DM:2:LEU:CD2    | 38:DM:46:ILE:HD11  | 2.42        | 0.50     |
| 1:CA:437:U:H4'     | 3:CD:153:ARG:NH1   | 2.27        | 0.50     |
| 1:CA:312:C:H2'     | 1:CA:313:A:C8      | 2.47        | 0.50     |
| 34:D3:21:PHE:CE1   | 34:D3:58:ILE:HG12  | 2.47        | 0.50     |
| 23:BB:2652:C:H2'   | 23:BB:2653:U:O4'   | 2.11        | 0.50     |
| 20:AB:96:LEU:N     | 20:AB:99:MET:HE3   | 2.25        | 0.50     |
| 51:DZ:14:THR:HA    | 51:DZ:28:ARG:CA    | 2.42        | 0.50     |
| 1:CA:925:G:C2      | 1:CA:927:G:C8      | 3.00        | 0.50     |
| 23:DB:2074:U:O2'   | 23:DB:2075:U:H5'   | 2.12        | 0.50     |
| 23:BB:2241:A:H2'   | 23:BB:2242:G:H8    | 1.76        | 0.50     |
| 1:AA:264:C:H4'     | 16:AQ:64:ARG:HD2   | 1.92        | 0.50     |
| 23:BB:649:G:H2'    | 23:BB:650:C:H6     | 1.77        | 0.50     |
| 23:BB:155:A:H2'    | 23:BB:156:A:H8     | 1.77        | 0.50     |
| 37:DL:4:ASN:HD22   | 37:DL:4:ASN:N      | 2.10        | 0.50     |
| 1:AA:401:C:H2'     | 1:AA:402:G:C8      | 2.47        | 0.50     |
| 20:CB:87:ASP:HB2   | 20:CB:224:ARG:CZ   | 2.42        | 0.50     |
| 20:CB:94:ARG:HD2   | 20:CB:142:LYS:HE2  | 1.93        | 0.50     |
| 20:CB:172:ILE:HG23 | 20:CB:182:VAL:HG11 | 1.94        | 0.50     |
| 10:AK:16:SER:HA    | 10:AK:77:GLY:O     | 2.12        | 0.50     |
| 9:AJ:92:LEU:HD13   | 9:AJ:92:LEU:N      | 2.27        | 0.50     |
| 1:AA:502:A:H2'     | 1:AA:503:C:H6      | 1.76        | 0.50     |
| 50:DT:32:LEU:N     | 50:DT:83:ALA:HB3   | 2.26        | 0.50     |
| 26:DD:133:THR:HG23 | 26:DD:134:HIS:N    | 2.27        | 0.50     |
| 23:DB:6:A:H2'      | 23:DB:7:G:C8       | 2.45        | 0.50     |
| 23:BB:2439:A:C8    | 23:BB:2586:U:H4'   | 2.46        | 0.50     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 29:BE:102:ARG:O   | 29:BE:106:LYS:HG3  | 2.12        | 0.50     |
| 4:AE:87:VAL:HG22  | 4:AE:88:HIS:N      | 2.27        | 0.50     |
| 3:CD:145:ARG:HB3  | 3:CD:147:LYS:HD2   | 1.93        | 0.50     |
| 23:DB:1053:C:H2'  | 23:DB:1054:A:H5'   | 1.94        | 0.50     |
| 17:AR:56:ARG:O    | 17:AR:60:ARG:HG2   | 2.12        | 0.50     |
| 1:CA:1426:G:O2'   | 1:CA:1427:C:H5'    | 2.12        | 0.50     |
| 10:CK:63:GLN:HG3  | 10:CK:98:ALA:HB2   | 1.93        | 0.50     |
| 1:AA:911:U:H2'    | 1:AA:912:C:C6      | 2.46        | 0.50     |
| 1:AA:49:U:O2'     | 1:AA:50:A:H2'      | 2.11        | 0.50     |
| 23:BB:2655:G:O2'  | 23:BB:2656:U:P     | 2.70        | 0.50     |
| 23:BB:2655:G:HO2' | 23:BB:2656:U:P     | 2.35        | 0.50     |
| 25:DC:222:THR:HA  | 25:DC:231:HIS:O    | 2.11        | 0.50     |
| 23:BB:2573:C:H3'  | 57:BB:3613:HOH:O   | 2.10        | 0.50     |
| 23:DB:2007:U:O2'  | 23:DB:2008:C:H5'   | 2.12        | 0.50     |
| 6:AG:30:MET:HG2   | 6:AG:31:VAL:N      | 2.26        | 0.50     |
| 5:AF:32:ALA:O     | 5:AF:33:GLU:HB2    | 2.12        | 0.50     |
| 46:BU:51:LEU:O    | 46:BU:52:ASN:HB2   | 2.11        | 0.50     |
| 23:DB:2203:U:C2'  | 23:DB:2204:G:OP2   | 2.60        | 0.50     |
| 41:BJ:133:ALA:C   | 41:BJ:135:GLN:H    | 2.16        | 0.50     |
| 10:AK:126:ARG:HB2 | 21:AU:33:ARG:CD    | 2.42        | 0.49     |
| 23:DB:946:C:H2'   | 23:DB:947:A:C8     | 2.46        | 0.49     |
| 44:DQ:16:ILE:O    | 44:DQ:18:LYS:N     | 2.43        | 0.49     |
| 48:DG:10:VAL:HG21 | 48:DG:49:LEU:HD13  | 1.94        | 0.49     |
| 37:DL:90:VAL:CB   | 37:DL:122:VAL:HG12 | 2.42        | 0.49     |
| 48:DG:84:LYS:HG2  | 48:DG:85:LYS:N     | 2.25        | 0.49     |
| 40:BH:77:THR:CG2  | 40:BH:79:THR:HG23  | 2.41        | 0.49     |
| 26:DD:193:VAL:HB  | 26:DD:194:PRO:HD2  | 1.94        | 0.49     |
| 1:AA:1220:G:H21   | 18:AS:53:GLY:HA2   | 1.76        | 0.49     |
| 23:DB:143:C:H2'   | 23:DB:144:A:C8     | 2.47        | 0.49     |
| 1:CA:598:U:H4'    | 7:CH:85:TYR:CG     | 2.47        | 0.49     |
| 23:BB:77:G:H2'    | 23:BB:78:U:O4'     | 2.12        | 0.49     |
| 24:DI:11:GLN:HA   | 24:DI:55:PRO:HA    | 1.93        | 0.49     |
| 47:BF:43:ILE:HG23 | 47:BF:44:ALA:N     | 2.15        | 0.49     |
| 29:BE:146:VAL:O   | 29:BE:167:VAL:HA   | 2.12        | 0.49     |
| 40:DH:125:THR:HA  | 40:DH:146:VAL:CB   | 2.40        | 0.49     |
| 40:DH:83:LYS:O    | 40:DH:90:LEU:HA    | 2.12        | 0.49     |
| 1:AA:865:A:H2'    | 1:AA:866:C:C6      | 2.47        | 0.49     |
| 23:DB:2809:A:H2'  | 23:DB:2810:A:C8    | 2.47        | 0.49     |
| 24:DI:23:VAL:HG12 | 24:DI:27:LEU:HD21  | 1.94        | 0.49     |
| 1:AA:1237:C:H3'   | 1:AA:1238:A:H5'    | 1.93        | 0.49     |
| 15:CP:67:ILE:HG23 | 15:CP:67:ILE:O     | 2.12        | 0.49     |
| 23:BB:729:G:C5    | 25:BC:206:LYS:HB2  | 2.47        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:DD:141:ARG:O   | 26:DD:141:ARG:HG3 | 2.11        | 0.49     |
| 24:DI:19:PRO:HB2  | 24:DI:22:PRO:HD2  | 1.94        | 0.49     |
| 3:CD:154:VAL:HG23 | 3:CD:155:LYS:HD2  | 1.94        | 0.49     |
| 49:BR:39:LEU:HB2  | 49:BR:49:ILE:HG12 | 1.94        | 0.49     |
| 6:CG:144:ALA:O    | 6:CG:145:GLU:HB3  | 2.12        | 0.49     |
| 26:DD:68:PHE:C    | 26:DD:73:VAL:HB   | 2.33        | 0.49     |
| 47:DF:163:GLU:HA  | 47:DF:166:ARG:HD3 | 1.93        | 0.49     |
| 1:CA:325:A:H2'    | 1:CA:326:G:O4'    | 2.12        | 0.49     |
| 28:DP:94:ALA:C    | 28:DP:95:LYS:HD2  | 2.32        | 0.49     |
| 28:BP:88:ARG:HB2  | 28:BP:112:ARG:NH1 | 2.26        | 0.49     |
| 40:BH:18:GLN:HE21 | 40:BH:44:ILE:HG21 | 1.74        | 0.49     |
| 1:AA:190:A:O5'    | 1:AA:190:A:H8     | 1.95        | 0.49     |
| 40:BH:47:PHE:CA   | 40:BH:50:ARG:HH21 | 2.24        | 0.49     |
| 23:BB:2191:A:H2'  | 23:BB:2192:U:O4'  | 2.12        | 0.49     |
| 2:CC:46:LEU:HB3   | 2:CC:49:ALA:HB3   | 1.93        | 0.49     |
| 42:BN:12:ARG:HG2  | 42:BN:16:HIS:HB2  | 1.94        | 0.49     |
| 1:CA:769:G:H4'    | 1:CA:1513:A:H4'   | 1.94        | 0.49     |
| 27:BK:2:ILE:HD12  | 27:BK:2:ILE:N     | 2.27        | 0.49     |
| 23:BB:956:G:OP2   | 38:BM:86:LYS:HE2  | 2.11        | 0.49     |
| 1:CA:1277:C:O2'   | 1:CA:1279:G:H8    | 1.95        | 0.49     |
| 23:BB:1535:A:H5'' | 23:BB:1536:C:H5   | 1.77        | 0.49     |
| 23:BB:1537:G:H5'' | 23:BB:1537:G:N3   | 2.27        | 0.49     |
| 12:CM:43:LYS:O    | 12:CM:46:GLU:HG3  | 2.11        | 0.49     |
| 41:DJ:89:PHE:CE1  | 41:DJ:93:ILE:HD13 | 2.47        | 0.49     |
| 23:DB:2677:G:H2'  | 23:DB:2678:C:H6   | 1.78        | 0.49     |
| 1:AA:693:G:H2'    | 1:AA:694:A:O4'    | 2.11        | 0.49     |
| 10:AK:52:ARG:NH1  | 10:AK:53:GLY:H    | 2.09        | 0.49     |
| 9:AJ:80:THR:HG21  | 9:AJ:82:LYS:NZ    | 2.27        | 0.49     |
| 23:BB:949:G:O2'   | 23:BB:950:G:H5'   | 2.12        | 0.49     |
| 23:DB:600:G:H2'   | 23:DB:601:C:C6    | 2.46        | 0.49     |
| 17:CR:61:ALA:HB3  | 17:CR:67:LEU:HD12 | 1.93        | 0.49     |
| 23:BB:1846:G:H2'  | 23:BB:1847:A:O4'  | 2.12        | 0.49     |
| 23:BB:1153:C:H2'  | 23:BB:1154:G:O4'  | 2.12        | 0.49     |
| 1:CA:90:C:H2'     | 1:CA:91:U:C6      | 2.47        | 0.49     |
| 23:DB:132:G:H2'   | 23:DB:133:U:H6    | 1.77        | 0.49     |
| 23:DB:2419:U:H2'  | 23:DB:2420:C:C6   | 2.46        | 0.49     |
| 1:CA:1423:G:H2'   | 1:CA:1424:U:H6    | 1.77        | 0.49     |
| 28:BP:62:LYS:HE3  | 28:BP:64:SER:OG   | 2.12        | 0.49     |
| 28:DP:8:GLU:HG2   | 28:DP:54:LEU:HD23 | 1.94        | 0.49     |
| 33:D1:29:LYS:N    | 33:D1:30:PRO:HD3  | 2.27        | 0.49     |
| 36:D2:13:ASN:O    | 36:D2:17:GLY:N    | 2.45        | 0.49     |
| 23:DB:730:A:O2'   | 23:DB:731:C:H5'   | 2.11        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:208:U:H6     | 1:CA:208:U:O5'    | 1.95        | 0.49     |
| 6:AG:121:ASN:N    | 6:AG:121:ASN:HD22 | 2.07        | 0.49     |
| 4:AE:42:ASN:O     | 4:AE:75:LEU:HD12  | 2.12        | 0.49     |
| 23:BB:1230:A:H2'  | 23:BB:1231:U:C6   | 2.46        | 0.49     |
| 44:DQ:96:ASP:C    | 44:DQ:98:ALA:N    | 2.65        | 0.49     |
| 1:AA:1148:U:H5'   | 8:AI:6:TYR:OH     | 2.12        | 0.49     |
| 26:DD:3:GLY:C     | 26:DD:4:LEU:HD22  | 2.32        | 0.49     |
| 1:AA:597:G:H2'    | 1:AA:598:U:H5'    | 1.94        | 0.49     |
| 42:DN:38:LEU:HD11 | 42:DN:42:LYS:HD2  | 1.94        | 0.49     |
| 39:BX:28:LEU:HB3  | 39:BX:43:LEU:HD21 | 1.93        | 0.49     |
| 41:BJ:42:ALA:O    | 41:BJ:44:TYR:N    | 2.45        | 0.49     |
| 42:BN:52:ILE:HD13 | 42:BN:87:PHE:CD2  | 2.47        | 0.49     |
| 1:AA:1076:U:H2'   | 1:AA:1077:G:C8    | 2.48        | 0.49     |
| 1:CA:1225:A:H5'   | 1:CA:1226:C:OP2   | 2.12        | 0.49     |
| 18:CS:42:ASN:H    | 18:CS:42:ASN:HD22 | 1.60        | 0.49     |
| 18:AS:61:VAL:HG12 | 18:AS:62:THR:N    | 2.27        | 0.49     |
| 50:DT:39:THR:HG22 | 50:DT:42:GLU:CG   | 2.35        | 0.49     |
| 50:DT:85:VAL:C    | 50:DT:86:THR:HG23 | 2.33        | 0.49     |
| 23:BB:160:A:H2'   | 23:BB:161:A:C8    | 2.47        | 0.49     |
| 23:BB:2037:A:H2'  | 23:BB:2038:G:H8   | 1.77        | 0.49     |
| 28:DP:96:LEU:HB3  | 28:DP:99:LEU:HB2  | 1.94        | 0.49     |
| 13:CN:52:ARG:HG3  | 13:CN:53:ASP:N    | 2.27        | 0.49     |
| 1:AA:1287:A:H2'   | 1:AA:1288:A:C8    | 2.46        | 0.49     |
| 1:AA:1349:A:H2'   | 1:AA:1350:A:O4'   | 2.12        | 0.49     |
| 15:CP:6:LEU:HD23  | 15:CP:17:TYR:HB2  | 1.92        | 0.49     |
| 45:BS:66:ILE:N    | 45:BS:66:ILE:HD13 | 2.19        | 0.49     |
| 20:AB:33:ALA:HB2  | 20:AB:38:HIS:ND1  | 2.27        | 0.49     |
| 23:DB:1737:G:H5'  | 23:DB:1738:G:OP2  | 2.12        | 0.49     |
| 40:DH:4:ILE:HG21  | 40:DH:51:ARG:HH22 | 1.75        | 0.49     |
| 1:CA:1411:C:H2'   | 1:CA:1412:C:H6    | 1.77        | 0.49     |
| 1:CA:310:G:H5''   | 15:CP:31:ARG:HB2  | 1.94        | 0.49     |
| 23:DB:8:C:O2'     | 23:DB:9:G:H5'     | 2.11        | 0.49     |
| 23:DB:1439:A:N7   | 23:DB:1440:U:C2   | 2.80        | 0.49     |
| 11:AL:52:CYS:SG   | 11:AL:66:ILE:HD11 | 2.52        | 0.49     |
| 51:BZ:14:THR:HA   | 51:BZ:28:ARG:CA   | 2.40        | 0.49     |
| 2:CC:113:LYS:HE3  | 2:CC:117:ASP:OD1  | 2.12        | 0.49     |
| 23:DB:278:A:C8    | 23:DB:361:G:N1    | 2.80        | 0.49     |
| 46:DU:35:VAL:HB   | 46:DU:38:ILE:CB   | 2.41        | 0.49     |
| 7:CH:40:LYS:HA    | 7:CH:45:ILE:HG13  | 1.94        | 0.49     |
| 14:AO:16:GLY:HA2  | 14:AO:27:VAL:HG22 | 1.92        | 0.49     |
| 23:DB:1139:G:O2'  | 23:DB:1143:A:N1   | 2.41        | 0.49     |
| 1:CA:858:G:O6     | 1:CA:869:G:H3'    | 2.12        | 0.49     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 12:CM:5:GLY:O      | 12:CM:7:ASN:N      | 2.45        | 0.49     |
| 23:DB:704:G:C2'    | 23:DB:726:G:H22    | 2.24        | 0.49     |
| 6:AG:63:VAL:HA     | 6:AG:66:GLU:CD     | 2.33        | 0.49     |
| 23:DB:1407:G:H2'   | 23:DB:1408:G:C8    | 2.45        | 0.49     |
| 23:DB:544:C:H2'    | 23:DB:545:U:C5     | 2.47        | 0.49     |
| 2:CC:139:ASN:O     | 2:CC:143:LEU:HD23  | 2.12        | 0.49     |
| 23:BB:1184:U:O2'   | 23:BB:1185:G:H5'   | 2.11        | 0.49     |
| 34:B3:41:ARG:HG3   | 34:B3:44:ARG:NH2   | 2.27        | 0.49     |
| 1:CA:182:A:O2'     | 1:CA:183:C:H3'     | 2.12        | 0.49     |
| 13:AN:14:ALA:C     | 13:AN:18:LYS:HE2   | 2.33        | 0.49     |
| 22:BA:109:A:H2'    | 22:BA:110:C:H6     | 1.74        | 0.49     |
| 13:CN:14:ALA:C     | 13:CN:18:LYS:HE2   | 2.33        | 0.49     |
| 37:DL:135:ILE:HG23 | 37:DL:136:GLU:N    | 2.28        | 0.49     |
| 17:AR:31:TYR:CD1   | 17:AR:54:LEU:HD11  | 2.48        | 0.49     |
| 23:BB:1774:C:O2    | 23:BB:1774:C:H2'   | 2.11        | 0.49     |
| 46:DU:13:LEU:HA    | 46:DU:18:LYS:HD3   | 1.92        | 0.49     |
| 1:CA:1247:U:O2'    | 1:CA:1248:A:H5'    | 2.11        | 0.49     |
| 8:CI:44:ARG:HG2    | 8:CI:44:ARG:HH11   | 1.75        | 0.49     |
| 23:DB:2655:G:O2'   | 23:DB:2656:U:P     | 2.69        | 0.49     |
| 3:CD:22:SER:H      | 3:CD:109:THR:HG22  | 1.77        | 0.49     |
| 23:BB:857:G:O2'    | 23:BB:858:G:H5'    | 2.11        | 0.49     |
| 10:CK:14:GLN:HA    | 10:CK:76:TYR:O     | 2.12        | 0.49     |
| 37:DL:120:VAL:HG12 | 37:DL:121:THR:N    | 2.27        | 0.49     |
| 37:BL:122:VAL:HG23 | 37:BL:143:GLU:OE1  | 2.12        | 0.49     |
| 20:AB:209:VAL:HG23 | 20:AB:210:THR:N    | 2.28        | 0.49     |
| 23:DB:2315:G:H5'   | 47:DF:156:THR:HG21 | 1.95        | 0.49     |
| 47:DF:31:GLU:O     | 47:DF:32:LYS:HD3   | 2.11        | 0.49     |
| 23:DB:2352:A:C6    | 52:DW:30:VAL:HG11  | 2.47        | 0.49     |
| 8:CI:83:THR:OG1    | 8:CI:97:LEU:HD13   | 2.13        | 0.49     |
| 1:CA:1349:A:H2'    | 1:CA:1350:A:O4'    | 2.12        | 0.49     |
| 44:DQ:73:ILE:HD11  | 44:DQ:77:LYS:HB3   | 1.93        | 0.49     |
| 8:AI:41:GLU:C      | 8:AI:43:ALA:H      | 2.15        | 0.49     |
| 35:DV:62:THR:CB    | 35:DV:71:LYS:HG2   | 2.42        | 0.49     |
| 44:BQ:83:LYS:HZ1   | 44:BQ:87:VAL:HA    | 1.77        | 0.49     |
| 40:DH:77:THR:HG22  | 40:DH:143:ILE:CB   | 2.34        | 0.49     |
| 29:BE:115:GLN:O    | 29:BE:117:ARG:HG3  | 2.12        | 0.49     |
| 47:DF:133:GLU:HA   | 47:DF:150:GLY:CA   | 2.42        | 0.49     |
| 21:AU:24:LYS:HB3   | 21:AU:24:LYS:NZ    | 2.28        | 0.49     |
| 1:CA:1080:A:H4'    | 4:CE:20:VAL:HG13   | 1.94        | 0.49     |
| 1:CA:763:G:H2'     | 1:CA:764:C:H6      | 1.77        | 0.49     |
| 18:CS:47:THR:HA    | 18:CS:60:PHE:CD1   | 2.48        | 0.49     |
| 23:BB:2868:A:H2'   | 23:BB:2869:G:H8    | 1.77        | 0.49     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 28:BP:96:LEU:HB3  | 28:BP:99:LEU:HB2   | 1.94        | 0.49     |
| 23:BB:674:G:H2'   | 23:BB:804:A:H61    | 1.78        | 0.49     |
| 50:DT:27:SER:O    | 50:DT:28:ASN:HB3   | 2.12        | 0.49     |
| 29:BE:29:HIS:C    | 29:BE:32:VAL:HG22  | 2.33        | 0.49     |
| 2:AC:110:LEU:HD21 | 2:AC:140:ALA:O     | 2.13        | 0.49     |
| 23:BB:972:A:C3'   | 23:BB:973:A:H5''   | 2.39        | 0.49     |
| 23:DB:2379:G:H4'  | 43:DO:21:LEU:HD11  | 1.94        | 0.49     |
| 35:DV:26:PHE:HE2  | 35:DV:44:HIS:HA    | 1.77        | 0.49     |
| 1:AA:1337:G:H5''  | 1:AA:1338:G:OP1    | 2.12        | 0.49     |
| 1:AA:1340:A:H2'   | 1:AA:1341:U:O4'    | 2.12        | 0.49     |
| 39:DX:23:ARG:HA   | 39:DX:26:PHE:HB3   | 1.95        | 0.49     |
| 23:DB:2680:U:OP2  | 26:DD:114:LYS:HB3  | 2.12        | 0.49     |
| 3:AD:158:LEU:HA   | 3:AD:161:ALA:CB    | 2.43        | 0.49     |
| 26:DD:69:ALA:HA   | 26:DD:73:VAL:HB    | 1.92        | 0.49     |
| 23:DB:1446:C:H2'  | 23:DB:1447:C:C6    | 2.48        | 0.49     |
| 29:DE:126:VAL:CG2 | 29:DE:133:LEU:HB2  | 2.42        | 0.49     |
| 23:BB:188:G:OP1   | 51:BZ:14:THR:HG23  | 2.13        | 0.49     |
| 46:DU:35:VAL:O    | 46:DU:38:ILE:HG22  | 2.12        | 0.49     |
| 3:AD:169:TRP:NE1  | 3:AD:170:LEU:HD23  | 2.27        | 0.49     |
| 23:BB:2840:C:H2'  | 23:BB:2841:C:C6    | 2.48        | 0.49     |
| 23:BB:1583:A:OP2  | 23:BB:1583:A:H2    | 1.94        | 0.49     |
| 29:BE:46:GLN:HB3  | 29:BE:86:ALA:CA    | 2.42        | 0.49     |
| 33:B1:47:ILE:HD12 | 33:B1:47:ILE:N     | 2.27        | 0.49     |
| 5:AF:53:LYS:C     | 5:AF:54:LEU:HD22   | 2.32        | 0.49     |
| 5:AF:54:LEU:N     | 5:AF:54:LEU:HD13   | 2.26        | 0.49     |
| 23:DB:1484:U:H2'  | 23:DB:1485:U:H6    | 1.77        | 0.49     |
| 45:DS:96:ILE:O    | 45:DS:96:ILE:HG23  | 2.12        | 0.49     |
| 1:AA:67:C:H4'     | 1:AA:172:A:O4'     | 2.12        | 0.49     |
| 23:DB:2458:G:H1'  | 23:DB:2460:U:O4    | 2.12        | 0.49     |
| 23:DB:2461:A:H2'  | 23:DB:2462:C:H6    | 1.75        | 0.49     |
| 23:DB:1400:U:H2'  | 23:DB:1401:G:C8    | 2.47        | 0.49     |
| 10:CK:16:SER:HA   | 10:CK:77:GLY:O     | 2.12        | 0.49     |
| 42:BN:65:LEU:O    | 42:BN:68:ALA:HB3   | 2.12        | 0.49     |
| 53:D6:10:THR:O    | 53:D6:14:MET:HG3   | 2.13        | 0.49     |
| 40:BH:67:ALA:HB1  | 40:BH:70:GLU:HG2   | 1.93        | 0.49     |
| 23:BB:1351:C:H2'  | 23:BB:1352:U:O4'   | 2.12        | 0.49     |
| 23:BB:1917:U:O2'  | 23:BB:1918:A:H5'   | 2.11        | 0.49     |
| 23:DB:680:C:H2'   | 23:DB:681:G:C8     | 2.46        | 0.49     |
| 23:BB:2260:C:O2'  | 23:BB:2261:C:H5'   | 2.12        | 0.49     |
| 40:DH:41:LYS:HA   | 40:DH:44:ILE:HG12  | 1.94        | 0.49     |
| 43:DO:102:ARG:O   | 43:DO:106:LEU:HD23 | 2.12        | 0.49     |
| 23:DB:2439:A:C8   | 23:DB:2586:U:H4'   | 2.48        | 0.49     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:169:C:O2'    | 1:CA:170:U:H5'     | 2.13        | 0.49     |
| 5:AF:18:VAL:O     | 5:AF:22:ILE:HG13   | 2.11        | 0.49     |
| 23:DB:303:G:H2'   | 23:DB:304:U:H6     | 1.78        | 0.49     |
| 23:DB:347:A:H2'   | 23:DB:348:A:H8     | 1.76        | 0.49     |
| 1:AA:821:G:H2'    | 1:AA:822:U:C6      | 2.48        | 0.49     |
| 17:AR:22:TYR:CE2  | 17:AR:23:LYS:HE3   | 2.47        | 0.49     |
| 1:AA:631:C:H5''   | 1:AA:632:U:O4'     | 2.12        | 0.49     |
| 23:BB:1037:G:O2'  | 23:BB:1038:G:H5'   | 2.12        | 0.49     |
| 23:BB:431:U:O2'   | 23:BB:432:A:H5'    | 2.13        | 0.49     |
| 23:BB:627:A:H4'   | 23:BB:628:G:OP1    | 2.12        | 0.49     |
| 23:DB:1414:C:H2'  | 23:DB:1415:U:H6    | 1.77        | 0.49     |
| 1:AA:1113:C:O2'   | 1:AA:1114:C:H5'    | 2.12        | 0.49     |
| 23:DB:1526:C:O2'  | 23:DB:1527:G:H5'   | 2.11        | 0.49     |
| 1:CA:124:C:O2'    | 1:CA:125:U:H5'     | 2.12        | 0.49     |
| 23:DB:2485:G:O2'  | 23:DB:2486:C:H5'   | 2.12        | 0.49     |
| 25:DC:80:LEU:HD11 | 25:DC:109:LEU:HG   | 1.94        | 0.49     |
| 21:CU:39:LYS:N    | 21:CU:40:PRO:CD    | 2.76        | 0.49     |
| 21:AU:39:LYS:N    | 21:AU:40:PRO:CD    | 2.76        | 0.49     |
| 20:AB:14:HIS:CD2  | 20:AB:202:ASN:H    | 2.30        | 0.49     |
| 53:D6:84:ARG:HH11 | 53:D6:92:PRO:HD2   | 1.78        | 0.49     |
| 40:BH:100:ALA:HA  | 40:BH:103:VAL:HG21 | 1.95        | 0.49     |
| 41:BJ:56:VAL:HG12 | 41:BJ:57:LEU:H     | 1.76        | 0.49     |
| 35:DV:56:PHE:O    | 35:DV:61:LEU:HD21  | 2.13        | 0.49     |
| 45:DS:1:MET:SD    | 45:DS:62:ASP:HB3   | 2.53        | 0.49     |
| 1:AA:598:U:H4'    | 7:AH:85:TYR:CG     | 2.47        | 0.49     |
| 30:DY:7:THR:HA    | 30:DY:34:THR:HA    | 1.94        | 0.49     |
| 46:BU:90:LYS:HB3  | 46:BU:92:VAL:HG23  | 1.95        | 0.49     |
| 1:AA:1080:A:H5''  | 4:AE:51:LYS:NZ     | 2.25        | 0.49     |
| 47:DF:140:ILE:O   | 47:DF:145:VAL:HG12 | 2.13        | 0.49     |
| 25:BC:196:ASN:C   | 25:BC:198:GLU:H    | 2.15        | 0.49     |
| 29:BE:59:PRO:HB2  | 29:BE:67:ARG:NH2   | 2.18        | 0.49     |
| 23:BB:672:C:H2'   | 23:BB:673:C:C6     | 2.47        | 0.49     |
| 23:DB:138:U:O4'   | 50:DT:1:MET:HA     | 2.12        | 0.49     |
| 23:DB:662:G:O2'   | 23:DB:663:G:H5'    | 2.12        | 0.49     |
| 21:AU:48:LYS:HA   | 21:AU:51:ALA:CB    | 2.36        | 0.49     |
| 23:BB:1080:A:O2'  | 23:BB:1081:U:H5'   | 2.11        | 0.49     |
| 24:DI:17:ALA:C    | 24:DI:19:PRO:HD3   | 2.32        | 0.49     |
| 3:CD:154:VAL:HG23 | 3:CD:155:LYS:N     | 2.27        | 0.49     |
| 27:BK:105:ARG:HD2 | 27:BK:122:VAL:HG11 | 1.93        | 0.49     |
| 49:DR:59:ILE:HG23 | 49:DR:101:ILE:H    | 1.77        | 0.49     |
| 9:CJ:7:ARG:NH1    | 9:CJ:101:SER:HB2   | 2.28        | 0.49     |
| 23:BB:2897:U:H2'  | 23:BB:2898:U:H6    | 1.75        | 0.49     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 24:BI:33:ASN:HD21  | 24:BI:64:ARG:NH1   | 2.06        | 0.49     |
| 51:DZ:17:ASN:HD22  | 51:DZ:25:THR:HB    | 1.77        | 0.49     |
| 29:DE:126:VAL:HG21 | 29:DE:133:LEU:HB2  | 1.93        | 0.49     |
| 23:BB:1654:A:H2'   | 23:BB:1655:A:C8    | 2.48        | 0.49     |
| 1:AA:33:A:O2'      | 1:AA:34:C:H5'      | 2.12        | 0.49     |
| 12:CM:80:MET:HA    | 12:CM:87:GLY:HA3   | 1.93        | 0.49     |
| 46:BU:35:VAL:O     | 46:BU:38:ILE:HG22  | 2.13        | 0.49     |
| 10:CK:80:ASN:H     | 10:CK:80:ASN:HD22  | 1.60        | 0.49     |
| 11:AL:106:VAL:HA   | 11:AL:107:LYS:NZ   | 2.27        | 0.49     |
| 23:BB:99:U:O2      | 23:BB:99:U:H5'     | 2.11        | 0.49     |
| 34:B3:62:PRO:HG2   | 37:BL:48:ARG:NH2   | 2.27        | 0.49     |
| 23:DB:96:C:O2'     | 23:DB:97:C:H5'     | 2.11        | 0.49     |
| 23:DB:1585:C:H2'   | 23:DB:1586:A:O4'   | 2.12        | 0.49     |
| 3:AD:11:SER:HA     | 3:AD:18:LEU:CD2    | 2.42        | 0.49     |
| 23:BB:1372:U:O2'   | 23:BB:1373:A:H5'   | 2.11        | 0.49     |
| 28:BP:25:VAL:HA    | 28:BP:85:VAL:HA    | 1.94        | 0.49     |
| 1:AA:502:A:H2'     | 1:AA:503:C:C6      | 2.47        | 0.49     |
| 41:DJ:13:ARG:O     | 41:DJ:14:ASP:HB2   | 2.12        | 0.49     |
| 20:AB:94:ARG:HG2   | 20:AB:94:ARG:O     | 2.12        | 0.49     |
| 23:BB:1535:A:H5''  | 23:BB:1536:C:C5    | 2.47        | 0.49     |
| 22:BA:46:A:H2'     | 22:BA:47:C:O4'     | 2.11        | 0.49     |
| 1:CA:415:A:H3'     | 1:CA:416:G:H8      | 1.77        | 0.49     |
| 23:BB:1717:A:H2'   | 23:BB:1718:G:O4'   | 2.12        | 0.49     |
| 23:BB:1856:U:H2'   | 23:BB:1857:G:H5'   | 1.94        | 0.49     |
| 23:DB:1495:A:H2'   | 23:DB:1496:A:H8    | 1.77        | 0.49     |
| 1:AA:160:A:H1'     | 1:AA:344:A:N7      | 2.27        | 0.49     |
| 23:BB:2756:U:C1'   | 23:BB:2757:A:H5''  | 2.42        | 0.49     |
| 23:DB:2204:G:O2'   | 23:DB:2205:A:H5'   | 2.11        | 0.49     |
| 1:AA:1247:U:O2'    | 1:AA:1248:A:H5'    | 2.12        | 0.49     |
| 7:AH:23:ALA:HB1    | 7:AH:61:THR:HA     | 1.94        | 0.49     |
| 23:BB:458:G:N2     | 23:BB:469:G:H2'    | 2.28        | 0.49     |
| 23:DB:1669:A:O3'   | 23:DB:2549:G:H5'   | 2.13        | 0.49     |
| 23:DB:1838:C:H4'   | 23:DB:1839:G:H8    | 1.77        | 0.49     |
| 33:B1:29:LYS:N     | 33:B1:30:PRO:HD3   | 2.28        | 0.49     |
| 28:DP:64:SER:O     | 28:DP:66:GLY:N     | 2.46        | 0.49     |
| 23:BB:67:U:H2'     | 23:BB:68:G:H8      | 1.77        | 0.49     |
| 2:AC:128:MET:H     | 2:AC:128:MET:CE    | 2.26        | 0.49     |
| 42:BN:9:GLN:O      | 42:BN:17:ARG:HD3   | 2.12        | 0.49     |
| 25:DC:128:THR:OG1  | 25:DC:190:THR:HG22 | 2.12        | 0.49     |
| 44:BQ:23:TYR:N     | 44:BQ:23:TYR:CD2   | 2.79        | 0.49     |
| 16:CQ:74:LEU:HD22  | 16:CQ:75:VAL:N     | 2.27        | 0.49     |
| 53:B6:52:LEU:HD11  | 53:B6:58:VAL:HG23  | 1.94        | 0.49     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 40:BH:94:ILE:CG2   | 40:BH:99:ILE:HD11 | 2.42        | 0.49     |
| 29:DE:60:TRP:C     | 29:DE:62:GLN:H    | 2.15        | 0.49     |
| 7:AH:94:VAL:CG2    | 7:AH:101:ALA:HB2  | 2.42        | 0.49     |
| 23:DB:2732:G:H5'   | 23:DB:2733:A:O4'  | 2.12        | 0.49     |
| 43:BO:36:TYR:CD2   | 43:BO:36:TYR:N    | 2.80        | 0.49     |
| 47:BF:27:VAL:O     | 47:BF:29:ARG:HD2  | 2.13        | 0.49     |
| 23:BB:321:U:O4'    | 29:BE:159:LEU:HG  | 2.13        | 0.49     |
| 1:CA:1079:G:H5''   | 4:CE:49:TYR:CE2   | 2.47        | 0.49     |
| 18:CS:50:VAL:HG23  | 18:CS:59:VAL:HG21 | 1.95        | 0.49     |
| 1:AA:1318:A:H4'    | 18:AS:9:PHE:CE1   | 2.47        | 0.49     |
| 23:DB:1188:U:O2'   | 23:DB:1189:A:H5'  | 2.12        | 0.49     |
| 53:B6:107:THR:HG22 | 53:B6:108:GLU:H   | 1.78        | 0.49     |
| 33:D1:7:LYS:HA     | 33:D1:23:THR:HG22 | 1.95        | 0.49     |
| 33:D1:7:LYS:CD     | 34:D3:33:THR:HG21 | 2.37        | 0.49     |
| 23:BB:2646:C:H2'   | 23:BB:2647:U:O4'  | 2.12        | 0.49     |
| 24:BI:122:GLU:CD   | 24:BI:122:GLU:H   | 2.16        | 0.49     |
| 29:DE:146:VAL:O    | 29:DE:167:VAL:HA  | 2.12        | 0.49     |
| 20:AB:186:VAL:O    | 20:AB:200:PRO:HA  | 2.12        | 0.49     |
| 3:CD:121:ALA:O     | 3:CD:122:ILE:HD13 | 2.13        | 0.49     |
| 35:BV:30:ILE:HB    | 35:BV:38:LEU:HB3  | 1.94        | 0.49     |
| 23:DB:1553:A:H2'   | 23:DB:1555:G:N7   | 2.27        | 0.49     |
| 28:DP:9:GLN:HA     | 28:DP:12:MET:SD   | 2.53        | 0.49     |
| 23:BB:116:C:H1'    | 23:BB:127:A:N3    | 2.27        | 0.49     |
| 3:AD:104:MET:CE    | 3:AD:170:LEU:HD13 | 2.41        | 0.49     |
| 3:AD:170:LEU:HB2   | 3:AD:180:THR:O    | 2.12        | 0.49     |
| 28:DP:31:VAL:CG1   | 28:DP:38:ARG:HG3  | 2.42        | 0.49     |
| 10:CK:17:ASP:HA    | 10:CK:80:ASN:O    | 2.12        | 0.49     |
| 4:CE:152:VAL:O     | 4:CE:156:ARG:HG2  | 2.13        | 0.49     |
| 1:CA:1522:U:O2'    | 1:CA:1523:G:H5'   | 2.12        | 0.49     |
| 3:CD:129:VAL:HG12  | 3:CD:130:ASN:N    | 2.27        | 0.49     |
| 25:BC:6:LYS:C      | 25:BC:8:THR:H     | 2.15        | 0.49     |
| 2:CC:70:ALA:HA     | 2:CC:105:VAL:CG2  | 2.43        | 0.49     |
| 23:BB:96:C:H2'     | 23:BB:97:C:H6     | 1.77        | 0.49     |
| 23:BB:2457:U:H2'   | 23:BB:2458:G:H5'  | 1.94        | 0.49     |
| 19:AT:57:VAL:HB    | 19:AT:71:ALA:HB1  | 1.95        | 0.49     |
| 23:BB:1040:A:H2'   | 23:BB:1041:G:H8   | 1.77        | 0.49     |
| 1:CA:1053:G:C4'    | 1:CA:1054:C:H5'   | 2.42        | 0.49     |
| 22:BA:6:G:H2'      | 22:BA:7:G:C8      | 2.47        | 0.49     |
| 23:DB:2756:U:C1'   | 23:DB:2757:A:H5'' | 2.43        | 0.49     |
| 23:BB:2539:C:O2'   | 23:BB:2540:C:H5'  | 2.13        | 0.49     |
| 23:BB:1351:C:H2'   | 23:BB:1352:U:C1'  | 2.42        | 0.49     |
| 22:DA:88:C:O2'     | 22:DA:89:U:H5''   | 2.12        | 0.49     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DC:2:VAL:HG23   | 25:DC:3:VAL:N     | 2.28        | 0.49     |
| 23:DB:1816:C:H3'   | 25:DC:61:TYR:CE2  | 2.48        | 0.49     |
| 23:BB:833:A:C1'    | 37:BL:52:GLY:H    | 2.26        | 0.49     |
| 1:AA:204:G:H2'     | 1:AA:205:A:C8     | 2.48        | 0.49     |
| 1:AA:204:G:O2'     | 1:AA:205:A:H5'    | 2.12        | 0.49     |
| 37:DL:136:GLU:HA   | 37:DL:140:GLY:HA3 | 1.94        | 0.49     |
| 23:DB:108:G:H2'    | 23:DB:109:C:C6    | 2.48        | 0.49     |
| 5:CF:86:ARG:NH1    | 17:CR:64:LEU:HD12 | 2.27        | 0.49     |
| 23:DB:79:C:HO2'    | 23:DB:346:A:H1'   | 1.77        | 0.49     |
| 1:AA:992:U:H1'     | 1:AA:993:G:C2     | 2.47        | 0.49     |
| 40:BH:59:ALA:C     | 40:BH:62:LEU:HG   | 2.32        | 0.49     |
| 23:DB:2303:G:H1'   | 47:DF:122:ASP:OD1 | 2.13        | 0.49     |
| 48:BG:53:PRO:HG3   | 48:BG:61:TRP:CD2  | 2.48        | 0.49     |
| 23:DB:251:A:H2'    | 23:DB:252:G:O4'   | 2.12        | 0.49     |
| 23:DB:620:G:H5'    | 23:DB:620:G:N3    | 2.27        | 0.49     |
| 14:AO:50:HIS:O     | 14:AO:53:ARG:HB3  | 2.12        | 0.49     |
| 1:AA:227:G:H2'     | 1:AA:228:A:C8     | 2.47        | 0.49     |
| 47:BF:10:GLU:O     | 47:BF:13:LYS:HG3  | 2.12        | 0.49     |
| 1:CA:409:U:OP1     | 3:CD:23:GLY:HA3   | 2.12        | 0.49     |
| 20:AB:130:LYS:O    | 20:AB:134:LEU:HG  | 2.12        | 0.49     |
| 1:CA:114:U:H2'     | 1:CA:115:G:C8     | 2.48        | 0.49     |
| 5:AF:51:ILE:O      | 5:AF:51:ILE:HG23  | 2.11        | 0.49     |
| 25:BC:132:ARG:O    | 25:BC:132:ARG:HG3 | 2.12        | 0.49     |
| 5:CF:51:ILE:HG23   | 5:CF:51:ILE:O     | 2.11        | 0.49     |
| 48:BG:133:LYS:H    | 48:BG:133:LYS:HD3 | 1.76        | 0.49     |
| 23:BB:1145:C:O2'   | 23:BB:1146:C:H5'  | 2.12        | 0.49     |
| 1:CA:790:A:H2'     | 1:CA:791:G:C8     | 2.48        | 0.49     |
| 23:BB:923:G:N3     | 52:BW:23:LYS:HE3  | 2.27        | 0.49     |
| 25:DC:183:VAL:HG22 | 25:DC:184:GLU:N   | 2.27        | 0.49     |
| 10:AK:14:GLN:HA    | 10:AK:76:TYR:O    | 2.12        | 0.49     |
| 5:CF:25:TYR:O      | 5:CF:29:ILE:HG13  | 2.12        | 0.49     |
| 26:BD:36:GLN:HG2   | 26:BD:37:VAL:N    | 2.26        | 0.49     |
| 40:BH:95:GLY:O     | 40:BH:99:ILE:HG12 | 2.11        | 0.49     |
| 8:CI:56:MET:SD     | 8:CI:57:VAL:N     | 2.84        | 0.49     |
| 26:DD:111:GLY:H    | 26:DD:194:PRO:HG3 | 1.78        | 0.49     |
| 53:B6:14:MET:HB3   | 53:B6:168:PHE:CG  | 2.47        | 0.49     |
| 42:BN:79:LEU:HA    | 42:BN:83:LEU:CD1  | 2.42        | 0.49     |
| 23:BB:2311:A:H1'   | 47:BF:84:ILE:HD13 | 1.94        | 0.49     |
| 10:AK:90:PRO:C     | 10:AK:92:ARG:H    | 2.15        | 0.49     |
| 1:CA:947:G:H2'     | 1:CA:948:C:H6     | 1.77        | 0.49     |
| 13:AN:27:LYS:HA    | 13:AN:31:SER:HB2  | 1.94        | 0.49     |
| 29:BE:58:LYS:CD    | 29:BE:58:LYS:N    | 2.75        | 0.49     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:673:C:O4'    | 29:BE:77:ILE:HD11  | 2.13        | 0.49     |
| 50:DT:1:MET:CG     | 50:DT:2:ILE:H      | 2.24        | 0.49     |
| 37:DL:116:VAL:HG13 | 37:DL:117:THR:N    | 2.19        | 0.49     |
| 41:BJ:84:ILE:HG23  | 41:BJ:84:ILE:O     | 2.12        | 0.49     |
| 45:DS:29:VAL:CA    | 45:DS:32:ALA:HB3   | 2.43        | 0.49     |
| 49:DR:78:ARG:HH21  | 49:DR:78:ARG:HG3   | 1.78        | 0.49     |
| 46:BU:46:LYS:HZ1   | 46:BU:47:PRO:HG2   | 1.76        | 0.49     |
| 23:DB:2270:A:H2'   | 23:DB:2271:G:O4'   | 2.13        | 0.49     |
| 23:DB:1029:A:H2'   | 23:DB:1030:C:O4'   | 2.13        | 0.49     |
| 43:DO:58:ILE:O     | 43:DO:62:LEU:HB2   | 2.12        | 0.49     |
| 26:DD:113:SER:HB3  | 26:DD:167:ASN:HA   | 1.94        | 0.49     |
| 24:DI:17:ALA:O     | 24:DI:18:ASN:HB3   | 2.13        | 0.49     |
| 44:BQ:109:VAL:O    | 44:BQ:113:LYS:HG3  | 2.11        | 0.49     |
| 44:DQ:97:ILE:HD11  | 44:DQ:108:LEU:HD11 | 1.95        | 0.49     |
| 49:DR:38:VAL:HG13  | 49:DR:54:VAL:HG12  | 1.94        | 0.49     |
| 37:DL:95:LEU:HB2   | 37:DL:101:ILE:HG13 | 1.93        | 0.49     |
| 4:CE:111:ARG:HG3   | 4:CE:112:ALA:N     | 2.27        | 0.49     |
| 8:CI:117:LEU:HB3   | 8:CI:122:ARG:O     | 2.12        | 0.49     |
| 4:CE:143:LEU:O     | 4:CE:146:MET:HG2   | 2.12        | 0.49     |
| 33:D1:47:ILE:HD12  | 33:D1:47:ILE:N     | 2.27        | 0.49     |
| 34:B3:61:LEU:HB2   | 34:B3:64:ALA:HB2   | 1.95        | 0.49     |
| 40:BH:3:VAL:HG12   | 40:BH:38:PRO:HA    | 1.94        | 0.49     |
| 23:BB:1389:G:O2'   | 23:BB:1390:U:H5'   | 2.13        | 0.49     |
| 6:CG:129:ASN:HA    | 6:CG:134:VAL:HG11  | 1.94        | 0.49     |
| 23:DB:2457:U:O2'   | 23:DB:2458:G:H5'   | 2.13        | 0.49     |
| 19:CT:85:LEU:HD23  | 19:CT:86:ALA:H     | 1.77        | 0.49     |
| 23:DB:521:U:H2'    | 23:DB:522:A:H8     | 1.74        | 0.49     |
| 3:AD:10:LEU:HD12   | 3:AD:20:LEU:CD1    | 2.43        | 0.49     |
| 1:AA:1144:G:N2     | 1:AA:1146:A:H62    | 2.11        | 0.49     |
| 1:CA:1142:G:H3'    | 1:CA:1143:G:H8     | 1.76        | 0.49     |
| 23:BB:1184:U:OP1   | 30:BY:29:ARG:HD3   | 2.11        | 0.49     |
| 1:AA:677:U:H2'     | 1:AA:678:U:H6      | 1.76        | 0.49     |
| 26:BD:125:TRP:CD1  | 26:BD:160:LYS:HB3  | 2.47        | 0.49     |
| 23:BB:2069:G:O2'   | 23:BB:2070:A:H5'   | 2.13        | 0.49     |
| 1:CA:1179:A:H2'    | 1:CA:1180:A:O4'    | 2.12        | 0.49     |
| 31:D0:12:ARG:HD2   | 31:D0:16:ARG:NH1   | 2.27        | 0.49     |
| 1:AA:1040:U:O2'    | 1:AA:1041:G:H5'    | 2.12        | 0.49     |
| 23:DB:1201:U:H2'   | 23:DB:1202:G:H8    | 1.76        | 0.49     |
| 23:BB:1163:G:O2'   | 23:BB:1164:C:H5'   | 2.13        | 0.49     |
| 23:DB:1252:G:N2    | 44:DQ:32:ARG:HB3   | 2.27        | 0.49     |
| 46:DU:13:LEU:HD12  | 46:DU:68:ASN:O     | 2.13        | 0.49     |
| 1:AA:1366:C:H2'    | 1:AA:1367:C:H6     | 1.77        | 0.49     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1147:A:O2'   | 23:DB:1148:U:H5'   | 2.13        | 0.49     |
| 23:BB:902:C:H2'    | 23:BB:903:C:C6     | 2.48        | 0.49     |
| 19:CT:14:GLU:OE2   | 19:CT:18:LYS:HE2   | 2.13        | 0.49     |
| 27:BK:17:ARG:HB2   | 27:BK:45:GLU:HB3   | 1.95        | 0.49     |
| 1:CA:218:U:H2'     | 1:CA:219:U:C6      | 2.48        | 0.49     |
| 27:DK:17:ARG:HB2   | 27:DK:45:GLU:HB3   | 1.94        | 0.49     |
| 33:D1:16:THR:OG1   | 33:D1:41:VAL:HG11  | 2.12        | 0.49     |
| 50:DT:62:VAL:HG12  | 50:DT:63:VAL:N     | 2.27        | 0.49     |
| 26:DD:46:ARG:HH12  | 26:DD:88:GLU:HG3   | 1.77        | 0.49     |
| 10:CK:126:ARG:HB2  | 21:CU:33:ARG:CD    | 2.43        | 0.49     |
| 53:B6:40:HIS:O     | 53:B6:41:LEU:C     | 2.49        | 0.49     |
| 8:CI:62:LEU:N      | 8:CI:62:LEU:HD13   | 2.28        | 0.49     |
| 41:BJ:55:ILE:HG22  | 41:BJ:123:LYS:HB2  | 1.94        | 0.49     |
| 41:BJ:29:ALA:O     | 41:BJ:32:LEU:HB2   | 2.11        | 0.49     |
| 23:DB:630:G:H22    | 23:DB:632:A:H3'    | 1.74        | 0.49     |
| 29:DE:58:LYS:HB2   | 29:DE:60:TRP:HB2   | 1.94        | 0.49     |
| 23:DB:2646:C:H2'   | 23:DB:2647:U:O4'   | 2.12        | 0.49     |
| 13:CN:61:ASN:O     | 13:CN:62:ARG:HB2   | 2.12        | 0.49     |
| 50:BT:42:GLU:O     | 50:BT:46:ALA:HB2   | 2.12        | 0.49     |
| 50:BT:29:THR:CA    | 50:BT:86:THR:HA    | 2.41        | 0.49     |
| 40:DH:127:GLU:HB2  | 40:DH:143:ILE:HG21 | 1.95        | 0.49     |
| 23:BB:345:A:N3     | 23:BB:346:A:N1     | 2.60        | 0.49     |
| 3:AD:160:LEU:HD23  | 3:AD:164:ARG:NH2   | 2.28        | 0.49     |
| 47:BF:131:VAL:HG22 | 47:BF:151:LEU:O    | 2.12        | 0.49     |
| 23:BB:2394:C:OP1   | 37:BL:63:LYS:HG2   | 2.12        | 0.49     |
| 29:BE:145:ASP:OD1  | 29:BE:183:PHE:HA   | 2.12        | 0.49     |
| 1:AA:1078:U:O2'    | 4:AE:137:ARG:NH1   | 2.46        | 0.49     |
| 41:DJ:82:GLY:O     | 41:DJ:84:ILE:HG22  | 2.13        | 0.49     |
| 43:DO:26:LEU:HD13  | 43:DO:39:VAL:CG2   | 2.43        | 0.49     |
| 29:BE:69:ARG:O     | 29:BE:70:SER:CB    | 2.56        | 0.49     |
| 23:BB:2789:C:H3'   | 23:BB:2893:A:H62   | 1.78        | 0.49     |
| 38:DM:26:VAL:HG23  | 38:DM:104:GLU:OE2  | 2.11        | 0.49     |
| 31:B0:41:HIS:HB2   | 42:BN:99:LYS:C     | 2.33        | 0.49     |
| 43:BO:49:VAL:HG11  | 43:BO:82:ALA:HA    | 1.94        | 0.49     |
| 48:BG:166:GLU:CG   | 48:BG:168:VAL:HG23 | 2.39        | 0.49     |
| 42:BN:72:ASP:C     | 42:BN:74:GLU:H     | 2.16        | 0.49     |
| 5:CF:4:TYR:O       | 5:CF:63:ASN:HA     | 2.12        | 0.49     |
| 2:CC:149:LYS:HB2   | 2:CC:168:ARG:HG3   | 1.94        | 0.49     |
| 40:BH:140:ALA:C    | 40:BH:141:LYS:HD3  | 2.33        | 0.49     |
| 49:DR:4:VAL:HB     | 49:DR:39:LEU:HG    | 1.95        | 0.49     |
| 3:AD:154:VAL:HG23  | 3:AD:155:LYS:N     | 2.28        | 0.49     |
| 44:DQ:7:VAL:O      | 44:DQ:11:ALA:HB2   | 2.12        | 0.49     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:BB:1103:A:H5''  | 23:BB:1104:C:C5   | 2.46        | 0.49     |
| 1:CA:998:C:H2'     | 1:CA:999:C:C6     | 2.47        | 0.49     |
| 20:CB:102:ASN:OD1  | 20:CB:105:THR:HB  | 2.13        | 0.49     |
| 4:AE:71:ILE:HD11   | 4:AE:144:GLU:HG3  | 1.93        | 0.49     |
| 43:DO:76:LYS:HG3   | 43:DO:113:ALA:CB  | 2.42        | 0.49     |
| 2:CC:26:LYS:HG3    | 2:CC:27:GLU:N     | 2.25        | 0.49     |
| 23:BB:2592:G:O2'   | 23:BB:2593:U:H5'  | 2.13        | 0.49     |
| 35:DV:76:ASP:H     | 35:DV:90:ASP:HB2  | 1.77        | 0.49     |
| 23:BB:150:U:H2'    | 23:BB:151:C:H6    | 1.78        | 0.49     |
| 23:BB:1805:A:N3    | 25:BC:49:THR:HG23 | 2.27        | 0.49     |
| 39:BX:14:LEU:O     | 39:BX:18:LEU:HB2  | 2.12        | 0.49     |
| 39:DX:41:HIS:O     | 39:DX:44:LYS:HB3  | 2.12        | 0.49     |
| 23:BB:2847:U:H5''  | 28:BP:94:ALA:HB2  | 1.93        | 0.49     |
| 1:AA:737:C:O2'     | 1:AA:738:C:H5'    | 2.13        | 0.49     |
| 23:BB:2218:G:O2'   | 23:BB:2219:U:H5'  | 2.12        | 0.49     |
| 23:DB:2854:G:H2'   | 23:DB:2855:C:C6   | 2.48        | 0.49     |
| 45:BS:96:ILE:HG23  | 45:BS:96:ILE:O    | 2.12        | 0.49     |
| 3:AD:18:LEU:HB2    | 3:AD:20:LEU:HG    | 1.94        | 0.49     |
| 20:CB:8:MET:CG     | 20:CB:9:LEU:N     | 2.76        | 0.49     |
| 23:DB:2197:U:O2'   | 23:DB:2198:A:H2'  | 2.13        | 0.49     |
| 1:CA:1308:U:H3'    | 12:CM:97:ARG:NH1  | 2.28        | 0.49     |
| 23:DB:4:U:H2'      | 23:DB:5:A:H8      | 1.78        | 0.49     |
| 22:DA:59:A:H2'     | 22:DA:60:C:O4'    | 2.13        | 0.49     |
| 1:AA:694:A:C2      | 1:AA:695:A:H1'    | 2.46        | 0.49     |
| 23:DB:1717:A:H2'   | 23:DB:1718:G:O4'  | 2.12        | 0.49     |
| 23:DB:2553:G:H2'   | 23:DB:2554:U:O4'  | 2.12        | 0.49     |
| 23:BB:2300:C:H2'   | 23:BB:2301:C:C6   | 2.47        | 0.49     |
| 1:CA:201:G:O2'     | 1:CA:469:C:H4'    | 2.12        | 0.49     |
| 1:AA:766:A:H2'     | 1:AA:767:A:O4'    | 2.13        | 0.49     |
| 23:BB:1848:A:H2'   | 23:BB:1849:G:H8   | 1.78        | 0.49     |
| 23:BB:621:A:H2'    | 23:BB:622:G:O4'   | 2.12        | 0.49     |
| 22:BA:33:G:O2'     | 22:BA:34:A:H5'    | 2.12        | 0.49     |
| 1:CA:179:A:H2'     | 1:CA:180:U:O4'    | 2.13        | 0.49     |
| 23:DB:1664:A:H1'   | 23:DB:2726:A:N1   | 2.28        | 0.49     |
| 23:DB:927:A:H2'    | 23:DB:928:A:C8    | 2.48        | 0.49     |
| 37:BL:25:SER:O     | 37:BL:27:LEU:HD12 | 2.13        | 0.49     |
| 29:DE:3:LEU:CB     | 29:DE:12:LEU:HB2  | 2.43        | 0.49     |
| 2:AC:57:GLU:HB2    | 2:AC:64:ARG:HB2   | 1.94        | 0.49     |
| 1:CA:935:A:O2'     | 1:CA:936:C:H5'    | 2.13        | 0.49     |
| 10:CK:115:ILE:HD11 | 17:CR:72:ARG:HH12 | 1.78        | 0.49     |
| 2:CC:54:ILE:O      | 2:CC:54:ILE:HG23  | 2.12        | 0.49     |
| 25:DC:132:ARG:HG3  | 25:DC:132:ARG:O   | 2.12        | 0.49     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 37:BL:2:ARG:HG2    | 37:BL:2:ARG:O      | 2.12        | 0.49     |
| 23:BB:1693:U:H4'   | 23:BB:1694:C:OP2   | 2.13        | 0.49     |
| 25:DC:90:ILE:HD12  | 25:DC:102:TYR:HB3  | 1.95        | 0.49     |
| 23:DB:945:A:H4'    | 23:DB:945:A:OP2    | 2.12        | 0.49     |
| 37:BL:90:VAL:CB    | 37:BL:122:VAL:HG12 | 2.42        | 0.49     |
| 40:BH:111:ALA:O    | 40:BH:114:GLU:HG2  | 2.12        | 0.49     |
| 53:B6:42:LYS:HE2   | 53:B6:49:HIS:O     | 2.13        | 0.49     |
| 53:B6:68:VAL:HB    | 53:B6:99:LEU:CG    | 2.42        | 0.49     |
| 20:CB:209:VAL:HG23 | 20:CB:210:THR:N    | 2.28        | 0.49     |
| 51:DZ:76:GLU:HG3   | 51:DZ:77:LYS:N     | 2.23        | 0.49     |
| 1:AA:1216:A:H5''   | 13:AN:4:SER:CB     | 2.42        | 0.49     |
| 47:BF:177:ARG:CZ   | 47:BF:177:ARG:HA   | 2.43        | 0.49     |
| 23:DB:143:C:H2'    | 23:DB:144:A:H8     | 1.78        | 0.49     |
| 50:BT:27:SER:O     | 50:BT:28:ASN:HB3   | 2.12        | 0.49     |
| 23:DB:1063:G:H4'   | 24:DI:135:MET:HG2  | 1.95        | 0.49     |
| 47:BF:110:ILE:CG2  | 47:BF:113:PHE:HB3  | 2.43        | 0.49     |
| 12:CM:70:ARG:NH2   | 47:DF:142:TYR:HB3  | 2.27        | 0.49     |
| 4:CE:89:THR:HG22   | 4:CE:90:GLY:N      | 2.28        | 0.49     |
| 12:CM:79:LEU:CD2   | 12:CM:86:ARG:HH21  | 2.26        | 0.49     |
| 45:BS:8:ARG:HB3    | 45:BS:102:HIS:CE1  | 2.47        | 0.49     |
| 29:BE:60:TRP:CZ3   | 29:BE:62:GLN:HA    | 2.48        | 0.49     |
| 23:BB:2886:A:H62   | 31:B0:39:ARG:CZ    | 2.23        | 0.49     |
| 15:AP:67:ILE:HG23  | 15:AP:67:ILE:O     | 2.13        | 0.49     |
| 23:DB:1654:A:H2'   | 23:DB:1655:A:H8    | 1.77        | 0.49     |
| 24:DI:21:PRO:CB    | 24:DI:22:PRO:HD3   | 2.38        | 0.49     |
| 22:DA:32:U:H4'     | 22:DA:52:A:H62     | 1.76        | 0.49     |
| 44:DQ:109:VAL:CG1  | 44:DQ:113:LYS:HE3  | 2.40        | 0.49     |
| 23:BB:2147:A:H5'   | 23:BB:2148:G:H4'   | 1.94        | 0.49     |
| 23:BB:851:C:O2'    | 30:BY:45:GLY:HA3   | 2.12        | 0.49     |
| 36:D2:21:ARG:CD    | 36:D2:43:THR:HG21  | 2.42        | 0.49     |
| 23:BB:1553:A:H2'   | 23:BB:1555:G:N7    | 2.27        | 0.49     |
| 34:D3:22:LYS:HB2   | 34:D3:48:MET:SD    | 2.53        | 0.49     |
| 11:AL:26:CYS:SG    | 11:AL:29:LYS:HE2   | 2.52        | 0.49     |
| 23:DB:171:U:H2'    | 23:DB:172:A:H8     | 1.75        | 0.49     |
| 23:DB:2527:C:O2'   | 23:DB:2528:U:H5'   | 2.13        | 0.49     |
| 4:AE:111:ARG:HG3   | 4:AE:112:ALA:N     | 2.27        | 0.49     |
| 42:BN:45:ARG:HG3   | 42:BN:95:THR:HG21  | 1.94        | 0.49     |
| 4:CE:152:VAL:HA    | 4:CE:155:LYS:HD3   | 1.93        | 0.49     |
| 6:AG:100:MET:O     | 6:AG:104:VAL:HG23  | 2.13        | 0.49     |
| 1:AA:401:C:H2'     | 1:AA:402:G:H8      | 1.77        | 0.49     |
| 20:AB:75:ALA:O     | 20:AB:79:VAL:HG23  | 2.13        | 0.49     |
| 20:CB:94:ARG:HG2   | 20:CB:94:ARG:O     | 2.13        | 0.49     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 2:AC:46:LEU:HB3    | 2:AC:49:ALA:HB3    | 1.93        | 0.49     |
| 3:AD:11:SER:HA     | 3:AD:18:LEU:HD22   | 1.95        | 0.49     |
| 3:AD:59:LYS:O      | 3:AD:63:ILE:HG13   | 2.12        | 0.49     |
| 50:BT:12:ARG:HB3   | 50:BT:12:ARG:HH11  | 1.74        | 0.49     |
| 1:AA:678:U:O2'     | 1:AA:679:C:H5'     | 2.13        | 0.49     |
| 3:CD:59:LYS:O      | 3:CD:63:ILE:HG13   | 2.12        | 0.49     |
| 1:CA:1472:U:H2'    | 1:CA:1473:G:C8     | 2.48        | 0.49     |
| 26:DD:125:TRP:CD1  | 26:DD:160:LYS:HB3  | 2.48        | 0.49     |
| 23:DB:231:A:H3'    | 23:DB:232:G:C8     | 2.48        | 0.49     |
| 1:CA:399:G:H2'     | 1:CA:400:C:H6      | 1.78        | 0.49     |
| 27:DK:109:SER:HB2  | 27:DK:111:LYS:HG2  | 1.93        | 0.49     |
| 23:DB:615:U:O4     | 29:DE:39:ALA:HB2   | 2.13        | 0.49     |
| 23:BB:2302:U:O2'   | 23:BB:2303:G:H5'   | 2.13        | 0.49     |
| 29:BE:37:ALA:C     | 29:BE:39:ALA:H     | 2.14        | 0.49     |
| 1:AA:852:G:H2'     | 1:AA:853:C:H6      | 1.77        | 0.49     |
| 23:BB:516:C:O2'    | 23:BB:517:C:H5'    | 2.13        | 0.49     |
| 17:AR:44:THR:C     | 17:AR:46:THR:H     | 2.15        | 0.49     |
| 46:DU:41:VAL:O     | 46:DU:42:LYS:HB2   | 2.13        | 0.49     |
| 23:BB:1613:G:H2'   | 23:BB:1617:C:H42   | 1.77        | 0.49     |
| 23:DB:688:U:O2'    | 23:DB:689:A:H5'    | 2.12        | 0.49     |
| 48:BG:173:ALA:HB3  | 48:BG:175:LYS:NZ   | 2.28        | 0.49     |
| 23:DB:2818:U:O2'   | 23:DB:2819:G:H5'   | 2.12        | 0.49     |
| 23:BB:736:C:H2'    | 23:BB:737:C:C6     | 2.48        | 0.49     |
| 25:BC:226:PRO:HA   | 25:BC:232:GLY:HA3  | 1.95        | 0.49     |
| 23:BB:659:G:H4'    | 29:BE:95:LYS:HB3   | 1.95        | 0.49     |
| 41:BJ:75:TYR:CD1   | 41:BJ:86:GLN:HB3   | 2.48        | 0.49     |
| 49:BR:84:ARG:HH21  | 49:BR:84:ARG:HG3   | 1.77        | 0.49     |
| 23:BB:452:G:OP1    | 29:BE:53:THR:HG23  | 2.13        | 0.49     |
| 23:DB:1842:G:H2'   | 23:DB:1843:C:C6    | 2.48        | 0.49     |
| 25:DC:6:LYS:C      | 25:DC:8:THR:H      | 2.16        | 0.49     |
| 23:DB:1099:G:H5''  | 24:DI:2:LYS:HB2    | 1.95        | 0.49     |
| 23:BB:852:U:H2'    | 23:BB:853:C:C6     | 2.48        | 0.49     |
| 25:BC:131:MET:HE1  | 25:BC:143:VAL:HG13 | 1.94        | 0.49     |
| 48:BG:10:VAL:HG21  | 48:BG:49:LEU:HD13  | 1.94        | 0.49     |
| 25:DC:183:VAL:HG22 | 25:DC:184:GLU:H    | 1.78        | 0.49     |
| 10:AK:70:ALA:O     | 10:AK:74:LYS:HB2   | 2.13        | 0.49     |
| 23:BB:2314:A:H2'   | 23:BB:2315:G:C8    | 2.48        | 0.49     |
| 26:BD:4:LEU:HD12   | 26:BD:32:ASN:HB2   | 1.94        | 0.49     |
| 23:DB:853:C:H2'    | 23:DB:854:C:H6     | 1.77        | 0.49     |
| 53:B6:92:PRO:HG3   | 53:B6:101:ILE:HG23 | 1.95        | 0.49     |
| 25:DC:196:ASN:C    | 25:DC:198:GLU:H    | 2.15        | 0.49     |
| 41:DJ:42:ALA:O     | 41:DJ:44:TYR:N     | 2.46        | 0.49     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 35:DV:1:MET:HG3    | 35:DV:2:PHE:N     | 2.28        | 0.49     |
| 30:DY:8:GLN:HB3    | 30:DY:31:ILE:O    | 2.13        | 0.49     |
| 25:BC:141:HIS:HB3  | 25:BC:190:THR:OG1 | 2.12        | 0.49     |
| 26:DD:31:ALA:O     | 26:DD:52:THR:HG23 | 2.13        | 0.49     |
| 35:BV:56:PHE:O     | 35:BV:61:LEU:HD21 | 2.13        | 0.49     |
| 35:BV:71:LYS:O     | 35:BV:94:ALA:HB2  | 2.13        | 0.49     |
| 13:CN:60:ARG:NE    | 13:CN:69:PRO:HB3  | 2.27        | 0.49     |
| 44:BQ:73:ILE:HD11  | 44:BQ:77:LYS:HB3  | 1.95        | 0.49     |
| 48:BG:17:LYS:O     | 48:BG:23:ILE:HG23 | 2.13        | 0.49     |
| 51:BZ:56:MET:HA    | 51:BZ:59:ILE:HG12 | 1.94        | 0.49     |
| 42:BN:87:PHE:C     | 42:BN:89:SER:H    | 2.15        | 0.49     |
| 12:CM:37:GLY:O     | 12:CM:38:ILE:HD13 | 2.13        | 0.49     |
| 47:DF:21:TYR:HD2   | 47:DF:27:VAL:HG12 | 1.78        | 0.49     |
| 1:CA:1361:G:C2'    | 1:CA:1362:A:H5''  | 2.41        | 0.49     |
| 20:AB:41:ASN:HD22  | 20:AB:44:LYS:HB3  | 1.78        | 0.49     |
| 29:BE:58:LYS:HB2   | 29:BE:60:TRP:HB2  | 1.94        | 0.49     |
| 29:BE:60:TRP:CE3   | 29:BE:60:TRP:HA   | 2.48        | 0.49     |
| 46:BU:81:ARG:N     | 46:BU:81:ARG:HH21 | 2.09        | 0.49     |
| 17:AR:38:ILE:HG23  | 17:AR:62:ARG:NH2  | 2.28        | 0.49     |
| 9:CJ:52:LEU:HB2    | 13:CN:80:ARG:HD2  | 1.95        | 0.49     |
| 38:DM:134:THR:HG22 | 38:DM:136:MET:H   | 1.78        | 0.49     |
| 39:BX:7:ARG:HH11   | 39:BX:7:ARG:HB2   | 1.77        | 0.49     |
| 25:BC:12:ARG:HA    | 25:BC:15:VAL:CG2  | 2.43        | 0.49     |
| 35:BV:77:VAL:HG23  | 35:BV:89:ILE:HG22 | 1.94        | 0.49     |
| 1:AA:85:U:O2       | 1:AA:85:U:H2'     | 2.11        | 0.49     |
| 4:AE:152:VAL:O     | 4:AE:156:ARG:HG2  | 2.12        | 0.49     |
| 29:DE:154:ASP:OD1  | 29:DE:156:ASN:HB3 | 2.11        | 0.49     |
| 23:BB:38:A:HO2'    | 29:BE:43:THR:HA   | 1.77        | 0.49     |
| 46:DU:11:ILE:O     | 46:DU:11:ILE:HD13 | 2.12        | 0.49     |
| 14:CO:70:LEU:HD12  | 14:CO:78:TYR:CB   | 2.43        | 0.49     |
| 23:DB:1681:G:H2'   | 23:DB:1757:A:N1   | 2.28        | 0.49     |
| 23:DB:2145:C:H3'   | 23:DB:2146:C:H5'' | 1.93        | 0.49     |
| 23:DB:91:A:H1'     | 23:DB:92:U:C6     | 2.48        | 0.49     |
| 28:DP:50:ARG:HB3   | 28:DP:57:ALA:N    | 2.28        | 0.49     |
| 23:BB:783:A:H8     | 23:BB:784:G:H4'   | 1.77        | 0.49     |
| 35:BV:76:ASP:H     | 35:BV:90:ASP:HB2  | 1.78        | 0.49     |
| 1:CA:1120:C:O2'    | 1:CA:1121:U:H5'   | 2.12        | 0.49     |
| 23:BB:154:U:H2'    | 23:BB:155:A:C8    | 2.48        | 0.49     |
| 39:DX:56:LEU:O     | 39:DX:57:LEU:HB3  | 2.12        | 0.49     |
| 5:AF:53:LYS:HB3    | 5:AF:54:LEU:HD22  | 1.95        | 0.49     |
| 23:BB:2458:G:H1'   | 23:BB:2460:U:O4   | 2.12        | 0.49     |
| 23:BB:2462:C:H2'   | 23:BB:2463:C:C6   | 2.48        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:2189:U:H2'  | 23:BB:2190:G:H8   | 1.77        | 0.49     |
| 1:AA:393:A:O2'    | 1:AA:394:G:H5'    | 2.13        | 0.49     |
| 10:AK:77:GLY:O    | 10:AK:79:LYS:HE3  | 2.12        | 0.49     |
| 20:CB:8:MET:O     | 20:CB:9:LEU:HB3   | 2.13        | 0.49     |
| 23:DB:2539:C:O2'  | 23:DB:2540:C:H5'  | 2.13        | 0.49     |
| 42:BN:59:SER:O    | 42:BN:63:ARG:HB2  | 2.13        | 0.49     |
| 23:DB:2069:G:O2'  | 23:DB:2070:A:H5'  | 2.13        | 0.49     |
| 20:AB:22:TRP:HA   | 20:AB:188:THR:HB  | 1.95        | 0.49     |
| 1:CA:511:C:O2'    | 1:CA:512:U:H5''   | 2.13        | 0.49     |
| 1:AA:585:G:H2'    | 1:AA:586:C:H6     | 1.78        | 0.49     |
| 1:CA:204:G:O2'    | 1:CA:205:A:H5'    | 2.12        | 0.49     |
| 1:CA:1450:U:H2'   | 1:CA:1452:C:C4    | 2.48        | 0.49     |
| 23:DB:2648:G:H2'  | 23:DB:2649:C:H6   | 1.77        | 0.49     |
| 6:AG:70:PRO:HA    | 6:AG:141:HIS:CE1  | 2.48        | 0.49     |
| 1:CA:62:U:H2'     | 1:CA:63:C:H6      | 1.78        | 0.49     |
| 23:DB:1464:G:H2'  | 23:DB:1465:G:C8   | 2.47        | 0.49     |
| 23:BB:2676:C:O2'  | 23:BB:2677:G:H5'  | 2.12        | 0.49     |
| 22:BA:64:G:H2'    | 22:BA:65:U:H6     | 1.77        | 0.49     |
| 1:CA:386:C:C2'    | 1:CA:387:U:H5'    | 2.43        | 0.49     |
| 23:BB:1369:G:O2'  | 23:BB:1370:C:H5'  | 2.13        | 0.49     |
| 23:BB:840:C:H2'   | 23:BB:841:G:H8    | 1.78        | 0.49     |
| 6:AG:38:ALA:O     | 6:AG:42:VAL:HG23  | 2.13        | 0.49     |
| 23:BB:2828:G:O2'  | 23:BB:2829:A:H5'  | 2.13        | 0.49     |
| 23:BB:2559:C:H2'  | 23:BB:2560:A:H8   | 1.77        | 0.49     |
| 23:DB:1344:U:H4'  | 23:DB:1384:A:C5   | 2.48        | 0.49     |
| 7:CH:23:ALA:HB1   | 7:CH:61:THR:HA    | 1.95        | 0.49     |
| 10:CK:35:ASP:OD1  | 10:CK:37:GLN:HB2  | 2.13        | 0.49     |
| 23:BB:1661:G:O2'  | 23:BB:1662:U:H5'  | 2.13        | 0.49     |
| 39:BX:15:ASN:O    | 39:BX:19:LEU:HD13 | 2.13        | 0.49     |
| 23:DB:734:A:O2'   | 23:DB:735:A:H5'   | 2.12        | 0.49     |
| 23:BB:1878:G:H2'  | 23:BB:1879:C:C6   | 2.48        | 0.49     |
| 23:BB:1051:G:H5'' | 23:BB:1052:C:OP2  | 2.13        | 0.49     |
| 6:AG:106:ALA:HB1  | 6:AG:132:THR:HB   | 1.95        | 0.49     |
| 48:BG:8:VAL:HG22  | 48:BG:68:ARG:HD3  | 1.95        | 0.49     |
| 48:DG:16:VAL:HG11 | 48:DG:44:HIS:CE1  | 2.47        | 0.49     |
| 26:BD:55:LYS:C    | 26:BD:57:ALA:H    | 2.17        | 0.49     |
| 23:DB:2314:A:H2'  | 23:DB:2315:G:C8   | 2.47        | 0.49     |
| 41:BJ:25:LEU:O    | 41:BJ:27:ARG:N    | 2.44        | 0.49     |
| 47:DF:84:ILE:HG22 | 47:DF:84:ILE:O    | 2.12        | 0.49     |
| 23:DB:672:C:H2'   | 23:DB:673:C:C6    | 2.47        | 0.49     |
| 39:BX:28:LEU:HD13 | 39:BX:37:LEU:CD1  | 2.40        | 0.49     |
| 41:BJ:45:THR:OG1  | 41:BJ:48:VAL:HB   | 2.13        | 0.49     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 44:BQ:60:TRP:C    | 44:BQ:64:ILE:HG12  | 2.33        | 0.49     |
| 53:B6:14:MET:HG2  | 53:B6:129:ILE:HG23 | 1.95        | 0.49     |
| 30:BY:11:SER:HA   | 30:BY:31:ILE:HG22  | 1.95        | 0.49     |
| 33:B1:26:LYS:HB2  | 33:B1:52:LYS:HZ3   | 1.78        | 0.49     |
| 47:BF:74:ALA:HB1  | 47:BF:76:PHE:CD2   | 2.48        | 0.49     |
| 46:DU:81:ARG:HH21 | 46:DU:81:ARG:N     | 2.10        | 0.49     |
| 29:BE:126:VAL:CG2 | 29:BE:133:LEU:HB2  | 2.43        | 0.49     |
| 42:DN:83:LEU:HD12 | 42:DN:84:GLY:N     | 2.28        | 0.49     |
| 1:CA:1225:A:N3    | 1:CA:1225:A:H2'    | 2.27        | 0.49     |
| 12:AM:52:ILE:HG23 | 12:AM:56:ARG:NH1   | 2.17        | 0.49     |
| 23:DB:483:A:O2'   | 46:DU:56:GLY:HA2   | 2.13        | 0.49     |
| 23:DB:1025:G:H1'  | 23:DB:1135:C:O5'   | 2.13        | 0.49     |
| 13:AN:16:ALA:HA   | 13:AN:54:SER:O     | 2.13        | 0.49     |
| 23:BB:981:A:H4'   | 23:BB:2037:A:H5'   | 1.95        | 0.49     |
| 31:B0:42:ILE:HG22 | 31:B0:43:THR:O     | 2.13        | 0.49     |
| 15:AP:67:ILE:HG13 | 15:AP:71:VAL:HG13  | 1.94        | 0.49     |
| 23:BB:973:A:OP1   | 23:BB:973:A:H8     | 1.95        | 0.49     |
| 25:BC:14:HIS:O    | 25:BC:16:VAL:HG23  | 2.13        | 0.49     |
| 27:DK:42:THR:O    | 27:DK:44:LYS:HG2   | 2.12        | 0.49     |
| 20:AB:16:GLY:HA2  | 20:AB:40:ILE:CG1   | 2.42        | 0.49     |
| 20:AB:16:GLY:HA3  | 20:AB:39:ILE:HA    | 1.94        | 0.49     |
| 38:BM:32:GLY:HA2  | 38:BM:117:PHE:CZ   | 2.48        | 0.49     |
| 31:D0:39:ARG:O    | 31:D0:40:HIS:HB2   | 2.12        | 0.49     |
| 35:BV:42:LEU:HD23 | 35:BV:42:LEU:N     | 2.25        | 0.49     |
| 27:DK:58:LEU:CD1  | 27:DK:86:LEU:HB3   | 2.39        | 0.49     |
| 1:CA:192:A:O2'    | 1:CA:193:C:H5'     | 2.12        | 0.49     |
| 46:BU:21:ARG:HD3  | 46:BU:72:PHE:CD2   | 2.48        | 0.49     |
| 23:DB:263:G:H2'   | 23:DB:264:C:O4'    | 2.12        | 0.49     |
| 11:AL:79:ILE:HD12 | 11:AL:96:THR:CG2   | 2.43        | 0.49     |
| 23:BB:629:G:H5''  | 23:BB:650:C:O2'    | 2.12        | 0.49     |
| 23:BB:1131:G:N2   | 23:BB:2024:G:N2    | 2.60        | 0.49     |
| 1:AA:490:C:H2'    | 1:AA:491:G:H8      | 1.77        | 0.49     |
| 6:AG:47:GLU:OE1   | 6:AG:57:GLU:HG2    | 2.12        | 0.49     |
| 23:DB:365:U:H2'   | 23:DB:366:C:H6     | 1.71        | 0.49     |
| 30:BY:6:ILE:HG21  | 30:BY:47:ILE:HD12  | 1.94        | 0.49     |
| 1:AA:1329:A:H5''  | 12:AM:24:VAL:HA    | 1.93        | 0.49     |
| 23:BB:2285:C:OP2  | 33:B1:5:ARG:HD3    | 2.12        | 0.49     |
| 19:AT:79:THR:O    | 19:AT:82:ILE:HG12  | 2.13        | 0.49     |
| 25:DC:116:GLN:O   | 25:DC:127:ASN:HA   | 2.13        | 0.49     |
| 23:BB:1407:G:H2'  | 23:BB:1408:G:C8    | 2.45        | 0.49     |
| 23:BB:1983:G:H4'  | 23:BB:2606:C:H4'   | 1.95        | 0.49     |
| 23:BB:2070:A:H2'  | 23:BB:2071:A:H8    | 1.78        | 0.49     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 26:BD:122:VAL:HA   | 26:BD:127:PHE:N    | 2.28        | 0.49     |
| 23:BB:2816:G:O2'   | 23:BB:2817:U:H5'   | 2.13        | 0.49     |
| 23:DB:1719:G:O2'   | 23:DB:1720:U:H5'   | 2.13        | 0.49     |
| 23:DB:2813:A:H2'   | 23:DB:2814:A:H8    | 1.75        | 0.49     |
| 29:DE:37:ALA:C     | 29:DE:39:ALA:H     | 2.16        | 0.49     |
| 23:DB:2834:G:H1'   | 23:DB:2883:A:N6    | 2.27        | 0.49     |
| 2:CC:179:ALA:HB3   | 2:CC:181:ILE:HD11  | 1.95        | 0.49     |
| 1:CA:811:C:H4'     | 1:CA:900:A:N6      | 2.27        | 0.49     |
| 17:CR:44:THR:OG1   | 17:CR:46:THR:HG22  | 2.13        | 0.49     |
| 1:CA:558:G:H8      | 1:CA:559:A:H2'     | 1.78        | 0.49     |
| 23:DB:2559:C:H2'   | 23:DB:2560:A:H8    | 1.78        | 0.49     |
| 40:BH:30:LEU:O     | 40:BH:35:LYS:HB2   | 2.13        | 0.49     |
| 33:D1:28:THR:O     | 33:D1:29:LYS:HD2   | 2.13        | 0.49     |
| 23:BB:516:C:H2'    | 23:BB:517:C:C6     | 2.48        | 0.49     |
| 1:CA:251:G:N3      | 1:CA:266:G:O6      | 2.46        | 0.49     |
| 28:BP:8:GLU:HG2    | 28:BP:54:LEU:HD23  | 1.94        | 0.49     |
| 6:CG:106:ALA:HB1   | 6:CG:132:THR:HB    | 1.94        | 0.49     |
| 10:AK:115:ILE:HD11 | 17:AR:72:ARG:HH12  | 1.78        | 0.49     |
| 9:AJ:35:GLN:HG2    | 9:AJ:78:GLU:OE1    | 2.13        | 0.49     |
| 1:AA:131:A:H2'     | 1:AA:132:C:C6      | 2.48        | 0.49     |
| 1:AA:1503:A:C8     | 1:AA:1531:A:N3     | 2.81        | 0.49     |
| 48:DG:133:LYS:H    | 48:DG:133:LYS:HD3  | 1.78        | 0.49     |
| 29:BE:88:ARG:HH21  | 29:BE:88:ARG:HG3   | 1.77        | 0.49     |
| 24:BI:2:LYS:NZ     | 24:BI:2:LYS:HB3    | 2.27        | 0.49     |
| 23:DB:1532:A:N3    | 23:DB:1532:A:H2'   | 2.25        | 0.49     |
| 23:BB:2327:A:H2'   | 23:BB:2328:A:C8    | 2.48        | 0.48     |
| 23:BB:2353:G:N3    | 52:BW:30:VAL:HG13  | 2.28        | 0.48     |
| 23:BB:2330:G:H1'   | 52:BW:38:ARG:HB3   | 1.95        | 0.48     |
| 25:DC:129:LEU:HB3  | 25:DC:134:ILE:HG22 | 1.93        | 0.48     |
| 44:BQ:29:ARG:NH1   | 44:BQ:29:ARG:HG2   | 2.28        | 0.48     |
| 16:CQ:62:GLU:HB2   | 16:CQ:72:TRP:CZ2   | 2.47        | 0.48     |
| 40:BH:97:ARG:HA    | 40:BH:112:LYS:CB   | 2.39        | 0.48     |
| 41:BJ:58:ASN:HA    | 41:BJ:127:GLY:HA2  | 1.94        | 0.48     |
| 35:DV:2:PHE:HD2    | 35:DV:59:GLU:OE1   | 1.97        | 0.48     |
| 23:BB:141:G:H5''   | 23:BB:142:A:O4'    | 2.13        | 0.48     |
| 26:DD:106:LYS:HD3  | 26:DD:106:LYS:N    | 2.28        | 0.48     |
| 12:AM:15:VAL:HG21  | 12:AM:40:GLU:HB3   | 1.95        | 0.48     |
| 3:CD:107:GLY:O     | 3:CD:157:ALA:HB1   | 2.12        | 0.48     |
| 13:AN:63:CYS:SG    | 13:AN:82:LYS:HG3   | 2.53        | 0.48     |
| 24:DI:131:THR:O    | 24:DI:135:MET:HG3  | 2.13        | 0.48     |
| 47:BF:16:MET:O     | 47:BF:20:ASN:HA    | 2.12        | 0.48     |
| 29:BE:153:LEU:HG   | 29:BE:154:ASP:N    | 2.28        | 0.48     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 12:AM:33:LEU:HD13 | 12:AM:39:ALA:O     | 2.13        | 0.48     |
| 12:AM:37:GLY:O    | 12:AM:38:ILE:HD13  | 2.13        | 0.48     |
| 50:DT:39:THR:O    | 50:DT:40:LYS:HB2   | 2.12        | 0.48     |
| 24:DI:27:LEU:HD23 | 24:DI:27:LEU:N     | 2.20        | 0.48     |
| 23:BB:1180:U:H2'  | 23:BB:1181:U:O4'   | 2.13        | 0.48     |
| 3:CD:173:ASP:CB   | 3:CD:178:GLU:HB2   | 2.36        | 0.48     |
| 11:CL:41:PRO:HB2  | 11:CL:88:ASP:HB3   | 1.96        | 0.48     |
| 23:DB:873:C:H2'   | 23:DB:874:G:C8     | 2.43        | 0.48     |
| 13:CN:52:ARG:C    | 13:CN:54:SER:H     | 2.15        | 0.48     |
| 18:CS:6:LYS:HD2   | 18:CS:6:LYS:N      | 2.28        | 0.48     |
| 27:DK:43:ILE:HG21 | 27:DK:46:ALA:HB2   | 1.95        | 0.48     |
| 22:BA:103:U:O2'   | 22:BA:104:A:H5'    | 2.12        | 0.48     |
| 23:BB:1198:U:H2'  | 23:BB:1199:U:H6    | 1.78        | 0.48     |
| 23:DB:847:U:O4'   | 23:DB:847:U:O2     | 2.31        | 0.48     |
| 22:DA:32:U:H4'    | 22:DA:52:A:N6      | 2.28        | 0.48     |
| 42:DN:65:LEU:O    | 42:DN:68:ALA:HB3   | 2.13        | 0.48     |
| 44:BQ:71:ASN:HD22 | 44:BQ:109:VAL:HG11 | 1.78        | 0.48     |
| 3:AD:123:MET:HA   | 3:AD:128:VAL:HA    | 1.95        | 0.48     |
| 28:DP:88:ARG:HB2  | 28:DP:112:ARG:NH1  | 2.28        | 0.48     |
| 23:DB:321:U:O4'   | 29:DE:159:LEU:HG   | 2.13        | 0.48     |
| 23:DB:1131:G:N2   | 23:DB:2024:G:N2    | 2.58        | 0.48     |
| 10:AK:110:THR:CG2 | 21:AU:4:LYS:HA     | 2.43        | 0.48     |
| 29:DE:46:GLN:HB3  | 29:DE:86:ALA:CA    | 2.42        | 0.48     |
| 1:CA:1522:U:H2'   | 1:CA:1523:G:H8     | 1.77        | 0.48     |
| 23:DB:2840:C:H2'  | 23:DB:2841:C:C6    | 2.48        | 0.48     |
| 50:DT:54:GLU:HB3  | 50:DT:88:LYS:HB2   | 1.94        | 0.48     |
| 1:CA:1084:G:H2'   | 1:CA:1085:U:C6     | 2.48        | 0.48     |
| 1:AA:1521:C:O2'   | 1:AA:1522:U:H5'    | 2.12        | 0.48     |
| 33:B1:3:GLY:C     | 33:B1:5:ARG:H      | 2.14        | 0.48     |
| 23:DB:1260:A:H2'  | 23:DB:1261:C:C6    | 2.47        | 0.48     |
| 23:DB:1000:A:H2'  | 23:DB:1001:A:H8    | 1.76        | 0.48     |
| 9:AJ:92:LEU:N     | 9:AJ:92:LEU:HD22   | 2.26        | 0.48     |
| 16:CQ:32:ILE:HG23 | 16:CQ:33:TYR:CD2   | 2.48        | 0.48     |
| 23:DB:1889:A:H2'  | 23:DB:1890:A:H8    | 1.75        | 0.48     |
| 23:DB:2686:G:H2'  | 23:DB:2687:U:C6    | 2.48        | 0.48     |
| 29:DE:102:ARG:O   | 29:DE:106:LYS:HG3  | 2.13        | 0.48     |
| 1:CA:201:G:H2'    | 1:CA:202:G:O4'     | 2.13        | 0.48     |
| 23:DB:656:G:H2'   | 23:DB:657:U:C6     | 2.48        | 0.48     |
| 23:DB:2008:C:H2'  | 23:DB:2009:A:H8    | 1.78        | 0.48     |
| 1:AA:558:G:C8     | 1:AA:559:A:H2'     | 2.48        | 0.48     |
| 23:BB:2201:G:O2'  | 23:BB:2202:U:H5'   | 2.12        | 0.48     |
| 23:DB:245:G:H2'   | 23:DB:246:C:H6     | 1.78        | 0.48     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 5:AF:42:TRP:HB2    | 5:AF:59:TYR:HB2    | 1.94        | 0.48     |
| 41:BJ:76:HIS:CE1   | 41:BJ:85:LYS:HB2   | 2.48        | 0.48     |
| 23:DB:736:C:H2'    | 23:DB:737:C:C6     | 2.48        | 0.48     |
| 37:BL:70:LYS:O     | 37:BL:73:ILE:HG12  | 2.13        | 0.48     |
| 22:DA:64:G:H2'     | 22:DA:65:U:C6      | 2.48        | 0.48     |
| 23:DB:527:C:O2     | 23:DB:527:C:O4'    | 2.30        | 0.48     |
| 18:AS:11:ASP:HB2   | 18:AS:14:LEU:HD23  | 1.94        | 0.48     |
| 2:AC:125:ARG:O     | 2:AC:126:ARG:HB2   | 2.13        | 0.48     |
| 48:BG:94:ARG:HB2   | 48:BG:127:GLN:HG3  | 1.95        | 0.48     |
| 20:AB:162:VAL:HG13 | 20:AB:184:ALA:CB   | 2.36        | 0.48     |
| 50:BT:1:MET:HB2    | 50:BT:2:ILE:HD13   | 1.94        | 0.48     |
| 47:BF:71:LYS:O     | 47:BF:72:SER:HB3   | 2.13        | 0.48     |
| 25:BC:106:PRO:O    | 25:BC:109:LEU:HD13 | 2.14        | 0.48     |
| 37:BL:4:ASN:N      | 37:BL:4:ASN:HD22   | 2.10        | 0.48     |
| 23:BB:321:U:H1'    | 29:BE:162:ARG:NH1  | 2.25        | 0.48     |
| 47:DF:113:PHE:HZ   | 47:DF:175:PRO:HB2  | 1.78        | 0.48     |
| 18:CS:39:ILE:HG21  | 18:CS:61:VAL:HG13  | 1.95        | 0.48     |
| 18:CS:46:LEU:O     | 18:CS:60:PHE:HA    | 2.12        | 0.48     |
| 13:AN:30:ILE:O     | 13:AN:40:ARG:HA    | 2.13        | 0.48     |
| 41:DJ:84:ILE:HG23  | 41:DJ:84:ILE:O     | 2.13        | 0.48     |
| 23:DB:138:U:O5'    | 23:DB:138:U:H6     | 1.95        | 0.48     |
| 9:AJ:52:LEU:HB2    | 13:AN:80:ARG:HD2   | 1.95        | 0.48     |
| 16:AQ:62:GLU:HB2   | 16:AQ:72:TRP:CZ2   | 2.48        | 0.48     |
| 29:DE:145:ASP:OD1  | 29:DE:183:PHE:HA   | 2.13        | 0.48     |
| 37:DL:2:ARG:O      | 37:DL:2:ARG:HG2    | 2.13        | 0.48     |
| 27:DK:43:ILE:CG2   | 27:DK:54:LYS:HA    | 2.42        | 0.48     |
| 49:DR:49:ILE:HG22  | 49:DR:54:VAL:HB    | 1.94        | 0.48     |
| 24:BI:21:PRO:CB    | 24:BI:22:PRO:HD3   | 2.40        | 0.48     |
| 23:DB:1438:U:H2'   | 23:DB:1439:A:O4'   | 2.12        | 0.48     |
| 29:BE:41:GLN:O     | 29:BE:42:GLY:O     | 2.31        | 0.48     |
| 46:BU:39:ASN:CG    | 46:BU:62:ALA:HB3   | 2.33        | 0.48     |
| 7:CH:58:LEU:CD2    | 7:CH:60:LEU:HB2    | 2.43        | 0.48     |
| 7:AH:11:THR:HA     | 7:AH:14:ARG:CZ     | 2.42        | 0.48     |
| 15:AP:43:ALA:HA    | 15:AP:46:LYS:HE3   | 1.95        | 0.48     |
| 13:AN:17:ASP:HA    | 13:AN:21:ALA:HB2   | 1.94        | 0.48     |
| 3:AD:129:VAL:HG12  | 3:AD:130:ASN:N     | 2.28        | 0.48     |
| 46:DU:48:VAL:O     | 46:DU:48:VAL:HG13  | 2.13        | 0.48     |
| 28:BP:50:ARG:HB3   | 28:BP:57:ALA:N     | 2.28        | 0.48     |
| 20:CB:20:ARG:HA    | 20:CB:20:ARG:NE    | 2.28        | 0.48     |
| 1:AA:1522:U:H2'    | 1:AA:1523:G:H8     | 1.78        | 0.48     |
| 46:BU:48:VAL:O     | 46:BU:48:VAL:HG13  | 2.13        | 0.48     |
| 1:CA:677:U:H2'     | 1:CA:678:U:H6      | 1.78        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:2026:U:H2'  | 23:BB:2027:G:C8   | 2.48        | 0.48     |
| 11:CL:106:VAL:HA  | 11:CL:107:LYS:NZ  | 2.29        | 0.48     |
| 6:CG:68:VAL:CG1   | 6:CG:133:ALA:HB1  | 2.42        | 0.48     |
| 42:BN:12:ARG:HG3  | 42:BN:13:ASN:N    | 2.28        | 0.48     |
| 23:BB:540:C:O2'   | 23:BB:541:A:H5'   | 2.13        | 0.48     |
| 11:CL:7:VAL:HG22  | 16:CQ:33:TYR:CD1  | 2.48        | 0.48     |
| 23:DB:2699:C:H2'  | 23:DB:2700:A:H8   | 1.77        | 0.48     |
| 22:BA:49:C:O2'    | 22:BA:50:A:H5'    | 2.13        | 0.48     |
| 22:BA:49:C:OP1    | 43:BO:101:GLY:HA3 | 2.13        | 0.48     |
| 23:DB:379:G:O4'   | 23:DB:2232:C:H5'' | 2.14        | 0.48     |
| 1:CA:1036:A:H2'   | 1:CA:1037:C:C6    | 2.48        | 0.48     |
| 41:BJ:13:ARG:O    | 41:BJ:14:ASP:HB2  | 2.12        | 0.48     |
| 22:BA:93:C:H2'    | 22:BA:94:A:H8     | 1.78        | 0.48     |
| 23:BB:325:G:H2'   | 23:BB:326:G:H8    | 1.78        | 0.48     |
| 37:BL:136:GLU:HA  | 37:BL:140:GLY:HA3 | 1.94        | 0.48     |
| 23:BB:942:G:O2'   | 23:BB:943:A:H5'   | 2.12        | 0.48     |
| 22:DA:35:C:H2'    | 22:DA:36:C:H5'    | 1.95        | 0.48     |
| 23:BB:779:U:H2'   | 23:BB:780:G:C8    | 2.48        | 0.48     |
| 4:CE:87:VAL:HG23  | 4:CE:92:ARG:HA    | 1.95        | 0.48     |
| 53:B6:4:LYS:HA    | 53:B6:7:TYR:HD2   | 1.77        | 0.48     |
| 24:BI:52:LEU:HD12 | 24:BI:52:LEU:N    | 2.28        | 0.48     |
| 23:BB:1234:U:H2'  | 23:BB:1235:G:O4'  | 2.12        | 0.48     |
| 29:BE:3:LEU:CB    | 29:BE:12:LEU:HB2  | 2.43        | 0.48     |
| 23:DB:2829:A:O2'  | 23:DB:2830:C:H5'  | 2.14        | 0.48     |
| 7:CH:23:ALA:CB    | 7:CH:61:THR:HA    | 2.44        | 0.48     |
| 24:DI:89:SER:HA   | 24:DI:97:VAL:HG11 | 1.96        | 0.48     |
| 23:DB:1038:G:O2'  | 23:DB:1039:A:H5'  | 2.13        | 0.48     |
| 23:DB:2611:C:O2'  | 23:DB:2612:C:H5'  | 2.12        | 0.48     |
| 23:DB:1693:U:H4'  | 23:DB:1694:C:OP2  | 2.13        | 0.48     |
| 1:AA:1379:G:O2'   | 1:AA:1380:U:H5'   | 2.13        | 0.48     |
| 4:CE:79:THR:OG1   | 4:CE:97:PRO:HA    | 2.13        | 0.48     |
| 40:DH:25:TYR:O    | 40:DH:30:LEU:HG   | 2.13        | 0.48     |
| 1:AA:409:U:OP1    | 3:AD:23:GLY:HA3   | 2.12        | 0.48     |
| 6:AG:94:ARG:NH1   | 6:AG:98:LEU:HD21  | 2.28        | 0.48     |
| 23:DB:1155:A:O2'  | 23:DB:1156:A:H2'  | 2.13        | 0.48     |
| 1:CA:1125:U:O2'   | 1:CA:1126:U:H2'   | 2.13        | 0.48     |
| 15:AP:12:LYS:C    | 15:AP:14:ARG:H    | 2.16        | 0.48     |
| 23:BB:2076:U:O4'  | 23:BB:2076:U:O2   | 2.28        | 0.48     |
| 1:CA:80:A:H2'     | 1:CA:81:A:C8      | 2.48        | 0.48     |
| 40:BH:27:ARG:O    | 40:BH:28:ASN:ND2  | 2.46        | 0.48     |
| 2:CC:125:ARG:O    | 2:CC:126:ARG:HB2  | 2.13        | 0.48     |
| 40:DH:27:ARG:O    | 40:DH:28:ASN:ND2  | 2.46        | 0.48     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BC:119:VAL:HG13 | 25:BC:133:ASN:HD21 | 1.79        | 0.48     |
| 23:DB:2355:G:O3'   | 52:DW:20:LEU:HD13  | 2.13        | 0.48     |
| 25:DC:89:ASN:O     | 25:DC:105:ALA:HB3  | 2.13        | 0.48     |
| 25:DC:188:ARG:HG2  | 25:DC:188:ARG:HH21 | 1.78        | 0.48     |
| 48:BG:91:VAL:HG23  | 48:BG:92:GLY:H     | 1.78        | 0.48     |
| 23:DB:572:A:C2     | 23:DB:2033:A:C2    | 3.01        | 0.48     |
| 20:AB:164:ASP:OD1  | 20:AB:203:ASP:HB2  | 2.12        | 0.48     |
| 40:BH:81:ALA:HB2   | 40:BH:147:VAL:HG23 | 1.95        | 0.48     |
| 53:B6:77:LYS:HE2   | 53:B6:94:ASN:ND2   | 2.07        | 0.48     |
| 44:DQ:91:ARG:NH1   | 49:DR:10:LYS:HB3   | 2.28        | 0.48     |
| 26:DD:54:ALA:HA    | 26:DD:76:GLY:N     | 2.29        | 0.48     |
| 48:DG:17:LYS:O     | 48:DG:23:ILE:HG23  | 2.13        | 0.48     |
| 1:CA:1014:A:H5''   | 18:CS:13:HIS:HB3   | 1.95        | 0.48     |
| 41:BJ:4:PHE:HB3    | 41:BJ:44:TYR:CE1   | 2.47        | 0.48     |
| 1:AA:1277:C:H1'    | 1:AA:1282:C:O2     | 2.13        | 0.48     |
| 47:BF:104:THR:C    | 47:BF:108:PRO:HG2  | 2.33        | 0.48     |
| 47:DF:142:TYR:CD1  | 47:DF:142:TYR:N    | 2.78        | 0.48     |
| 18:AS:44:ILE:HA    | 18:AS:61:VAL:CG1   | 2.43        | 0.48     |
| 29:BE:56:GLY:O     | 29:BE:58:LYS:HD3   | 2.13        | 0.48     |
| 41:BJ:81:ILE:HG12  | 41:BJ:82:GLY:N     | 2.27        | 0.48     |
| 8:AI:33:SER:HB3    | 8:AI:36:GLN:HE21   | 1.78        | 0.48     |
| 8:AI:33:SER:HB3    | 8:AI:36:GLN:NE2    | 2.28        | 0.48     |
| 28:DP:99:LEU:O     | 28:DP:99:LEU:HD13  | 2.13        | 0.48     |
| 23:BB:2732:G:H5'   | 23:BB:2733:A:O4'   | 2.13        | 0.48     |
| 45:BS:55:ILE:CD1   | 45:BS:107:VAL:HG21 | 2.43        | 0.48     |
| 25:BC:15:VAL:HA    | 25:BC:203:VAL:HG12 | 1.95        | 0.48     |
| 29:DE:115:GLN:O    | 29:DE:117:ARG:HG3  | 2.13        | 0.48     |
| 27:DK:54:LYS:HD2   | 27:DK:54:LYS:N     | 2.20        | 0.48     |
| 44:DQ:71:ASN:HD22  | 44:DQ:109:VAL:HG11 | 1.77        | 0.48     |
| 3:AD:154:VAL:HG23  | 3:AD:155:LYS:HD2   | 1.94        | 0.48     |
| 20:CB:67:LEU:HA    | 20:CB:89:PHE:O     | 2.12        | 0.48     |
| 11:AL:81:ILE:HG23  | 11:AL:94:TYR:HB3   | 1.94        | 0.48     |
| 20:AB:122:ASP:O    | 20:AB:125:PHE:HD2  | 1.96        | 0.48     |
| 46:BU:39:ASN:CB    | 46:BU:62:ALA:HB3   | 2.42        | 0.48     |
| 10:AK:17:ASP:HA    | 10:AK:80:ASN:O     | 2.13        | 0.48     |
| 1:AA:309:A:O2'     | 1:AA:310:G:H5'     | 2.13        | 0.48     |
| 19:CT:70:LYS:HA    | 19:CT:73:ARG:NH1   | 2.28        | 0.48     |
| 1:CA:338:A:H2'     | 1:CA:339:C:H6      | 1.78        | 0.48     |
| 1:CA:1124:G:H5''   | 9:CJ:37:ARG:O      | 2.13        | 0.48     |
| 3:CD:170:LEU:HB2   | 3:CD:180:THR:O     | 2.13        | 0.48     |
| 1:AA:17:U:O2'      | 1:AA:18:C:H5'      | 2.14        | 0.48     |
| 23:BB:1810:A:H2'   | 23:BB:1811:G:O4'   | 2.13        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:DD:14:ILE:O    | 26:DD:14:ILE:HG23 | 2.14        | 0.48     |
| 1:AA:169:C:O2'    | 1:AA:170:U:H5'    | 2.13        | 0.48     |
| 1:AA:66:A:H5''    | 1:AA:199:A:H4'    | 1.95        | 0.48     |
| 23:BB:2028:U:H2'  | 23:BB:2029:G:C8   | 2.48        | 0.48     |
| 23:BB:1327:A:H2'  | 23:BB:1328:A:O4'  | 2.13        | 0.48     |
| 23:BB:2074:U:O2'  | 23:BB:2075:U:H5'  | 2.13        | 0.48     |
| 23:DB:100:U:OP1   | 23:DB:101:A:O5'   | 2.31        | 0.48     |
| 23:DB:2799:A:O3'  | 23:DB:2800:A:O4'  | 2.31        | 0.48     |
| 23:BB:231:A:H3'   | 23:BB:232:G:H8    | 1.78        | 0.48     |
| 1:AA:586:C:O2'    | 1:AA:587:G:H5'    | 2.14        | 0.48     |
| 1:CA:694:A:C2     | 1:CA:695:A:H1'    | 2.49        | 0.48     |
| 50:BT:32:LEU:N    | 50:BT:83:ALA:HB3  | 2.27        | 0.48     |
| 12:AM:22:TYR:O    | 12:AM:68:LEU:HD12 | 2.13        | 0.48     |
| 1:CA:586:C:O2'    | 1:CA:587:G:H5'    | 2.13        | 0.48     |
| 23:DB:1047:G:H1'  | 23:DB:1111:A:N6   | 2.28        | 0.48     |
| 23:DB:106:C:H2'   | 23:DB:107:G:C8    | 2.47        | 0.48     |
| 27:BK:25:LEU:HD11 | 27:BK:40:LYS:N    | 2.28        | 0.48     |
| 23:BB:1495:A:O2'  | 23:BB:1496:A:H5'  | 2.13        | 0.48     |
| 23:DB:2597:G:C6   | 23:DB:2598:A:N6   | 2.81        | 0.48     |
| 1:AA:363:A:P      | 11:AL:57:THR:HG21 | 2.54        | 0.48     |
| 42:DN:64:ARG:O    | 42:DN:67:PHE:HB3  | 2.12        | 0.48     |
| 23:DB:1266:G:N2   | 23:DB:2012:G:H2'  | 2.27        | 0.48     |
| 23:DB:2798:U:O5'  | 23:DB:2798:U:H6   | 1.95        | 0.48     |
| 23:DB:1064:C:H2'  | 23:DB:1065:U:O4'  | 2.14        | 0.48     |
| 5:CF:32:ALA:O     | 5:CF:33:GLU:HB2   | 2.13        | 0.48     |
| 23:DB:769:U:H2'   | 23:DB:770:G:C8    | 2.49        | 0.48     |
| 23:BB:858:G:H21   | 23:BB:2268:A:H3'  | 1.78        | 0.48     |
| 23:BB:2365:G:O2'  | 52:BW:59:PHE:HE1  | 1.96        | 0.48     |
| 25:BC:185:ALA:C   | 25:BC:187:CYS:H   | 2.17        | 0.48     |
| 23:DB:2752:C:H2'  | 23:DB:2753:A:O4'  | 2.13        | 0.48     |
| 23:DB:919:U:H2'   | 23:DB:920:A:H8    | 1.72        | 0.48     |
| 52:DW:66:VAL:HA   | 52:DW:81:ILE:HG22 | 1.95        | 0.48     |
| 50:BT:2:ILE:HG12  | 50:BT:3:ARG:H     | 1.79        | 0.48     |
| 48:BG:36:LEU:N    | 48:BG:36:LEU:HD22 | 2.29        | 0.48     |
| 42:BN:8:ARG:HB2   | 42:BN:43:GLU:OE1  | 2.13        | 0.48     |
| 1:AA:947:G:H4'    | 12:AM:107:THR:OG1 | 2.14        | 0.48     |
| 23:BB:988:A:C8    | 30:BY:13:ILE:HD12 | 2.48        | 0.48     |
| 4:CE:132:PRO:O    | 4:CE:136:VAL:HG12 | 2.13        | 0.48     |
| 18:CS:61:VAL:HG12 | 18:CS:62:THR:N    | 2.27        | 0.48     |
| 18:CS:62:THR:H    | 18:CS:65:MET:HB3  | 1.78        | 0.48     |
| 10:CK:92:ARG:NH2  | 21:CU:24:LYS:HG2  | 2.27        | 0.48     |
| 13:CN:30:ILE:O    | 13:CN:40:ARG:HA   | 2.13        | 0.48     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:2547:A:H4'   | 27:BK:29:HIS:CE1   | 2.48        | 0.48     |
| 25:BC:16:VAL:N     | 25:BC:203:VAL:HG12 | 2.28        | 0.48     |
| 20:AB:16:GLY:HA2   | 20:AB:40:ILE:HD12  | 1.95        | 0.48     |
| 3:CD:123:MET:HA    | 3:CD:128:VAL:HA    | 1.95        | 0.48     |
| 31:D0:32:THR:OG1   | 31:D0:50:GLY:HA2   | 2.13        | 0.48     |
| 49:BR:38:VAL:HG13  | 49:BR:54:VAL:HG12  | 1.94        | 0.48     |
| 9:CJ:8:ILE:N       | 9:CJ:8:ILE:HD12    | 2.29        | 0.48     |
| 20:AB:101:THR:HG23 | 20:AB:102:ASN:N    | 2.28        | 0.48     |
| 37:BL:99:ASN:O     | 37:BL:100:ILE:HB   | 2.13        | 0.48     |
| 45:DS:50:VAL:HA    | 45:DS:53:SER:HB3   | 1.95        | 0.48     |
| 10:AK:80:ASN:CB    | 10:AK:105:ARG:HB3  | 2.44        | 0.48     |
| 23:BB:2821:A:OP2   | 26:BD:115:GLY:HA3  | 2.14        | 0.48     |
| 38:BM:31:PHE:HB3   | 38:BM:130:PHE:CZ   | 2.48        | 0.48     |
| 4:CE:45:VAL:HG13   | 4:CE:117:ALA:HA    | 1.94        | 0.48     |
| 1:CA:490:C:H2'     | 1:CA:491:G:H8      | 1.78        | 0.48     |
| 41:BJ:100:VAL:O    | 41:BJ:104:ALA:HB2  | 2.14        | 0.48     |
| 1:AA:265:G:H4'     | 16:AQ:67:SER:HA    | 1.95        | 0.48     |
| 8:CI:9:GLY:HA2     | 8:CI:80:HIS:HD2    | 1.76        | 0.48     |
| 1:AA:236:A:H2'     | 1:AA:237:G:H8      | 1.78        | 0.48     |
| 36:D2:9:VAL:CG1    | 36:D2:10:LEU:N     | 2.77        | 0.48     |
| 39:DX:55:THR:O     | 39:DX:58:ASN:HB3   | 2.14        | 0.48     |
| 23:DB:540:C:O2'    | 23:DB:541:A:H5'    | 2.13        | 0.48     |
| 1:CA:401:C:H2'     | 1:CA:402:G:H8      | 1.79        | 0.48     |
| 23:BB:1999:C:O2'   | 23:BB:2000:C:H5'   | 2.14        | 0.48     |
| 23:BB:1874:C:H2'   | 23:BB:1875:G:O4'   | 2.13        | 0.48     |
| 20:CB:71:THR:HG23  | 20:CB:94:ARG:H     | 1.79        | 0.48     |
| 23:BB:2100:G:C6    | 23:BB:2190:G:C6    | 3.02        | 0.48     |
| 14:CO:8:THR:O      | 14:CO:11:ILE:HG22  | 2.12        | 0.48     |
| 38:BM:69:PRO:HA    | 38:BM:94:ALA:HB2   | 1.95        | 0.48     |
| 9:CJ:92:LEU:HD13   | 9:CJ:92:LEU:N      | 2.28        | 0.48     |
| 9:CJ:83:THR:O      | 9:CJ:86:ALA:HB3    | 2.13        | 0.48     |
| 1:AA:448:A:H2'     | 1:AA:449:G:C8      | 2.48        | 0.48     |
| 23:BB:2854:G:H2'   | 23:BB:2855:C:H6    | 1.77        | 0.48     |
| 23:BB:818:G:N1     | 23:BB:1187:G:H2'   | 2.28        | 0.48     |
| 1:AA:663:A:H5'     | 1:AA:836:G:OP1     | 2.13        | 0.48     |
| 23:BB:935:C:O2'    | 23:BB:936:A:H5'    | 2.14        | 0.48     |
| 23:BB:2784:U:H2'   | 23:BB:2785:C:H6    | 1.78        | 0.48     |
| 22:BA:88:C:O2'     | 22:BA:89:U:H5''    | 2.14        | 0.48     |
| 23:DB:1047:G:H3'   | 23:DB:1048:A:H5'   | 1.96        | 0.48     |
| 23:BB:2529:G:H4'   | 48:BG:174:LYS:HB2  | 1.94        | 0.48     |
| 1:CA:98:A:H2'      | 1:CA:99:C:H6       | 1.78        | 0.48     |
| 23:BB:2678:C:H2'   | 23:BB:2679:A:H8    | 1.77        | 0.48     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 43:DO:100:HIS:C   | 43:DO:104:GLN:HB2  | 2.34        | 0.48     |
| 10:AK:63:GLN:O    | 10:AK:67:GLU:HG2   | 2.13        | 0.48     |
| 23:BB:2597:G:C6   | 23:BB:2598:A:N6    | 2.81        | 0.48     |
| 23:BB:429:A:H2'   | 23:BB:430:A:C8     | 2.48        | 0.48     |
| 23:DB:789:A:H5''  | 57:DB:3670:HOH:O   | 2.12        | 0.48     |
| 23:DB:1798:U:OP1  | 25:DC:257:ARG:HB2  | 2.13        | 0.48     |
| 8:CI:42:THR:O     | 8:CI:45:MET:HG2    | 2.13        | 0.48     |
| 23:BB:1838:C:H4'  | 23:BB:1839:G:H8    | 1.78        | 0.48     |
| 23:DB:283:G:H2'   | 23:DB:284:U:O4'    | 2.13        | 0.48     |
| 23:DB:67:U:H2'    | 23:DB:68:G:H8      | 1.77        | 0.48     |
| 23:DB:112:U:H2'   | 23:DB:113:U:H5'    | 1.96        | 0.48     |
| 23:BB:2519:U:C6   | 23:BB:2542:A:N6    | 2.82        | 0.48     |
| 23:DB:1799:G:H4'  | 23:DB:1800:C:O5'   | 2.14        | 0.48     |
| 52:DW:30:VAL:HA   | 52:DW:60:ALA:O     | 2.13        | 0.48     |
| 53:B6:78:ALA:O    | 53:B6:82:ALA:HB2   | 2.13        | 0.48     |
| 53:B6:92:PRO:CG   | 53:B6:101:ILE:HG12 | 2.43        | 0.48     |
| 40:BH:99:ILE:HD12 | 40:BH:130:VAL:HG11 | 1.96        | 0.48     |
| 44:DQ:94:LEU:HD21 | 49:DR:11:GLN:HB2   | 1.94        | 0.48     |
| 8:AI:16:ALA:HA    | 8:AI:66:VAL:HA     | 1.96        | 0.48     |
| 5:AF:3:HIS:CE1    | 5:AF:95:ALA:H      | 2.31        | 0.48     |
| 13:AN:60:ARG:NE   | 13:AN:69:PRO:HB3   | 2.29        | 0.48     |
| 23:DB:496:G:H4'   | 45:DS:61:ASN:ND2   | 2.29        | 0.48     |
| 7:AH:77:VAL:HG11  | 7:AH:124:ILE:HG21  | 1.95        | 0.48     |
| 41:BJ:44:TYR:C    | 41:BJ:44:TYR:CD2   | 2.86        | 0.48     |
| 45:BS:17:VAL:HG11 | 45:BS:103:ILE:HG12 | 1.96        | 0.48     |
| 33:D1:33:LEU:HD12 | 33:D1:34:GLU:H     | 1.77        | 0.48     |
| 43:DO:49:VAL:HG11 | 43:DO:82:ALA:HA    | 1.95        | 0.48     |
| 31:B0:39:ARG:O    | 31:B0:40:HIS:HB2   | 2.13        | 0.48     |
| 13:CN:30:ILE:CG2  | 13:CN:41:TRP:HB2   | 2.40        | 0.48     |
| 35:DV:77:VAL:CG1  | 38:DM:136:MET:HB3  | 2.44        | 0.48     |
| 20:AB:15:PHE:CD1  | 20:AB:16:GLY:N     | 2.81        | 0.48     |
| 8:CI:87:MET:HE2   | 8:CI:87:MET:O      | 2.13        | 0.48     |
| 1:CA:332:G:OP2    | 19:CT:4:LYS:HB2    | 2.14        | 0.48     |
| 38:BM:26:VAL:HA   | 38:BM:66:ARG:HH21  | 1.78        | 0.48     |
| 49:BR:39:LEU:N    | 49:BR:39:LEU:HD23  | 2.29        | 0.48     |
| 37:DL:96:LYS:HD3  | 37:DL:103:ILE:HA   | 1.96        | 0.48     |
| 23:BB:2143:C:N3   | 23:BB:2148:G:O6    | 2.46        | 0.48     |
| 38:BM:55:ARG:CA   | 38:BM:55:ARG:HH21  | 2.22        | 0.48     |
| 1:AA:906:A:C2'    | 1:AA:907:A:H5''    | 2.43        | 0.48     |
| 46:DU:21:ARG:HD3  | 46:DU:72:PHE:CD2   | 2.48        | 0.48     |
| 26:BD:69:ALA:HA   | 26:BD:73:VAL:HB    | 1.95        | 0.48     |
| 22:BA:101:A:H4'   | 23:BB:864:G:H4'    | 1.94        | 0.48     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:2015:A:H2'   | 23:BB:2016:U:O4'   | 2.13        | 0.48     |
| 38:DM:4:PRO:HG2    | 38:DM:70:ASP:HA    | 1.94        | 0.48     |
| 23:DB:150:U:H2'    | 23:DB:151:C:H6     | 1.78        | 0.48     |
| 1:AA:474:G:H2'     | 1:AA:475:C:H6      | 1.78        | 0.48     |
| 37:DL:3:LEU:O      | 37:DL:5:THR:N      | 2.45        | 0.48     |
| 1:CA:1460:C:H2'    | 1:CA:1461:G:C8     | 2.49        | 0.48     |
| 23:DB:15:G:O2'     | 23:DB:16:C:H5'     | 2.14        | 0.48     |
| 1:AA:1330:U:H2'    | 1:AA:1331:G:H5'    | 1.95        | 0.48     |
| 12:CM:19:THR:HA    | 12:CM:24:VAL:HG23  | 1.95        | 0.48     |
| 1:AA:807:A:H2'     | 1:AA:808:C:C6      | 2.48        | 0.48     |
| 23:BB:1000:A:H2'   | 23:BB:1001:A:H8    | 1.77        | 0.48     |
| 11:CL:54:VAL:HG12  | 11:CL:55:ARG:N     | 2.29        | 0.48     |
| 6:AG:135:LYS:HE2   | 6:AG:139:ASP:OD2   | 2.14        | 0.48     |
| 23:DB:1924:C:O2'   | 23:DB:1925:C:H5'   | 2.14        | 0.48     |
| 23:BB:2699:C:H2'   | 23:BB:2700:A:H8    | 1.78        | 0.48     |
| 23:DB:876:C:H3'    | 23:DB:877:A:C8     | 2.48        | 0.48     |
| 3:CD:115:GLN:HE21  | 3:CD:119:HIS:CE1   | 2.31        | 0.48     |
| 40:BH:67:ALA:HB1   | 40:BH:70:GLU:CG    | 2.43        | 0.48     |
| 41:DJ:72:LYS:CB    | 41:DJ:89:PHE:H     | 2.26        | 0.48     |
| 6:CG:89:GLU:OE1    | 6:CG:152:HIS:NE2   | 2.47        | 0.48     |
| 23:DB:2545:G:O2'   | 23:DB:2546:U:H5'   | 2.13        | 0.48     |
| 5:CF:86:ARG:HH11   | 17:CR:64:LEU:HD12  | 1.78        | 0.48     |
| 1:AA:1477:U:H2'    | 1:AA:1478:U:H6     | 1.78        | 0.48     |
| 43:DO:100:HIS:CA   | 43:DO:104:GLN:HB2  | 2.44        | 0.48     |
| 7:AH:118:ALA:HB3   | 7:AH:120:LEU:CD2   | 2.43        | 0.48     |
| 1:CA:224:U:H2'     | 1:CA:225:C:H6      | 1.78        | 0.48     |
| 1:AA:1244:G:H2'    | 1:AA:1245:C:C6     | 2.48        | 0.48     |
| 1:AA:178:C:O2'     | 1:AA:179:A:H5'     | 2.14        | 0.48     |
| 50:DT:61:LEU:HD12  | 50:DT:62:VAL:O     | 2.13        | 0.48     |
| 23:DB:2011:U:H2'   | 23:DB:2012:G:O4'   | 2.14        | 0.48     |
| 1:AA:542:G:O2'     | 1:AA:543:U:H5'     | 2.12        | 0.48     |
| 41:DJ:133:ALA:C    | 41:DJ:135:GLN:H    | 2.17        | 0.48     |
| 23:DB:2588:G:H2'   | 23:DB:2589:A:O4'   | 2.13        | 0.48     |
| 1:CA:64:G:H3'      | 1:CA:64:G:OP1      | 2.13        | 0.48     |
| 44:BQ:20:ALA:HA    | 44:BQ:23:TYR:CE1   | 2.49        | 0.48     |
| 47:BF:91:ARG:O     | 47:BF:92:GLY:C     | 2.51        | 0.48     |
| 20:AB:209:VAL:HG23 | 20:AB:210:THR:H    | 1.79        | 0.48     |
| 26:BD:106:LYS:N    | 26:BD:106:LYS:HD3  | 2.28        | 0.48     |
| 53:D6:80:GLU:CA    | 53:D6:83:ILE:HG12  | 2.41        | 0.48     |
| 8:CI:120:ALA:O     | 8:CI:121:ARG:HG2   | 2.14        | 0.48     |
| 35:DV:71:LYS:O     | 35:DV:94:ALA:HB2   | 2.14        | 0.48     |
| 1:CA:1493:A:OP1    | 55:CA:1662:PAR:H51 | 2.12        | 0.48     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 13:AN:9:GLU:HB2    | 13:AN:62:ARG:NE    | 2.29        | 0.48     |
| 47:DF:148:VAL:O    | 47:DF:149:ARG:HG2  | 2.13        | 0.48     |
| 1:AA:1283:U:O2'    | 1:AA:1284:C:H5'    | 2.13        | 0.48     |
| 23:BB:1076:C:H4'   | 24:BI:94:LYS:NZ    | 2.28        | 0.48     |
| 45:DS:17:VAL:HG11  | 45:DS:103:ILE:HG12 | 1.95        | 0.48     |
| 47:DF:168:LEU:HD13 | 47:DF:172:PHE:HE2  | 1.79        | 0.48     |
| 18:CS:42:ASN:N     | 18:CS:42:ASN:HD22  | 2.10        | 0.48     |
| 13:AN:20:PHE:CB    | 13:AN:24:ALA:HB2   | 2.44        | 0.48     |
| 16:AQ:60:ILE:HD13  | 16:AQ:60:ILE:H     | 1.78        | 0.48     |
| 23:BB:1176:U:H2'   | 23:BB:1177:G:O4'   | 2.13        | 0.48     |
| 52:BW:9:THR:OG1    | 52:BW:10:ARG:N     | 2.45        | 0.48     |
| 23:DB:587:C:O2'    | 37:DL:19:LEU:HD13  | 2.14        | 0.48     |
| 23:DB:2869:G:H2'   | 23:DB:2870:C:C6    | 2.48        | 0.48     |
| 48:DG:163:TYR:O    | 48:DG:165:ASP:N    | 2.47        | 0.48     |
| 23:DB:549:G:H2'    | 41:DJ:2:LYS:CE     | 2.43        | 0.48     |
| 1:CA:719:C:H2'     | 17:CR:38:ILE:HD11  | 1.96        | 0.48     |
| 23:BB:1278:C:O3'   | 42:BN:34:ILE:HG23  | 2.13        | 0.48     |
| 31:D0:42:ILE:HG12  | 42:DN:99:LYS:O     | 2.13        | 0.48     |
| 24:DI:100:ILE:O    | 24:DI:139:VAL:HG13 | 2.14        | 0.48     |
| 36:B2:21:ARG:CD    | 36:B2:43:THR:HG21  | 2.44        | 0.48     |
| 4:AE:143:LEU:O     | 4:AE:146:MET:HG2   | 2.13        | 0.48     |
| 4:AE:151:MET:O     | 4:AE:154:ALA:HB3   | 2.13        | 0.48     |
| 33:B1:7:LYS:HA     | 33:B1:23:THR:HG22  | 1.94        | 0.48     |
| 23:DB:1579:A:H2'   | 23:DB:1580:A:H8    | 1.78        | 0.48     |
| 3:AD:90:LEU:O      | 3:AD:93:LEU:HB2    | 2.14        | 0.48     |
| 1:AA:1048:G:H4'    | 13:AN:2:LYS:HZ2    | 1.76        | 0.48     |
| 1:AA:194:C:O2'     | 1:AA:195:A:H5'     | 2.14        | 0.48     |
| 37:DL:4:ASN:ND2    | 37:DL:4:ASN:N      | 2.60        | 0.48     |
| 27:BK:75:SER:HB2   | 28:BP:73:PHE:HA    | 1.94        | 0.48     |
| 28:BP:56:SER:O     | 28:BP:74:GLN:HA    | 2.14        | 0.48     |
| 28:BP:94:ALA:C     | 28:BP:95:LYS:HD2   | 2.34        | 0.48     |
| 13:CN:17:ASP:HA    | 13:CN:21:ALA:HB2   | 1.94        | 0.48     |
| 39:BX:10:SER:HA    | 39:BX:57:LEU:HD13  | 1.94        | 0.48     |
| 1:AA:1124:G:H5''   | 9:AJ:37:ARG:O      | 2.13        | 0.48     |
| 29:BE:21:ARG:HG3   | 29:BE:22:ASP:O     | 2.13        | 0.48     |
| 1:CA:377:G:H2'     | 1:CA:378:G:H8      | 1.77        | 0.48     |
| 7:CH:113:ARG:NH2   | 7:CH:114:ALA:HA    | 2.29        | 0.48     |
| 2:CC:131:ARG:HG2   | 2:CC:131:ARG:NH1   | 2.25        | 0.48     |
| 23:BB:6:A:H2'      | 23:BB:7:G:C8       | 2.47        | 0.48     |
| 23:DB:1968:G:H5''  | 57:DB:3572:HOH:O   | 2.13        | 0.48     |
| 23:DB:6:A:H4'      | 41:DJ:131:ASN:O    | 2.14        | 0.48     |
| 23:BB:1570:A:H2'   | 23:BB:1571:A:C8    | 2.49        | 0.48     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:2368:C:H2'  | 23:DB:2369:A:H8    | 1.77        | 0.48     |
| 23:DB:629:G:H5''  | 23:DB:650:C:O2'    | 2.13        | 0.48     |
| 4:AE:32:PHE:CE2   | 4:AE:55:VAL:HG22   | 2.49        | 0.48     |
| 43:DO:40:ILE:HG22 | 43:DO:44:GLY:HA2   | 1.95        | 0.48     |
| 23:DB:257:C:H2'   | 23:DB:258:G:O4'    | 2.14        | 0.48     |
| 1:AA:810:C:O2'    | 1:AA:811:C:H5'     | 2.14        | 0.48     |
| 1:CA:26:A:H61     | 1:CA:558:G:H1'     | 1.79        | 0.48     |
| 1:AA:886:G:O2'    | 1:AA:887:G:H5'     | 2.13        | 0.48     |
| 37:BL:119:PRO:HA  | 37:BL:138:ALA:O    | 2.13        | 0.48     |
| 23:BB:359:G:O2'   | 23:BB:360:U:H5'    | 2.14        | 0.48     |
| 23:DB:516:C:O2'   | 23:DB:517:C:H5'    | 2.14        | 0.48     |
| 23:BB:56:A:H2'    | 23:BB:57:C:C6      | 2.48        | 0.48     |
| 20:CB:118:THR:O   | 20:CB:121:GLN:HB3  | 2.14        | 0.48     |
| 23:DB:1671:U:H2'  | 23:DB:1673:G:OP2   | 2.14        | 0.48     |
| 23:BB:2328:A:H2'  | 23:BB:2329:U:H6    | 1.76        | 0.48     |
| 48:BG:68:ARG:NH1  | 48:BG:72:ASN:HD22  | 2.09        | 0.48     |
| 44:DQ:29:ARG:HG2  | 44:DQ:29:ARG:HH11  | 1.77        | 0.48     |
| 26:BD:54:ALA:HA   | 26:BD:76:GLY:N     | 2.28        | 0.48     |
| 47:DF:91:ARG:O    | 47:DF:92:GLY:C     | 2.51        | 0.48     |
| 8:AI:5:TYR:HB3    | 8:AI:88:GLU:OE2    | 2.14        | 0.48     |
| 8:AI:75:ALA:HA    | 8:AI:78:ILE:HD12   | 1.96        | 0.48     |
| 26:DD:55:LYS:C    | 26:DD:57:ALA:H     | 2.17        | 0.48     |
| 22:DA:29:A:H2'    | 22:DA:30:C:O4'     | 2.14        | 0.48     |
| 48:DG:18:ILE:HA   | 48:DG:22:VAL:O     | 2.14        | 0.48     |
| 29:DE:60:TRP:CE3  | 29:DE:60:TRP:HA    | 2.48        | 0.48     |
| 38:DM:24:THR:HG23 | 38:DM:34:LYS:HE3   | 1.95        | 0.48     |
| 41:BJ:31:GLU:O    | 41:BJ:34:ARG:HB2   | 2.13        | 0.48     |
| 41:BJ:43:GLU:O    | 41:BJ:45:THR:HG22  | 2.14        | 0.48     |
| 23:BB:1652:A:OP1  | 42:BN:8:ARG:HD3    | 2.14        | 0.48     |
| 25:BC:89:ASN:O    | 25:BC:105:ALA:HB3  | 2.12        | 0.48     |
| 22:BA:28:C:N4     | 22:BA:56:G:C6      | 2.82        | 0.48     |
| 43:BO:35:ILE:HG21 | 43:BO:71:ALA:CB    | 2.43        | 0.48     |
| 37:BL:4:ASN:ND2   | 37:BL:4:ASN:N      | 2.61        | 0.48     |
| 24:DI:52:LEU:HD13 | 24:DI:81:LYS:HZ3   | 1.79        | 0.48     |
| 47:BF:108:PRO:O   | 47:BF:110:ILE:HG23 | 2.13        | 0.48     |
| 40:DH:86:ASP:C    | 40:DH:88:GLY:H     | 2.17        | 0.48     |
| 42:DN:106:ASP:OD1 | 42:DN:108:ALA:HB3  | 2.14        | 0.48     |
| 29:DE:29:HIS:C    | 29:DE:32:VAL:HG22  | 2.34        | 0.48     |
| 50:DT:50:LEU:C    | 50:DT:52:GLU:H     | 2.17        | 0.48     |
| 25:DC:202:ARG:NH1 | 25:DC:213:ARG:NE   | 2.60        | 0.48     |
| 23:BB:662:G:O2'   | 23:BB:663:G:H5'    | 2.13        | 0.48     |
| 23:BB:1029:A:H2'  | 23:BB:1030:C:O4'   | 2.13        | 0.48     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 9:CJ:55:PRO:HA     | 13:CN:80:ARG:HH22  | 1.72        | 0.48     |
| 35:DV:30:ILE:HB    | 35:DV:38:LEU:HB3   | 1.95        | 0.48     |
| 23:DB:2465:C:O2'   | 23:DB:2466:C:H5'   | 2.14        | 0.48     |
| 53:D6:1:MET:CG     | 53:D6:2:THR:H      | 2.26        | 0.48     |
| 20:CB:15:PHE:CD1   | 20:CB:16:GLY:N     | 2.82        | 0.48     |
| 31:D0:42:ILE:HG22  | 31:D0:43:THR:O     | 2.14        | 0.48     |
| 44:DQ:105:PHE:HA   | 44:DQ:108:LEU:HG   | 1.95        | 0.48     |
| 24:DI:129:GLU:HB3  | 24:DI:133:ARG:NH1  | 2.28        | 0.48     |
| 23:DB:1439:A:N7    | 23:DB:1440:U:C6    | 2.82        | 0.48     |
| 4:AE:80:LEU:HD13   | 4:AE:95:MET:HB3    | 1.96        | 0.48     |
| 25:DC:43:ASN:ND2   | 25:DC:44:ASN:N     | 2.57        | 0.48     |
| 29:DE:126:VAL:HG22 | 29:DE:127:GLU:H    | 1.77        | 0.48     |
| 20:CB:101:THR:HG23 | 20:CB:102:ASN:H    | 1.78        | 0.48     |
| 20:CB:102:ASN:O    | 20:CB:106:VAL:HG23 | 2.14        | 0.48     |
| 1:CA:714:G:H2'     | 1:CA:715:A:C8      | 2.49        | 0.48     |
| 31:D0:31:LYS:N     | 31:D0:31:LYS:HD2   | 2.26        | 0.48     |
| 3:AD:169:TRP:CD1   | 3:AD:170:LEU:HD23  | 2.49        | 0.48     |
| 4:CE:151:MET:O     | 4:CE:154:ALA:HB3   | 2.13        | 0.48     |
| 23:DB:265:A:O2'    | 23:DB:266:G:H4'    | 2.14        | 0.48     |
| 29:DE:41:GLN:O     | 29:DE:42:GLY:O     | 2.32        | 0.48     |
| 1:CA:621:A:H2'     | 1:CA:622:A:H8      | 1.77        | 0.48     |
| 20:AB:20:ARG:HA    | 20:AB:20:ARG:NE    | 2.28        | 0.48     |
| 1:AA:1009:U:O2     | 1:AA:1009:U:H2'    | 2.13        | 0.48     |
| 7:AH:55:LYS:NZ     | 7:AH:55:LYS:HA     | 2.27        | 0.48     |
| 23:BB:2244:U:H2'   | 23:BB:2245:U:O4'   | 2.14        | 0.48     |
| 1:AA:1053:G:C4'    | 1:AA:1054:C:H5'    | 2.43        | 0.48     |
| 1:AA:212:G:H2'     | 1:AA:213:G:H8      | 1.78        | 0.48     |
| 23:BB:2700:A:H2'   | 23:BB:2701:U:C6    | 2.49        | 0.48     |
| 3:CD:11:SER:HA     | 3:CD:18:LEU:HD22   | 1.96        | 0.48     |
| 23:BB:1045:C:H5''  | 23:BB:1047:G:O4'   | 2.14        | 0.48     |
| 51:BZ:69:ALA:HA    | 51:BZ:72:ARG:NH1   | 2.28        | 0.48     |
| 16:AQ:32:ILE:HG23  | 16:AQ:33:TYR:CD2   | 2.48        | 0.48     |
| 23:DB:1416:G:O2'   | 23:DB:1417:C:H6    | 1.96        | 0.48     |
| 20:CB:129:THR:C    | 20:CB:131:LYS:N    | 2.67        | 0.48     |
| 29:DE:37:ALA:HB1   | 29:DE:92:HIS:O     | 2.13        | 0.48     |
| 2:CC:13:ILE:C      | 2:CC:15:LYS:H      | 2.17        | 0.48     |
| 23:DB:2834:G:O6    | 23:DB:2879:A:H2'   | 2.13        | 0.48     |
| 23:BB:2358:A:H61   | 37:BL:54:GLN:HE22  | 1.60        | 0.48     |
| 43:DO:94:ARG:HD2   | 43:DO:97:PHE:O     | 2.14        | 0.48     |
| 47:BF:120:SER:OG   | 47:BF:129:MET:HB3  | 2.13        | 0.48     |
| 23:BB:235:U:H2'    | 23:BB:236:C:C6     | 2.49        | 0.48     |
| 23:BB:1848:A:H2'   | 23:BB:1849:G:C8    | 2.49        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 29:BE:37:ALA:HB1  | 29:BE:92:HIS:O    | 2.13        | 0.48     |
| 23:DB:1576:U:O2'  | 23:DB:1577:C:H5'  | 2.14        | 0.48     |
| 23:DB:78:U:H2'    | 23:DB:79:C:C6     | 2.49        | 0.48     |
| 23:DB:1747:U:H2'  | 23:DB:1748:C:C6   | 2.48        | 0.48     |
| 48:BG:133:LYS:N   | 48:BG:133:LYS:HD3 | 2.27        | 0.48     |
| 23:BB:620:G:H5'   | 23:BB:620:G:N3    | 2.27        | 0.48     |
| 23:BB:771:G:O2'   | 23:BB:772:C:H5'   | 2.14        | 0.48     |
| 51:BZ:53:ALA:O    | 51:BZ:55:GLY:N    | 2.38        | 0.48     |
| 29:BE:97:ASN:ND2  | 29:BE:100:MET:HG3 | 2.29        | 0.48     |
| 9:CJ:26:VAL:HG12  | 9:CJ:30:LYS:HE2   | 1.95        | 0.48     |
| 10:CK:27:ASN:O    | 10:CK:56:LYS:HD2  | 2.12        | 0.48     |
| 1:CA:1379:G:O2'   | 1:CA:1380:U:H5'   | 2.14        | 0.48     |
| 1:AA:1132:C:H2'   | 1:AA:1133:G:C8    | 2.47        | 0.48     |
| 42:DN:9:GLN:O     | 42:DN:17:ARG:HD3  | 2.13        | 0.48     |
| 6:CG:16:LYS:HD2   | 6:CG:43:TYR:CD1   | 2.49        | 0.48     |
| 2:CC:182:ASP:HB2  | 2:CC:203:LYS:HE2  | 1.95        | 0.48     |
| 10:CK:125:LYS:O   | 21:CU:33:ARG:NH2  | 2.46        | 0.48     |
| 23:BB:18:U:OP1    | 44:BQ:29:ARG:NH2  | 2.47        | 0.48     |
| 44:DQ:23:TYR:CD2  | 44:DQ:23:TYR:N    | 2.79        | 0.48     |
| 26:BD:176:ASP:HB2 | 26:BD:190:LYS:HG2 | 1.94        | 0.48     |
| 41:BJ:18:VAL:CG1  | 41:BJ:54:ILE:HD11 | 2.43        | 0.48     |
| 13:AN:9:GLU:O     | 13:AN:13:VAL:HG23 | 2.13        | 0.48     |
| 13:CN:63:CYS:SG   | 13:CN:82:LYS:HG3  | 2.53        | 0.48     |
| 43:DO:35:ILE:HG21 | 43:DO:71:ALA:HA   | 1.96        | 0.48     |
| 24:BI:74:PRO:O    | 24:BI:77:VAL:HG22 | 2.13        | 0.48     |
| 1:AA:1278:G:H4'   | 1:AA:1279:G:O4'   | 2.13        | 0.48     |
| 47:BF:7:TYR:HA    | 47:BF:11:VAL:HB   | 1.95        | 0.48     |
| 29:BE:138:LEU:O   | 29:BE:142:ALA:N   | 2.47        | 0.48     |
| 49:DR:20:VAL:HG12 | 49:DR:21:ARG:N    | 2.29        | 0.48     |
| 12:CM:109:LYS:HG3 | 12:CM:110:GLY:N   | 2.29        | 0.48     |
| 23:DB:1244:A:O2'  | 23:DB:1245:G:H5'  | 2.13        | 0.48     |
| 23:DB:138:U:H2'   | 23:DB:140:C:C1'   | 2.44        | 0.48     |
| 7:CH:31:LEU:O     | 7:CH:35:ILE:HG13  | 2.13        | 0.48     |
| 23:BB:1244:A:O2'  | 23:BB:1245:G:H5'  | 2.14        | 0.48     |
| 13:AN:52:ARG:HD2  | 13:AN:58:ARG:HH21 | 1.78        | 0.48     |
| 43:DO:55:GLU:HB2  | 43:DO:58:ILE:HD12 | 1.96        | 0.48     |
| 35:DV:9:ARG:HH21  | 35:DV:12:GLN:HA   | 1.74        | 0.48     |
| 23:BB:2645:G:H4'  | 23:BB:2732:G:H2'  | 1.96        | 0.48     |
| 27:BK:43:ILE:HG21 | 27:BK:46:ALA:HB2  | 1.96        | 0.48     |
| 20:CB:38:HIS:O    | 20:CB:39:ILE:HD13 | 2.13        | 0.48     |
| 20:CB:16:GLY:HA3  | 20:CB:40:ILE:H    | 1.78        | 0.48     |
| 43:BO:58:ILE:O    | 43:BO:62:LEU:HB2  | 2.13        | 0.48     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:BK:79:PHE:HZ   | 27:BK:104:THR:HG23 | 1.78        | 0.48     |
| 23:BB:1287:A:H3'  | 23:BB:1288:G:H21   | 1.76        | 0.48     |
| 25:DC:159:THR:H   | 25:DC:194:VAL:CG1  | 2.27        | 0.48     |
| 1:AA:1074:G:O4'   | 20:AB:102:ASN:HB2  | 2.14        | 0.48     |
| 2:CC:185:THR:HG22 | 2:CC:198:LYS:HA    | 1.95        | 0.48     |
| 31:D0:30:ASP:OD2  | 31:D0:31:LYS:HD2   | 2.13        | 0.48     |
| 26:BD:68:PHE:C    | 26:BD:73:VAL:HB    | 2.33        | 0.48     |
| 1:CA:472:U:H2'    | 1:CA:473:U:C6      | 2.49        | 0.48     |
| 19:AT:70:LYS:HA   | 19:AT:73:ARG:NH1   | 2.29        | 0.48     |
| 22:BA:113:C:H2'   | 22:BA:114:C:C6     | 2.49        | 0.48     |
| 29:BE:48:THR:O    | 29:BE:52:VAL:HG23  | 2.14        | 0.48     |
| 33:B1:36:LYS:HA   | 33:B1:46:VAL:O     | 2.13        | 0.48     |
| 22:DA:13:G:H1'    | 22:DA:69:G:N2      | 2.29        | 0.48     |
| 23:BB:1854:A:H61  | 23:BB:1888:G:H1'   | 1.78        | 0.48     |
| 45:BS:44:ALA:C    | 45:BS:46:LEU:H     | 2.16        | 0.48     |
| 5:CF:53:LYS:C     | 5:CF:54:LEU:HD22   | 2.33        | 0.48     |
| 19:CT:57:VAL:HB   | 19:CT:71:ALA:HB1   | 1.95        | 0.48     |
| 1:CA:678:U:O2'    | 1:CA:679:C:H5'     | 2.14        | 0.48     |
| 7:CH:101:ALA:HB3  | 7:CH:112:ASP:HB3   | 1.96        | 0.48     |
| 23:DB:543:G:H21   | 23:DB:545:U:H5'    | 1.78        | 0.48     |
| 14:AO:8:THR:O     | 14:AO:11:ILE:HG22  | 2.13        | 0.48     |
| 52:BW:77:LYS:HZ2  | 52:BW:77:LYS:H     | 1.60        | 0.48     |
| 23:DB:2700:A:O2'  | 23:DB:2701:U:H5'   | 2.14        | 0.48     |
| 23:BB:2852:G:H2'  | 23:BB:2853:C:H6    | 1.77        | 0.48     |
| 43:BO:28:VAL:HG21 | 43:BO:106:LEU:HD21 | 1.96        | 0.48     |
| 42:BN:19:ALA:C    | 42:BN:21:PHE:N     | 2.67        | 0.48     |
| 23:DB:2784:U:H2'  | 23:DB:2785:C:H6    | 1.79        | 0.48     |
| 23:BB:175:G:O2'   | 23:BB:176:A:H5'    | 2.14        | 0.48     |
| 23:BB:1708:C:H2'  | 23:BB:1709:U:H6    | 1.78        | 0.48     |
| 25:BC:2:VAL:HG23  | 25:BC:3:VAL:N      | 2.27        | 0.48     |
| 7:CH:29:SER:OG    | 7:CH:32:LYS:HG3    | 2.13        | 0.48     |
| 48:DG:87:GLN:HE21 | 48:DG:164:ALA:HA   | 1.77        | 0.48     |
| 1:AA:591:U:H2'    | 1:AA:592:G:C8      | 2.49        | 0.48     |
| 23:BB:807:U:H2'   | 23:BB:808:G:C8     | 2.49        | 0.48     |
| 23:BB:656:G:H2'   | 23:BB:657:U:C6     | 2.49        | 0.48     |
| 46:BU:31:GLY:O    | 46:BU:66:VAL:HG12  | 2.14        | 0.48     |
| 7:CH:55:LYS:NZ    | 7:CH:55:LYS:HA     | 2.29        | 0.48     |
| 23:BB:598:U:H2'   | 23:BB:599:A:C8     | 2.49        | 0.48     |
| 23:DB:1369:G:O2'  | 23:DB:1370:C:H5'   | 2.14        | 0.48     |
| 46:DU:4:ILE:HG13  | 46:DU:66:VAL:HG23  | 1.95        | 0.48     |
| 29:DE:11:ALA:O    | 29:DE:12:LEU:HD22  | 2.13        | 0.48     |
| 48:DG:133:LYS:N   | 48:DG:133:LYS:HD3  | 2.28        | 0.48     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:AA:26:A:H61      | 1:AA:558:G:H1'    | 1.78        | 0.48     |
| 32:B4:13:ASN:O     | 32:B4:27:CYS:HA   | 2.13        | 0.48     |
| 12:AM:71:GLU:HA    | 12:AM:74:MET:SD   | 2.54        | 0.48     |
| 28:BP:77:SER:O     | 28:BP:80:VAL:HG12 | 2.14        | 0.48     |
| 32:B4:19:ARG:O     | 32:B4:20:ASP:HB2  | 2.13        | 0.48     |
| 13:AN:42:ASN:O     | 13:AN:45:LEU:HB3  | 2.14        | 0.48     |
| 23:DB:553:G:O2'    | 23:DB:554:U:H5'   | 2.13        | 0.48     |
| 36:B2:3:ARG:NE     | 36:B2:3:ARG:HA    | 2.29        | 0.48     |
| 38:DM:33:LEU:HD22  | 38:DM:128:THR:OG1 | 2.14        | 0.48     |
| 23:DB:1099:G:O2'   | 23:DB:1100:C:H5'  | 2.14        | 0.48     |
| 25:DC:181:ARG:HD3  | 25:DC:182:LYS:H   | 1.77        | 0.48     |
| 44:BQ:30:VAL:CG1   | 44:BQ:31:TYR:H    | 1.97        | 0.48     |
| 48:DG:8:VAL:HG22   | 48:DG:68:ARG:HD3  | 1.96        | 0.48     |
| 37:DL:122:VAL:HG23 | 37:DL:143:GLU:OE1 | 2.13        | 0.48     |
| 20:AB:14:HIS:HB2   | 20:AB:208:ALA:CB  | 2.44        | 0.48     |
| 20:AB:187:ASP:HB3  | 20:AB:201:GLY:O   | 2.14        | 0.48     |
| 53:D6:41:LEU:HD13  | 53:D6:52:LEU:HD13 | 1.95        | 0.48     |
| 47:DF:87:LYS:CG    | 47:DF:88:VAL:H    | 2.20        | 0.48     |
| 1:CA:1350:A:H2'    | 1:CA:1351:U:C6    | 2.49        | 0.48     |
| 20:CB:162:VAL:HG13 | 20:CB:184:ALA:CB  | 2.36        | 0.48     |
| 20:CB:187:ASP:HB3  | 20:CB:201:GLY:O   | 2.14        | 0.48     |
| 8:AI:24:ASN:CG     | 8:AI:25:GLY:H     | 2.17        | 0.48     |
| 44:BQ:63:ARG:NH1   | 44:BQ:96:ASP:HB2  | 2.16        | 0.48     |
| 51:BZ:33:LEU:HA    | 51:BZ:51:VAL:O    | 2.14        | 0.48     |
| 3:AD:25:ARG:O      | 3:AD:26:ALA:HB3   | 2.14        | 0.48     |
| 47:BF:39:VAL:CG2   | 47:BF:48:LEU:HG   | 2.43        | 0.48     |
| 42:DN:79:LEU:C     | 42:DN:81:ASN:H    | 2.17        | 0.48     |
| 40:DH:125:THR:HA   | 40:DH:146:VAL:CG1 | 2.44        | 0.48     |
| 45:DS:13:SER:OG    | 45:DS:16:LYS:HB2  | 2.14        | 0.48     |
| 47:DF:104:THR:C    | 47:DF:108:PRO:HG2 | 2.34        | 0.48     |
| 1:CA:947:G:H2'     | 1:CA:948:C:C6     | 2.48        | 0.48     |
| 29:BE:61:ARG:HH12  | 29:BE:64:GLY:HA3  | 1.77        | 0.48     |
| 23:BB:811:U:OP2    | 37:BL:20:GLY:HA2  | 2.13        | 0.48     |
| 23:BB:973:A:H1'    | 23:BB:1188:U:C5   | 2.48        | 0.48     |
| 38:DM:135:VAL:O    | 38:DM:136:MET:HG3 | 2.13        | 0.48     |
| 39:BX:7:ARG:HG3    | 39:BX:7:ARG:O     | 2.14        | 0.48     |
| 27:BK:43:ILE:CG2   | 27:BK:46:ALA:HB2  | 2.44        | 0.48     |
| 23:BB:26:G:H1'     | 23:BB:514:A:N6    | 2.28        | 0.48     |
| 20:CB:33:ALA:HB2   | 20:CB:38:HIS:ND1  | 2.29        | 0.48     |
| 10:CK:28:ASN:HD22  | 10:CK:46:ALA:HB3  | 1.79        | 0.48     |
| 9:AJ:15:HIS:O      | 9:AJ:18:ILE:HG22  | 2.14        | 0.48     |
| 24:BI:62:ALA:C     | 24:BI:64:ARG:H    | 2.16        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 28:BP:6:GLN:NE2   | 28:BP:7:LEU:N     | 2.62        | 0.48     |
| 26:BD:114:LYS:HG2 | 26:BD:166:GLY:HA2 | 1.95        | 0.48     |
| 42:BN:24:MET:SD   | 42:BN:44:LEU:HD22 | 2.54        | 0.48     |
| 1:AA:310:G:H5''   | 15:AP:31:ARG:HB2  | 1.96        | 0.48     |
| 11:CL:23:LEU:O    | 11:CL:25:ALA:N    | 2.46        | 0.48     |
| 35:BV:78:GLN:O    | 35:BV:87:GLN:N    | 2.44        | 0.48     |
| 6:AG:41:ILE:HG21  | 6:AG:115:MET:CG   | 2.43        | 0.48     |
| 33:D1:36:LYS:HA   | 33:D1:46:VAL:O    | 2.12        | 0.48     |
| 6:CG:100:MET:O    | 6:CG:104:VAL:HG23 | 2.14        | 0.48     |
| 23:BB:1825:U:H2'  | 23:BB:1826:G:C8   | 2.49        | 0.48     |
| 23:BB:1432:G:H2'  | 23:BB:1433:A:H8   | 1.77        | 0.48     |
| 23:BB:705:A:N6    | 23:BB:726:G:O2'   | 2.46        | 0.48     |
| 30:BY:7:THR:HA    | 30:BY:34:THR:HA   | 1.95        | 0.48     |
| 42:DN:49:GLU:HA   | 42:DN:94:TYR:HD2  | 1.77        | 0.48     |
| 23:DB:1868:C:H2'  | 23:DB:1869:G:O4'  | 2.13        | 0.48     |
| 43:DO:7:ARG:HA    | 43:DO:10:ARG:HD2  | 1.95        | 0.48     |
| 20:CB:23:ASN:HD22 | 20:CB:24:PRO:CD   | 2.26        | 0.48     |
| 23:BB:2455:G:O2'  | 23:BB:2456:C:H5'  | 2.14        | 0.48     |
| 23:BB:912:C:H2'   | 23:BB:913:U:C6    | 2.49        | 0.48     |
| 42:DN:19:ALA:C    | 42:DN:21:PHE:N    | 2.67        | 0.48     |
| 3:AD:77:GLU:OE1   | 3:AD:80:ARG:HD3   | 2.14        | 0.48     |
| 23:DB:1536:C:H4'  | 23:DB:1537:G:C4   | 2.49        | 0.48     |
| 22:DA:87:U:H2'    | 22:DA:88:C:H5''   | 1.95        | 0.48     |
| 1:CA:54:C:H2'     | 1:CA:352:C:N4     | 2.29        | 0.48     |
| 1:AA:590:U:H2'    | 1:AA:591:U:H6     | 1.79        | 0.48     |
| 1:CA:201:G:O2'    | 1:CA:202:G:H5'    | 2.14        | 0.48     |
| 43:BO:104:GLN:O   | 43:BO:107:ALA:HB3 | 2.14        | 0.48     |
| 23:DB:1339:G:H21  | 23:DB:1603:A:H1'  | 1.79        | 0.48     |
| 53:B6:7:TYR:OH    | 53:B6:157:ALA:HA  | 2.13        | 0.48     |
| 6:CG:119:LEU:O    | 6:CG:123:LEU:HG   | 2.13        | 0.48     |
| 1:CA:1366:C:H2'   | 1:CA:1367:C:C6    | 2.47        | 0.48     |
| 1:CA:106:C:O2'    | 1:CA:107:G:H5'    | 2.14        | 0.48     |
| 8:AI:11:ARG:CZ    | 8:AI:106:ASP:OD1  | 2.62        | 0.48     |
| 23:DB:696:G:O2'   | 23:DB:697:G:H5'   | 2.14        | 0.48     |
| 1:AA:631:C:H3'    | 1:AA:632:U:H5'    | 1.96        | 0.48     |
| 7:AH:23:ALA:CB    | 7:AH:61:THR:HA    | 2.44        | 0.48     |
| 23:DB:2300:C:H2'  | 23:DB:2301:C:C6   | 2.48        | 0.48     |
| 23:DB:2588:G:H3'  | 57:DB:3589:HOH:O  | 2.13        | 0.48     |
| 1:AA:37:U:H2'     | 1:AA:38:G:C8      | 2.49        | 0.48     |
| 51:DZ:39:TRP:HB2  | 51:DZ:46:PHE:CE2  | 2.49        | 0.48     |
| 1:AA:201:G:O2'    | 1:AA:469:C:H4'    | 2.13        | 0.48     |
| 23:BB:195:A:H61   | 23:BB:198:C:H3'   | 1.79        | 0.48     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 27:DK:11:ALA:O     | 27:DK:100:PHE:N    | 2.47        | 0.48     |
| 23:DB:2297:A:N6    | 23:DB:2319:G:H1'   | 2.29        | 0.48     |
| 6:AG:16:LYS:HD2    | 6:AG:43:TYR:CD1    | 2.49        | 0.48     |
| 2:CC:38:VAL:HG23   | 2:CC:39:ARG:N      | 2.29        | 0.48     |
| 2:CC:128:MET:H     | 2:CC:128:MET:CE    | 2.26        | 0.48     |
| 1:AA:434:U:H3'     | 1:AA:435:A:H8      | 1.77        | 0.48     |
| 23:BB:2081:U:H2'   | 23:BB:2082:A:C8    | 2.49        | 0.48     |
| 23:BB:796:C:H2'    | 23:BB:797:G:C8     | 2.48        | 0.48     |
| 23:BB:2330:G:H1'   | 52:BW:38:ARG:CB    | 2.44        | 0.48     |
| 23:BB:2387:U:H1'   | 52:BW:38:ARG:CZ    | 2.44        | 0.48     |
| 25:DC:185:ALA:C    | 25:DC:187:CYS:H    | 2.16        | 0.48     |
| 44:BQ:18:LYS:C     | 44:BQ:20:ALA:N     | 2.67        | 0.48     |
| 21:AU:40:PRO:C     | 21:AU:42:THR:H     | 2.17        | 0.48     |
| 10:CK:12:ARG:HD3   | 10:CK:76:TYR:CE1   | 2.49        | 0.48     |
| 53:B6:41:LEU:HD21  | 53:B6:88:LEU:CD1   | 2.44        | 0.48     |
| 13:AN:13:VAL:HG22  | 13:AN:59:GLN:HG2   | 1.96        | 0.48     |
| 12:AM:13:HIS:HB2   | 12:AM:16:ILE:HG22  | 1.96        | 0.48     |
| 1:AA:947:G:H2'     | 1:AA:948:C:H6      | 1.78        | 0.48     |
| 25:BC:91:ALA:HB3   | 25:BC:105:ALA:HB2  | 1.94        | 0.48     |
| 25:BC:83:ASP:HB2   | 25:BC:90:ILE:HB    | 1.96        | 0.48     |
| 47:BF:141:ASP:O    | 47:BF:145:VAL:HG13 | 2.13        | 0.48     |
| 40:DH:121:VAL:O    | 40:DH:122:LEU:HB2  | 2.14        | 0.48     |
| 47:DF:138:PRO:HA   | 47:DF:142:TYR:CE2  | 2.49        | 0.48     |
| 35:BV:80:HIS:CD2   | 35:BV:82:TYR:H     | 2.13        | 0.48     |
| 24:BI:56:VAL:CG2   | 24:BI:68:PHE:HB2   | 2.43        | 0.48     |
| 1:AA:980:C:H4'     | 13:AN:58:ARG:HH12  | 1.78        | 0.48     |
| 20:CB:218:ALA:HA   | 20:CB:221:ARG:HG2  | 1.96        | 0.48     |
| 23:BB:2267:A:C8    | 23:BB:2267:A:O5'   | 2.65        | 0.48     |
| 32:D4:22:VAL:O     | 32:D4:24:ARG:HG3   | 2.14        | 0.48     |
| 45:BS:26:GLY:O     | 45:BS:28:LYS:N     | 2.46        | 0.48     |
| 23:DB:2466:C:OP1   | 32:D4:4:ARG:HB3    | 2.14        | 0.48     |
| 37:DL:99:ASN:O     | 37:DL:100:ILE:HB   | 2.14        | 0.48     |
| 1:AA:1389:C:H2'    | 1:AA:1390:U:H6     | 1.78        | 0.48     |
| 45:DS:44:ALA:C     | 45:DS:46:LEU:H     | 2.16        | 0.48     |
| 1:CA:672:U:H2'     | 1:CA:673:A:C8      | 2.49        | 0.48     |
| 20:CB:98:GLY:O     | 20:CB:102:ASN:N    | 2.46        | 0.48     |
| 40:DH:115:VAL:HG23 | 40:DH:132:PHE:HA   | 1.95        | 0.48     |
| 41:BJ:103:ILE:HD12 | 41:BJ:104:ALA:N    | 2.29        | 0.48     |
| 1:CA:320:A:H2'     | 1:CA:321:A:H8      | 1.74        | 0.48     |
| 12:AM:2:ARG:CG     | 12:AM:6:ILE:H      | 2.25        | 0.48     |
| 23:BB:2794:C:H2'   | 23:BB:2795:C:C6    | 2.49        | 0.48     |
| 4:CE:80:LEU:HD13   | 4:CE:95:MET:HB3    | 1.96        | 0.48     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 35:BV:78:GLN:HB2  | 35:BV:88:HIS:O     | 2.13        | 0.48     |
| 3:AD:22:SER:H     | 3:AD:109:THR:HG22  | 1.79        | 0.48     |
| 1:CA:394:G:O2'    | 1:CA:395:C:H5'     | 2.14        | 0.48     |
| 23:DB:1570:A:H2'  | 23:DB:1571:A:C8    | 2.49        | 0.48     |
| 7:CH:94:VAL:CG2   | 7:CH:101:ALA:HB2   | 2.44        | 0.48     |
| 23:DB:2247:A:H2'  | 23:DB:2248:C:C6    | 2.49        | 0.48     |
| 1:AA:482:A:C2     | 1:AA:483:C:H1'     | 2.49        | 0.48     |
| 50:BT:45:ALA:O    | 50:BT:48:GLN:HB2   | 2.14        | 0.48     |
| 22:BA:97:C:H2'    | 22:BA:98:G:H5'     | 1.96        | 0.48     |
| 1:AA:611:C:H2'    | 1:AA:612:C:C6      | 2.49        | 0.48     |
| 1:AA:1035:A:H2'   | 1:AA:1036:A:C8     | 2.48        | 0.48     |
| 23:BB:2776:A:H4'  | 23:BB:2777:G:C5'   | 2.44        | 0.48     |
| 23:BB:1341:G:H5'  | 50:BT:61:LEU:HD22  | 1.96        | 0.48     |
| 25:DC:42:ARG:HG3  | 25:DC:46:GLY:O     | 2.14        | 0.48     |
| 24:BI:116:MET:SD  | 24:BI:124:MET:HB2  | 2.54        | 0.48     |
| 1:CA:1096:C:H2'   | 1:CA:1097:C:C6     | 2.48        | 0.48     |
| 23:BB:1464:G:H2'  | 23:BB:1465:G:C8    | 2.48        | 0.48     |
| 24:BI:52:LEU:HD21 | 24:BI:81:LYS:NZ    | 2.29        | 0.48     |
| 21:CU:31:VAL:HG12 | 21:CU:31:VAL:O     | 2.13        | 0.48     |
| 23:DB:1050:A:H2'  | 23:DB:1051:G:C8    | 2.49        | 0.48     |
| 23:DB:351:C:H2'   | 23:DB:352:A:C8     | 2.48        | 0.48     |
| 28:DP:62:LYS:HE3  | 28:DP:64:SER:OG    | 2.14        | 0.48     |
| 25:BC:226:PRO:HG3 | 25:BC:233:GLY:H    | 1.79        | 0.48     |
| 41:DJ:75:TYR:CD1  | 41:DJ:86:GLN:HB3   | 2.49        | 0.48     |
| 44:BQ:45:ALA:O    | 44:BQ:49:ARG:N     | 2.42        | 0.48     |
| 1:AA:462:G:H2'    | 1:AA:463:U:C6      | 2.49        | 0.48     |
| 31:D0:54:ILE:H    | 42:DN:118:ARG:HH12 | 1.62        | 0.48     |
| 48:BG:28:LYS:O    | 48:BG:29:ASN:HB3   | 2.14        | 0.48     |
| 1:AA:218:U:H2'    | 1:AA:219:U:C6      | 2.49        | 0.48     |
| 1:CA:742:G:H2'    | 1:CA:743:A:H8      | 1.79        | 0.48     |
| 23:DB:2478:A:H5'  | 32:D4:32:LYS:HE3   | 1.96        | 0.48     |
| 1:AA:323:U:H2'    | 1:AA:324:G:O4'     | 2.14        | 0.48     |
| 23:DB:1916:A:H2'  | 23:DB:1917:U:O4'   | 2.13        | 0.48     |
| 1:AA:610:U:O2     | 1:AA:610:U:O4'     | 2.32        | 0.48     |
| 35:DV:46:LYS:HD2  | 35:DV:46:LYS:N     | 2.29        | 0.48     |
| 23:DB:2076:U:O2   | 23:DB:2076:U:O4'   | 2.28        | 0.48     |
| 37:DL:142:ILE:N   | 37:DL:142:ILE:HD12 | 2.28        | 0.48     |
| 23:BB:257:C:H2'   | 23:BB:258:G:O4'    | 2.14        | 0.48     |
| 20:CB:130:LYS:HA  | 20:CB:133:ALA:HB3  | 1.96        | 0.48     |
| 25:DC:83:ASP:HB2  | 25:DC:90:ILE:HB    | 1.95        | 0.47     |
| 21:AU:35:GLU:HB3  | 21:AU:36:PHE:H     | 1.53        | 0.47     |
| 37:DL:89:VAL:HG13 | 37:DL:89:VAL:O     | 2.15        | 0.47     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 37:BL:120:VAL:HG12 | 37:BL:121:THR:N    | 2.29        | 0.47     |
| 53:D6:38:LEU:CD1   | 53:D6:66:LEU:HD23  | 2.43        | 0.47     |
| 40:BH:79:THR:HG22  | 40:BH:145:ASN:HB2  | 1.96        | 0.47     |
| 40:BH:83:LYS:CB    | 40:BH:91:PHE:HB2   | 2.39        | 0.47     |
| 53:B6:76:LEU:HD23  | 53:B6:77:LYS:CE    | 2.44        | 0.47     |
| 20:CB:205:ALA:O    | 20:CB:209:VAL:HG22 | 2.14        | 0.47     |
| 8:AI:62:LEU:N      | 8:AI:62:LEU:HD13   | 2.29        | 0.47     |
| 51:DZ:77:LYS:CD    | 51:DZ:78:TYR:H     | 2.27        | 0.47     |
| 47:DF:71:LYS:O     | 47:DF:72:SER:HB3   | 2.14        | 0.47     |
| 13:AN:60:ARG:HE    | 13:AN:62:ARG:HG2   | 1.79        | 0.47     |
| 38:DM:12:MET:HB2   | 38:DM:72:PRO:HG2   | 1.96        | 0.47     |
| 23:DB:2444:G:OP2   | 29:DE:63:LYS:HD2   | 2.14        | 0.47     |
| 29:DE:56:GLY:O     | 29:DE:58:LYS:HD3   | 2.13        | 0.47     |
| 1:CA:1014:A:H4'    | 18:CS:13:HIS:CD2   | 2.48        | 0.47     |
| 50:BT:50:LEU:O     | 50:BT:51:PHE:HB2   | 2.14        | 0.47     |
| 25:DC:75:ALA:HB1   | 25:DC:93:VAL:HG22  | 1.96        | 0.47     |
| 2:CC:63:ILE:HD12   | 2:CC:98:ALA:CB     | 2.35        | 0.47     |
| 47:DF:3:LEU:HB2    | 47:DF:100:GLU:OE1  | 2.14        | 0.47     |
| 53:D6:45:TYR:CZ    | 53:D6:75:ALA:HB2   | 2.48        | 0.47     |
| 12:AM:3:ILE:HA     | 12:AM:56:ARG:CG    | 2.40        | 0.47     |
| 12:AM:52:ILE:HD12  | 12:AM:55:LEU:CD1   | 2.43        | 0.47     |
| 53:B6:109:GLU:O    | 53:B6:112:LYS:HG3  | 2.14        | 0.47     |
| 23:BB:2271:G:H2'   | 23:BB:2272:U:C6    | 2.48        | 0.47     |
| 53:D6:31:GLY:CA    | 53:D6:106:LEU:HD13 | 2.39        | 0.47     |
| 45:BS:27:LYS:CD    | 45:BS:27:LYS:H     | 2.27        | 0.47     |
| 49:DR:49:ILE:HG21  | 49:DR:53:PHE:C     | 2.34        | 0.47     |
| 3:AD:122:ILE:HG22  | 3:AD:123:MET:N     | 2.29        | 0.47     |
| 53:B6:114:LEU:HG   | 53:B6:183:ILE:HD11 | 1.95        | 0.47     |
| 23:DB:278:A:N7     | 23:DB:361:G:N1     | 2.62        | 0.47     |
| 20:CB:101:THR:HG23 | 20:CB:102:ASN:N    | 2.29        | 0.47     |
| 23:DB:2146:C:H4'   | 23:DB:2148:G:O4'   | 2.13        | 0.47     |
| 1:AA:672:U:H2'     | 1:AA:673:A:C8      | 2.49        | 0.47     |
| 1:CA:265:G:H4'     | 16:CQ:67:SER:HA    | 1.96        | 0.47     |
| 23:DB:718:A:H5'    | 23:DB:719:C:C5     | 2.49        | 0.47     |
| 23:DB:1508:A:H5'   | 23:DB:1509:A:N6    | 2.29        | 0.47     |
| 29:DE:21:ARG:HG3   | 29:DE:22:ASP:O     | 2.14        | 0.47     |
| 39:BX:51:ALA:O     | 39:BX:55:THR:N     | 2.41        | 0.47     |
| 3:CD:2:ARG:HB3     | 3:CD:114:ARG:HH22  | 1.78        | 0.47     |
| 23:BB:2461:A:N1    | 23:BB:2490:G:N2    | 2.61        | 0.47     |
| 1:AA:394:G:O2'     | 1:AA:395:C:H5'     | 2.12        | 0.47     |
| 23:DB:544:C:O2'    | 23:DB:545:U:O5'    | 2.32        | 0.47     |
| 23:DB:2064:C:H1'   | 23:DB:2450:A:C6    | 2.49        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:1958:C:H2'  | 23:DB:1959:G:H8   | 1.79        | 0.47     |
| 3:AD:16:THR:HG22  | 3:AD:17:ASP:H     | 1.79        | 0.47     |
| 1:AA:1036:A:H2'   | 1:AA:1037:C:C6    | 2.48        | 0.47     |
| 3:AD:115:GLN:HE21 | 3:AD:119:HIS:CE1  | 2.32        | 0.47     |
| 1:CA:505:G:H2'    | 1:CA:506:G:C8     | 2.49        | 0.47     |
| 1:AA:1450:U:H2'   | 1:AA:1452:C:C4    | 2.49        | 0.47     |
| 24:DI:37:PHE:HB2  | 24:DI:66:PHE:CE2  | 2.49        | 0.47     |
| 1:CA:1488:G:H2'   | 1:CA:1489:G:C8    | 2.49        | 0.47     |
| 22:DA:93:C:O2'    | 22:DA:94:A:H5'    | 2.14        | 0.47     |
| 49:DR:14:VAL:HG21 | 49:DR:98:ILE:HG12 | 1.94        | 0.47     |
| 1:CA:317:U:H2'    | 1:CA:318:G:C8     | 2.49        | 0.47     |
| 12:CM:22:TYR:O    | 12:CM:68:LEU:HD12 | 2.14        | 0.47     |
| 20:CB:93:HIS:HB2  | 20:CB:145:ASN:O   | 2.14        | 0.47     |
| 7:CH:54:THR:HG23  | 7:CH:55:LYS:N     | 2.29        | 0.47     |
| 23:BB:1576:U:O2'  | 23:BB:1577:C:H5'  | 2.13        | 0.47     |
| 23:DB:283:G:H2'   | 23:DB:284:U:C4'   | 2.44        | 0.47     |
| 9:AJ:41:PRO:O     | 9:AJ:42:LEU:HB2   | 2.14        | 0.47     |
| 1:AA:106:C:H2'    | 1:AA:107:G:H8     | 1.79        | 0.47     |
| 3:CD:106:PHE:CD1  | 3:CD:144:ILE:HD11 | 2.49        | 0.47     |
| 23:DB:2452:C:H2'  | 23:DB:2453:A:C8   | 2.49        | 0.47     |
| 1:AA:1109:C:H2'   | 1:AA:1110:A:O4'   | 2.14        | 0.47     |
| 23:BB:734:A:O2'   | 23:BB:735:A:H5'   | 2.14        | 0.47     |
| 23:BB:553:G:O2'   | 23:BB:554:U:H5'   | 2.13        | 0.47     |
| 48:DG:53:PRO:HG3  | 48:DG:61:TRP:CD2  | 2.48        | 0.47     |
| 23:BB:2221:G:O2'  | 23:BB:2222:C:H5'  | 2.14        | 0.47     |
| 23:BB:2234:G:O2'  | 23:BB:2235:G:H5'  | 2.13        | 0.47     |
| 23:DB:1184:U:O2'  | 23:DB:1185:G:H5'  | 2.14        | 0.47     |
| 1:CA:1113:C:O2'   | 1:CA:1114:C:H5'   | 2.13        | 0.47     |
| 53:B6:141:LYS:NZ  | 53:B6:141:LYS:HB3 | 2.29        | 0.47     |
| 50:DT:67:VAL:HG23 | 50:DT:75:GLY:O    | 2.14        | 0.47     |
| 23:DB:2386:A:C2   | 52:DW:38:ARG:HD2  | 2.48        | 0.47     |
| 25:DC:20:ASN:OD1  | 25:DC:22:GLU:HG2  | 2.14        | 0.47     |
| 47:BF:57:ALA:HB2  | 47:BF:64:PRO:HG2  | 1.96        | 0.47     |
| 23:BB:2313:C:O3'  | 47:BF:87:LYS:HE2  | 2.14        | 0.47     |
| 53:B6:80:GLU:O    | 53:B6:83:ILE:HG12 | 2.14        | 0.47     |
| 41:DJ:43:GLU:O    | 41:DJ:45:THR:HG22 | 2.14        | 0.47     |
| 44:DQ:60:TRP:C    | 44:DQ:64:ILE:HG12 | 2.33        | 0.47     |
| 25:BC:75:ALA:HB1  | 25:BC:93:VAL:HG22 | 1.95        | 0.47     |
| 41:DJ:25:LEU:O    | 41:DJ:27:ARG:N    | 2.44        | 0.47     |
| 48:DG:36:LEU:N    | 48:DG:36:LEU:HD22 | 2.29        | 0.47     |
| 1:CA:599:C:H2'    | 1:CA:600:A:H8     | 1.79        | 0.47     |
| 50:BT:29:THR:HB   | 50:BT:86:THR:HG22 | 1.96        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 48:BG:22:VAL:HG13 | 48:BG:36:LEU:HD13 | 1.95        | 0.47     |
| 51:BZ:5:CYS:SG    | 51:BZ:8:THR:HG23  | 2.54        | 0.47     |
| 13:AN:63:CYS:HB2  | 13:AN:79:SER:HB3  | 1.95        | 0.47     |
| 46:BU:86:PHE:HB3  | 46:BU:90:LYS:O    | 2.14        | 0.47     |
| 23:BB:1241:A:H2'  | 23:BB:1242:U:C5'  | 2.40        | 0.47     |
| 23:BB:2882:A:OP1  | 42:BN:96:ARG:HD2  | 2.14        | 0.47     |
| 40:DH:94:ILE:CG2  | 40:DH:95:GLY:N    | 2.77        | 0.47     |
| 1:AA:1080:A:OP1   | 4:AE:51:LYS:HD2   | 2.13        | 0.47     |
| 47:DF:12:VAL:O    | 47:DF:16:MET:HG2  | 2.14        | 0.47     |
| 21:AU:3:ILE:HG23  | 21:AU:18:PHE:CD1  | 2.48        | 0.47     |
| 21:AU:3:ILE:HG21  | 21:AU:19:LYS:CG   | 2.44        | 0.47     |
| 1:CA:947:G:H4'    | 12:CM:107:THR:OG1 | 2.14        | 0.47     |
| 10:CK:95:THR:HG23 | 10:CK:96:ILE:N    | 2.29        | 0.47     |
| 23:DB:2271:G:H2'  | 23:DB:2272:U:C6   | 2.49        | 0.47     |
| 20:AB:218:ALA:HA  | 20:AB:221:ARG:HG2 | 1.96        | 0.47     |
| 21:CU:24:LYS:HZ3  | 21:CU:25:ALA:N    | 2.11        | 0.47     |
| 48:BG:148:ARG:HA  | 48:BG:161:VAL:CG1 | 2.45        | 0.47     |
| 15:CP:67:ILE:HG13 | 15:CP:71:VAL:HG13 | 1.95        | 0.47     |
| 27:DK:54:LYS:H    | 27:DK:54:LYS:CD   | 2.21        | 0.47     |
| 38:BM:63:ILE:HA   | 38:BM:104:GLU:O   | 2.14        | 0.47     |
| 3:CD:158:LEU:HA   | 3:CD:161:ALA:CB   | 2.44        | 0.47     |
| 27:BK:105:ARG:HD2 | 27:BK:122:VAL:CG1 | 2.45        | 0.47     |
| 35:BV:38:LEU:HG   | 35:BV:40:ILE:HG23 | 1.96        | 0.47     |
| 23:DB:1779:U:C5   | 23:DB:1784:A:N7   | 2.81        | 0.47     |
| 23:DB:1551:A:H2'  | 23:DB:1552:A:O4'  | 2.14        | 0.47     |
| 23:BB:2186:G:H2'  | 23:BB:2187:U:O4'  | 2.14        | 0.47     |
| 20:CB:147:LEU:O   | 20:CB:151:LYS:HB3 | 2.14        | 0.47     |
| 40:DH:50:ARG:HA   | 40:DH:53:GLU:HB3  | 1.96        | 0.47     |
| 1:CA:1001:C:H2'   | 1:CA:1002:G:H8    | 1.79        | 0.47     |
| 1:CA:35:G:H2'     | 1:CA:36:C:H6      | 1.78        | 0.47     |
| 23:DB:61:C:O2'    | 23:DB:62:U:H5'    | 2.14        | 0.47     |
| 3:CD:90:LEU:O     | 3:CD:93:LEU:HB2   | 2.15        | 0.47     |
| 1:AA:555:U:H2'    | 1:AA:556:C:C6     | 2.49        | 0.47     |
| 1:CA:1072:G:H2'   | 1:CA:1073:U:C6    | 2.48        | 0.47     |
| 10:CK:80:ASN:CB   | 10:CK:105:ARG:HB3 | 2.43        | 0.47     |
| 23:BB:559:G:H2'   | 23:BB:560:C:O4'   | 2.15        | 0.47     |
| 3:CD:171:GLU:O    | 3:CD:180:THR:N    | 2.47        | 0.47     |
| 23:DB:1854:A:H61  | 23:DB:1888:G:H1'  | 1.77        | 0.47     |
| 1:CA:401:C:H1'    | 1:CA:622:A:H1'    | 1.96        | 0.47     |
| 49:DR:2:TYR:HB2   | 49:DR:42:ALA:N    | 2.29        | 0.47     |
| 1:AA:859:G:O2'    | 1:AA:860:A:H5'    | 2.14        | 0.47     |
| 42:DN:45:ARG:HG3  | 42:DN:95:THR:HG21 | 1.95        | 0.47     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 26:BD:133:THR:HG23 | 26:BD:134:HIS:CD2  | 2.49        | 0.47     |
| 1:CA:392:C:H2'     | 1:CA:393:A:H8      | 1.78        | 0.47     |
| 22:DA:114:C:H2'    | 22:DA:115:A:H8     | 1.78        | 0.47     |
| 12:AM:100:ARG:HH11 | 12:AM:103:THR:HB   | 1.79        | 0.47     |
| 38:BM:69:PRO:HG2   | 38:BM:70:ASP:H     | 1.79        | 0.47     |
| 50:BT:73:ARG:NH2   | 50:BT:73:ARG:HB3   | 2.29        | 0.47     |
| 23:DB:2199:A:H3'   | 23:DB:2200:C:C6    | 2.49        | 0.47     |
| 43:BO:40:ILE:HG22  | 43:BO:44:GLY:HA2   | 1.96        | 0.47     |
| 24:BI:85:ILE:CD1   | 24:BI:137:LEU:HD21 | 2.44        | 0.47     |
| 18:CS:11:ASP:HB2   | 18:CS:14:LEU:HD23  | 1.96        | 0.47     |
| 23:DB:7:G:H4'      | 41:DJ:15:TRP:CZ2   | 2.49        | 0.47     |
| 28:DP:100:ARG:HB3  | 28:DP:101:GLU:H    | 1.49        | 0.47     |
| 22:DA:60:C:H2'     | 22:DA:61:G:C8      | 2.48        | 0.47     |
| 22:BA:59:A:H2'     | 22:BA:60:C:O4'     | 2.13        | 0.47     |
| 1:CA:513:C:H2'     | 1:CA:514:C:H6      | 1.79        | 0.47     |
| 23:DB:2369:A:H2'   | 23:DB:2370:G:C8    | 2.49        | 0.47     |
| 23:DB:2491:U:H5''  | 23:DB:2570:G:C5'   | 2.44        | 0.47     |
| 1:AA:1499:A:H2'    | 1:AA:1500:A:H8     | 1.78        | 0.47     |
| 1:AA:996:A:H2'     | 1:AA:997:U:C6      | 2.49        | 0.47     |
| 25:DC:226:PRO:HG3  | 25:DC:233:GLY:N    | 2.29        | 0.47     |
| 28:BP:29:VAL:HA    | 28:BP:79:VAL:O     | 2.13        | 0.47     |
| 51:BZ:39:TRP:HB2   | 51:BZ:46:PHE:CE2   | 2.48        | 0.47     |
| 1:AA:1363:A:O2'    | 1:AA:1365:G:N7     | 2.40        | 0.47     |
| 48:DG:29:ASN:HD21  | 48:DG:81:GLY:HA2   | 1.80        | 0.47     |
| 23:DB:1689:A:H2'   | 23:DB:1690:A:C8    | 2.49        | 0.47     |
| 23:BB:1111:A:N3    | 23:BB:1112:G:H1'   | 2.29        | 0.47     |
| 1:AA:882:C:O2'     | 1:AA:883:C:H5'     | 2.14        | 0.47     |
| 3:CD:12:ARG:O      | 3:CD:37:PRO:HG3    | 2.14        | 0.47     |
| 47:BF:68:LYS:N     | 47:BF:68:LYS:HD2   | 2.29        | 0.47     |
| 23:BB:2798:U:O5'   | 23:BB:2798:U:H6    | 1.97        | 0.47     |
| 23:BB:853:C:H2'    | 23:BB:854:C:C6     | 2.48        | 0.47     |
| 52:BW:18:LYS:O     | 52:BW:34:SER:HA    | 2.14        | 0.47     |
| 23:DB:2330:G:N3    | 52:DW:38:ARG:HB3   | 2.30        | 0.47     |
| 23:BB:2315:G:H5'   | 47:BF:156:THR:HG21 | 1.95        | 0.47     |
| 26:BD:91:THR:HG23  | 26:BD:92:VAL:N     | 2.25        | 0.47     |
| 53:D6:40:HIS:O     | 53:D6:41:LEU:C     | 2.52        | 0.47     |
| 8:CI:16:ALA:HA     | 8:CI:66:VAL:HA     | 1.96        | 0.47     |
| 8:CI:66:VAL:HG11   | 8:CI:78:ILE:HD11   | 1.96        | 0.47     |
| 41:BJ:24:THR:O     | 41:BJ:25:LEU:HB3   | 2.14        | 0.47     |
| 41:DJ:3:THR:HB     | 41:DJ:44:TYR:OH    | 2.13        | 0.47     |
| 51:DZ:32:ASN:O     | 51:DZ:33:LEU:O     | 2.31        | 0.47     |
| 41:DJ:18:VAL:HG22  | 41:DJ:19:ASP:N     | 2.29        | 0.47     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 29:DE:58:LYS:CD   | 29:DE:58:LYS:N     | 2.77        | 0.47     |
| 23:DB:2733:A:H3'  | 23:DB:2733:A:C8    | 2.49        | 0.47     |
| 46:DU:3:LYS:NZ    | 46:DU:82:VAL:HB    | 2.30        | 0.47     |
| 46:BU:85:ARG:HA   | 46:BU:85:ARG:CZ    | 2.44        | 0.47     |
| 47:BF:78:ILE:HA   | 47:BF:79:ARG:HH11  | 1.79        | 0.47     |
| 47:BF:11:VAL:O    | 47:BF:12:VAL:HB    | 2.14        | 0.47     |
| 25:BC:180:MET:CB  | 25:BC:268:ARG:H    | 2.27        | 0.47     |
| 47:DF:27:VAL:O    | 47:DF:29:ARG:HD2   | 2.14        | 0.47     |
| 4:CE:33:THR:HB    | 4:CE:49:TYR:CE1    | 2.49        | 0.47     |
| 25:DC:180:MET:CB  | 25:DC:268:ARG:H    | 2.27        | 0.47     |
| 28:BP:92:ARG:HH11 | 28:BP:92:ARG:HG3   | 1.77        | 0.47     |
| 9:AJ:56:HIS:O     | 9:AJ:57:VAL:HG12   | 2.13        | 0.47     |
| 23:DB:139:U:H3    | 50:DT:49:LYS:NZ    | 2.12        | 0.47     |
| 28:DP:92:ARG:HH11 | 28:DP:92:ARG:HG3   | 1.78        | 0.47     |
| 53:D6:146:GLU:HG3 | 53:D6:147:LEU:HG   | 1.95        | 0.47     |
| 23:DB:1656:C:P    | 26:DD:141:ARG:HH11 | 2.37        | 0.47     |
| 24:DI:18:ASN:N    | 24:DI:19:PRO:CD    | 2.77        | 0.47     |
| 3:CD:126:GLY:O    | 3:CD:127:ARG:HD2   | 2.15        | 0.47     |
| 49:DR:16:GLU:HG2  | 49:DR:101:ILE:HB   | 1.96        | 0.47     |
| 23:DB:2895:G:H2'  | 23:DB:2896:C:H6    | 1.76        | 0.47     |
| 1:CA:313:A:H2'    | 1:CA:314:C:H6      | 1.79        | 0.47     |
| 44:DQ:14:LYS:O    | 44:DQ:15:LYS:C     | 2.51        | 0.47     |
| 6:CG:144:ALA:O    | 6:CG:146:ALA:N     | 2.45        | 0.47     |
| 23:BB:851:C:O4'   | 30:BY:46:MET:HG2   | 2.14        | 0.47     |
| 25:BC:159:THR:N   | 25:BC:194:VAL:CG1  | 2.77        | 0.47     |
| 28:BP:9:GLN:HA    | 28:BP:12:MET:SD    | 2.54        | 0.47     |
| 51:BZ:14:THR:HA   | 51:BZ:28:ARG:HB2   | 1.95        | 0.47     |
| 5:AF:5:GLU:HA     | 5:AF:63:ASN:HA     | 1.97        | 0.47     |
| 23:BB:1324:G:H1'  | 23:BB:1616:A:C6    | 2.50        | 0.47     |
| 48:BG:115:GLN:CD  | 48:BG:115:GLN:N    | 2.63        | 0.47     |
| 11:AL:54:VAL:HG12 | 11:AL:55:ARG:N     | 2.29        | 0.47     |
| 22:BA:115:A:O2'   | 22:BA:116:G:H5'    | 2.13        | 0.47     |
| 38:DM:69:PRO:HG2  | 38:DM:70:ASP:H     | 1.78        | 0.47     |
| 1:CA:401:C:H2'    | 1:CA:402:G:C8      | 2.48        | 0.47     |
| 1:CA:737:C:O2'    | 1:CA:738:C:H5'     | 2.14        | 0.47     |
| 1:CA:1329:A:H5''  | 12:CM:24:VAL:HA    | 1.95        | 0.47     |
| 2:CC:42:LEU:O     | 2:CC:46:LEU:HD23   | 2.15        | 0.47     |
| 23:DB:935:C:O2'   | 23:DB:936:A:H5'    | 2.14        | 0.47     |
| 25:BC:166:ARG:CB  | 25:BC:171:VAL:HG22 | 2.45        | 0.47     |
| 30:BY:29:ARG:H    | 30:BY:33:HIS:HD2   | 1.58        | 0.47     |
| 50:BT:69:ARG:HB3  | 50:BT:74:ILE:HA    | 1.96        | 0.47     |
| 3:CD:18:LEU:HB2   | 3:CD:20:LEU:HG     | 1.94        | 0.47     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 24:BI:135:MET:HG3  | 24:BI:137:LEU:HG  | 1.96        | 0.47     |
| 23:BB:2286:G:C8    | 23:BB:2286:G:H5'  | 2.49        | 0.47     |
| 1:CA:478:A:H2'     | 1:CA:479:U:O4'    | 2.14        | 0.47     |
| 1:AA:511:C:O2'     | 1:AA:512:U:H5''   | 2.15        | 0.47     |
| 1:CA:585:G:H2'     | 1:CA:586:C:C6     | 2.49        | 0.47     |
| 1:AA:825:A:H2'     | 1:AA:826:C:C6     | 2.48        | 0.47     |
| 29:BE:18:THR:HG22  | 29:BE:106:LYS:NZ  | 2.29        | 0.47     |
| 1:CA:766:A:H2'     | 1:CA:767:A:O4'    | 2.14        | 0.47     |
| 23:BB:807:U:OP2    | 37:BL:36:LYS:HD3  | 2.14        | 0.47     |
| 23:DB:1499:C:O2'   | 23:DB:1500:G:H5'  | 2.14        | 0.47     |
| 46:BU:14:THR:O     | 46:BU:18:LYS:HG2  | 2.13        | 0.47     |
| 23:DB:787:C:H5''   | 23:DB:788:A:H5'   | 1.96        | 0.47     |
| 16:CQ:28:VAL:O     | 16:CQ:36:PHE:HA   | 2.14        | 0.47     |
| 23:DB:840:C:H2'    | 23:DB:841:G:C8    | 2.50        | 0.47     |
| 1:AA:1246:A:H2'    | 1:AA:1247:U:C6    | 2.49        | 0.47     |
| 6:CG:15:PRO:HG2    | 6:CG:43:TYR:OH    | 2.14        | 0.47     |
| 7:CH:34:ALA:O      | 7:CH:38:VAL:HG23  | 2.13        | 0.47     |
| 1:CA:342:C:O2'     | 1:CA:343:U:H5'    | 2.14        | 0.47     |
| 1:AA:929:G:O2'     | 1:AA:930:C:H5'    | 2.14        | 0.47     |
| 23:DB:1516:G:O2'   | 23:DB:1517:G:H5'  | 2.14        | 0.47     |
| 44:DQ:35:PHE:O     | 44:DQ:39:ILE:HG12 | 2.14        | 0.47     |
| 23:BB:2856:A:H2'   | 23:BB:2857:G:C8   | 2.49        | 0.47     |
| 1:AA:208:U:O5'     | 1:AA:208:U:H6     | 1.96        | 0.47     |
| 23:DB:838:C:O2'    | 23:DB:839:U:H5'   | 2.15        | 0.47     |
| 6:CG:94:ARG:NH1    | 6:CG:98:LEU:HD21  | 2.29        | 0.47     |
| 23:DB:2201:G:O2'   | 23:DB:2202:U:H5'  | 2.14        | 0.47     |
| 25:DC:34:GLU:HG3   | 25:DC:34:GLU:O    | 2.14        | 0.47     |
| 53:D6:71:TRP:CD1   | 53:D6:71:TRP:N    | 2.82        | 0.47     |
| 23:BB:963:U:O2'    | 23:BB:964:C:H5'   | 2.14        | 0.47     |
| 41:DJ:76:HIS:CE1   | 41:DJ:85:LYS:HB2  | 2.48        | 0.47     |
| 39:DX:15:ASN:O     | 39:DX:19:LEU:HD13 | 2.14        | 0.47     |
| 23:BB:1147:A:O2'   | 23:BB:1148:U:H5'  | 2.13        | 0.47     |
| 23:DB:1100:C:H41   | 24:DI:1:ALA:N     | 2.12        | 0.47     |
| 23:BB:2332:C:H4'   | 23:BB:2336:A:C6   | 2.49        | 0.47     |
| 25:DC:140:VAL:HG12 | 25:DC:141:HIS:N   | 2.29        | 0.47     |
| 37:BL:124:GLY:O    | 37:BL:125:LEU:HG  | 2.14        | 0.47     |
| 26:BD:109:VAL:HG11 | 26:BD:193:VAL:CG1 | 2.44        | 0.47     |
| 26:BD:193:VAL:HB   | 26:BD:194:PRO:HD2 | 1.95        | 0.47     |
| 8:CI:66:VAL:HG22   | 8:CI:67:LYS:N     | 2.30        | 0.47     |
| 37:DL:78:ARG:HB3   | 37:DL:113:ALA:HB2 | 1.97        | 0.47     |
| 7:AH:101:ALA:HB3   | 7:AH:112:ASP:HB3  | 1.96        | 0.47     |
| 44:BQ:79:ILE:HD13  | 44:BQ:79:ILE:C    | 2.35        | 0.47     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:AA:947:G:H2'     | 1:AA:948:C:C6     | 2.49        | 0.47     |
| 47:BF:169:LEU:HD22 | 47:BF:174:PHE:CE1 | 2.49        | 0.47     |
| 29:BE:152:GLU:O    | 29:BE:153:LEU:HB3 | 2.14        | 0.47     |
| 12:AM:56:ARG:O     | 12:AM:59:VAL:HG12 | 2.14        | 0.47     |
| 23:BB:672:C:O2'    | 23:BB:673:C:H5'   | 2.14        | 0.47     |
| 23:DB:1189:A:H2'   | 23:DB:1190:G:O4'  | 2.13        | 0.47     |
| 46:BU:47:PRO:CD    | 46:BU:55:GLY:HA3  | 2.39        | 0.47     |
| 23:DB:1654:A:H2'   | 23:DB:1655:A:C8   | 2.49        | 0.47     |
| 23:DB:844:A:C2     | 23:DB:845:A:N1    | 2.82        | 0.47     |
| 23:BB:847:U:O4'    | 23:BB:847:U:O2    | 2.30        | 0.47     |
| 1:CA:1337:G:H5''   | 1:CA:1338:G:OP1   | 2.14        | 0.47     |
| 40:DH:47:PHE:HB3   | 40:DH:51:ARG:HH21 | 1.77        | 0.47     |
| 49:BR:59:ILE:HG23  | 49:BR:101:ILE:H   | 1.78        | 0.47     |
| 48:DG:75:VAL:O     | 48:DG:78:VAL:HG22 | 2.14        | 0.47     |
| 6:CG:145:GLU:C     | 6:CG:147:ASN:N    | 2.68        | 0.47     |
| 23:DB:1441:G:H2'   | 23:DB:1442:U:H6   | 1.79        | 0.47     |
| 23:DB:30:G:H2'     | 23:DB:31:C:H6     | 1.74        | 0.47     |
| 23:BB:62:U:H2'     | 23:BB:63:A:O4'    | 2.14        | 0.47     |
| 20:CB:96:LEU:N     | 20:CB:99:MET:HE3  | 2.26        | 0.47     |
| 2:AC:185:THR:HG22  | 2:AC:198:LYS:HA   | 1.97        | 0.47     |
| 23:DB:1427:A:H4'   | 23:DB:1428:C:O5'  | 2.14        | 0.47     |
| 3:AD:100:VAL:HG21  | 3:AD:136:VAL:HG21 | 1.97        | 0.47     |
| 1:AA:617:G:H4'     | 15:AP:46:LYS:HE2  | 1.94        | 0.47     |
| 23:BB:2420:C:O2'   | 23:BB:2421:G:H5'  | 2.14        | 0.47     |
| 23:BB:2078:C:O2'   | 23:BB:2079:U:H5'  | 2.14        | 0.47     |
| 39:DX:17:GLU:HB3   | 39:DX:53:VAL:CG1  | 2.45        | 0.47     |
| 6:AG:58:LEU:HA     | 6:AG:61:PHE:HB3   | 1.95        | 0.47     |
| 23:BB:727:A:OP1    | 23:BB:1431:A:O2'  | 2.30        | 0.47     |
| 20:CB:63:LYS:HB3   | 20:CB:87:ASP:OD2  | 2.14        | 0.47     |
| 1:CA:1330:U:H2'    | 1:CA:1331:G:H5'   | 1.96        | 0.47     |
| 25:BC:86:ARG:HB3   | 25:BC:86:ARG:CZ   | 2.43        | 0.47     |
| 40:BH:57:LYS:HA    | 40:BH:60:GLU:OE2  | 2.14        | 0.47     |
| 37:DL:65:GLY:O     | 37:DL:66:PHE:HB3  | 2.15        | 0.47     |
| 1:AA:1225:A:H5'    | 1:AA:1226:C:OP2   | 2.15        | 0.47     |
| 19:AT:50:PHE:HD2   | 19:AT:78:LEU:HD13 | 1.79        | 0.47     |
| 23:BB:1064:C:H5'   | 24:BI:88:GLY:HA3  | 1.95        | 0.47     |
| 30:DY:29:ARG:H     | 30:DY:33:HIS:HD2  | 1.61        | 0.47     |
| 22:BA:60:C:O2'     | 22:BA:61:G:H5'    | 2.14        | 0.47     |
| 23:DB:1535:A:H5''  | 23:DB:1536:C:C5   | 2.49        | 0.47     |
| 23:DB:528:A:H8     | 23:DB:528:A:H3'   | 1.79        | 0.47     |
| 1:CA:1039:G:H2'    | 1:CA:1040:U:H6    | 1.80        | 0.47     |
| 25:BC:42:ARG:HG3   | 25:BC:46:GLY:O    | 2.14        | 0.47     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 2:CC:13:ILE:O      | 2:CC:15:LYS:N     | 2.48        | 0.47     |
| 17:CR:22:TYR:CE2   | 17:CR:23:LYS:HE3  | 2.50        | 0.47     |
| 1:CA:821:G:H2'     | 1:CA:822:U:C6     | 2.49        | 0.47     |
| 1:AA:821:G:H2'     | 1:AA:822:U:H6     | 1.79        | 0.47     |
| 1:AA:1366:C:H2'    | 1:AA:1367:C:C6    | 2.49        | 0.47     |
| 23:BB:226:A:H5''   | 23:BB:257:C:O2'   | 2.14        | 0.47     |
| 48:DG:29:ASN:ND2   | 48:DG:77:GLY:O    | 2.47        | 0.47     |
| 37:DL:70:LYS:O     | 37:DL:73:ILE:HG12 | 2.14        | 0.47     |
| 1:CA:624:C:H2'     | 1:CA:625:U:C6     | 2.50        | 0.47     |
| 23:DB:2555:U:H2'   | 23:DB:2556:C:O4'  | 2.14        | 0.47     |
| 1:AA:961:U:OP1     | 1:AA:1223:C:H4'   | 2.14        | 0.47     |
| 23:BB:2153:C:H2'   | 23:BB:2153:C:O2   | 2.14        | 0.47     |
| 8:CI:71:ILE:HD12   | 8:CI:71:ILE:N     | 2.29        | 0.47     |
| 23:BB:1689:A:H2'   | 23:BB:1690:A:C8   | 2.49        | 0.47     |
| 23:BB:2494:G:H4'   | 38:BM:79:ALA:HB2  | 1.97        | 0.47     |
| 1:AA:1207:G:O2'    | 1:AA:1208:C:H5'   | 2.14        | 0.47     |
| 23:DB:2332:C:H4'   | 23:DB:2336:A:C6   | 2.49        | 0.47     |
| 48:BG:103:ASN:HA   | 48:BG:113:ASP:OD1 | 2.14        | 0.47     |
| 44:DQ:30:VAL:CG1   | 44:DQ:31:TYR:N    | 2.65        | 0.47     |
| 47:BF:32:LYS:HA    | 47:BF:95:MET:CG   | 2.44        | 0.47     |
| 53:D6:56:ALA:HB2   | 53:D6:79:ILE:CD1  | 2.39        | 0.47     |
| 53:B6:93:SER:O     | 53:B6:99:LEU:HD22 | 2.14        | 0.47     |
| 1:CA:1352:C:H2'    | 1:CA:1353:G:C8    | 2.50        | 0.47     |
| 8:AI:24:ASN:O      | 8:AI:60:LEU:N     | 2.48        | 0.47     |
| 51:DZ:56:MET:HA    | 51:DZ:59:ILE:HG12 | 1.96        | 0.47     |
| 1:AA:982:U:OP2     | 13:AN:60:ARG:NH1  | 2.47        | 0.47     |
| 1:AA:1014:A:H5''   | 18:AS:13:HIS:HB3  | 1.95        | 0.47     |
| 30:DY:12:ALA:HB2   | 30:DY:53:MET:HE1  | 1.95        | 0.47     |
| 50:BT:85:VAL:C     | 50:BT:86:THR:HG23 | 2.34        | 0.47     |
| 23:BB:397:U:H2'    | 23:BB:398:C:C6    | 2.49        | 0.47     |
| 22:BA:29:A:H2'     | 22:BA:30:C:O4'    | 2.14        | 0.47     |
| 10:AK:113:THR:HG21 | 21:AU:28:LEU:HD12 | 1.96        | 0.47     |
| 50:DT:50:LEU:O     | 50:DT:51:PHE:HB2  | 2.14        | 0.47     |
| 50:DT:29:THR:CA    | 50:DT:86:THR:HA   | 2.40        | 0.47     |
| 23:BB:2809:A:H2'   | 23:BB:2810:A:C8   | 2.49        | 0.47     |
| 23:BB:1175:A:H2'   | 23:BB:1175:A:N3   | 2.27        | 0.47     |
| 13:AN:50:LEU:HB3   | 13:AN:51:PRO:HD3  | 1.95        | 0.47     |
| 15:AP:71:VAL:HG13  | 15:AP:72:ALA:N    | 2.30        | 0.47     |
| 23:DB:1028:A:N6    | 23:DB:1125:G:H2'  | 2.29        | 0.47     |
| 13:CN:16:ALA:HA    | 13:CN:54:SER:O    | 2.14        | 0.47     |
| 43:BO:26:LEU:HD13  | 43:BO:39:VAL:HG23 | 1.96        | 0.47     |
| 35:DV:38:LEU:HG    | 35:DV:40:ILE:HG23 | 1.96        | 0.47     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 15:CP:71:VAL:HG13  | 15:CP:72:ALA:N    | 2.29        | 0.47     |
| 27:DK:43:ILE:CG2   | 27:DK:46:ALA:HB2  | 2.43        | 0.47     |
| 20:AB:16:GLY:HA3   | 20:AB:40:ILE:H    | 1.79        | 0.47     |
| 20:AB:57:ASN:HD22  | 20:AB:223:GLY:CA  | 2.28        | 0.47     |
| 1:CA:1340:A:H2'    | 1:CA:1341:U:O4'   | 2.13        | 0.47     |
| 49:DR:39:LEU:HD23  | 49:DR:39:LEU:N    | 2.29        | 0.47     |
| 49:DR:59:ILE:HA    | 49:DR:101:ILE:H   | 1.78        | 0.47     |
| 21:CU:48:LYS:HA    | 21:CU:51:ALA:CB   | 2.41        | 0.47     |
| 38:DM:19:GLY:H     | 38:DM:38:ARG:NH1  | 2.09        | 0.47     |
| 9:CJ:7:ARG:O       | 9:CJ:100:ILE:HA   | 2.14        | 0.47     |
| 28:DP:6:GLN:NE2    | 28:DP:7:LEU:N     | 2.62        | 0.47     |
| 23:DB:2103:C:H2'   | 23:DB:2104:C:O4'  | 2.14        | 0.47     |
| 1:AA:1072:G:H2'    | 1:AA:1073:U:C6    | 2.49        | 0.47     |
| 2:CC:129:PHE:CE2   | 2:CC:165:GLU:HG2  | 2.42        | 0.47     |
| 23:DB:560:C:H3'    | 23:DB:561:G:C8    | 2.49        | 0.47     |
| 11:CL:51:VAL:HG12  | 11:CL:52:CYS:N    | 2.25        | 0.47     |
| 23:BB:582:A:H2'    | 23:BB:583:G:C8    | 2.50        | 0.47     |
| 1:AA:552:U:H2'     | 1:AA:553:A:C8     | 2.49        | 0.47     |
| 2:CC:26:LYS:HE2    | 2:CC:27:GLU:CG    | 2.44        | 0.47     |
| 1:CA:9:G:H5'       | 4:CE:107:GLY:CA   | 2.44        | 0.47     |
| 4:CE:158:LYS:HZ3   | 7:CH:65:PHE:HA    | 1.80        | 0.47     |
| 3:CD:167:PRO:HG3   | 3:CD:170:LEU:HD11 | 1.96        | 0.47     |
| 23:DB:642:U:O2'    | 23:DB:644:A:N7    | 2.44        | 0.47     |
| 23:BB:947:A:H2'    | 23:BB:948:C:H6    | 1.77        | 0.47     |
| 23:BB:1825:U:H2'   | 23:BB:1826:G:H8   | 1.79        | 0.47     |
| 23:DB:2026:U:H2'   | 23:DB:2027:G:C8   | 2.49        | 0.47     |
| 49:BR:2:TYR:CB     | 49:BR:42:ALA:HB2  | 2.42        | 0.47     |
| 1:AA:68:G:H5'      | 1:AA:171:A:O2'    | 2.13        | 0.47     |
| 23:DB:1809:A:H2'   | 23:DB:1810:A:C8   | 2.49        | 0.47     |
| 23:DB:1454:C:H5'   | 42:DN:63:ARG:CZ   | 2.45        | 0.47     |
| 1:AA:833:G:H2'     | 1:AA:834:U:C6     | 2.49        | 0.47     |
| 37:BL:135:ILE:HG23 | 37:BL:136:GLU:N   | 2.29        | 0.47     |
| 23:DB:1535:A:H5''  | 23:DB:1536:C:H5   | 1.80        | 0.47     |
| 23:BB:314:C:O2'    | 23:BB:315:G:H5'   | 2.13        | 0.47     |
| 26:DD:122:VAL:HA   | 26:DD:127:PHE:N   | 2.29        | 0.47     |
| 1:CA:204:G:H2'     | 1:CA:205:A:C8     | 2.48        | 0.47     |
| 23:DB:1163:G:O2'   | 23:DB:1164:C:H5'  | 2.14        | 0.47     |
| 44:DQ:40:LYS:HD2   | 44:DQ:44:TYR:CE1  | 2.49        | 0.47     |
| 12:CM:23:GLY:HA3   | 12:CM:68:LEU:CD1  | 2.44        | 0.47     |
| 1:CA:996:A:H2'     | 1:CA:997:U:C6     | 2.50        | 0.47     |
| 26:BD:141:ARG:HG3  | 26:BD:141:ARG:O   | 2.15        | 0.47     |
| 43:DO:104:GLN:O    | 43:DO:107:ALA:HB3 | 2.14        | 0.47     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:DB:1842:G:H2'   | 23:DB:1843:C:H6   | 1.79        | 0.47     |
| 23:DB:2296:U:H4'   | 23:DB:2297:A:OP1  | 2.13        | 0.47     |
| 23:BB:1155:A:O2'   | 23:BB:1156:A:H2'  | 2.15        | 0.47     |
| 1:CA:1435:G:H2'    | 1:CA:1436:U:C6    | 2.50        | 0.47     |
| 23:DB:2187:U:H2'   | 23:DB:2188:U:H6   | 1.80        | 0.47     |
| 1:AA:77:A:H8       | 1:AA:77:A:O5'     | 1.97        | 0.47     |
| 1:CA:580:C:H2'     | 1:CA:581:G:O4'    | 2.14        | 0.47     |
| 23:DB:2047:C:H2'   | 23:DB:2048:G:H8   | 1.80        | 0.47     |
| 32:D4:19:ARG:O     | 32:D4:20:ASP:HB2  | 2.14        | 0.47     |
| 25:BC:170:TYR:CE2  | 25:BC:184:GLU:HA  | 2.50        | 0.47     |
| 10:AK:41:LEU:HD22  | 10:AK:76:TYR:CE2  | 2.50        | 0.47     |
| 5:CF:3:HIS:CE1     | 5:CF:95:ALA:H     | 2.33        | 0.47     |
| 48:DG:94:ARG:HB2   | 48:DG:127:GLN:HG3 | 1.96        | 0.47     |
| 26:BD:55:LYS:H     | 26:BD:76:GLY:H    | 1.62        | 0.47     |
| 40:BH:100:ALA:HB1  | 40:BH:132:PHE:CE1 | 2.44        | 0.47     |
| 41:BJ:16:TYR:O     | 41:BJ:55:ILE:HG12 | 2.15        | 0.47     |
| 20:CB:14:HIS:HB2   | 20:CB:208:ALA:CB  | 2.43        | 0.47     |
| 23:DB:986:C:O2'    | 23:DB:987:C:H5'   | 2.13        | 0.47     |
| 25:BC:93:VAL:HG12  | 25:BC:101:ARG:O   | 2.14        | 0.47     |
| 26:DD:55:LYS:H     | 26:DD:76:GLY:H    | 1.61        | 0.47     |
| 1:CA:599:C:H5'     | 7:CH:86:LYS:O     | 2.14        | 0.47     |
| 13:AN:70:HIS:O     | 13:AN:72:PHE:N    | 2.48        | 0.47     |
| 42:BN:38:LEU:CB    | 42:BN:39:PRO:HD3  | 2.41        | 0.47     |
| 42:BN:106:ASP:OD1  | 42:BN:108:ALA:HB3 | 2.14        | 0.47     |
| 1:CA:948:C:O2'     | 1:CA:949:A:H5'    | 2.14        | 0.47     |
| 23:BB:1023:U:H2'   | 23:BB:1024:G:C5'  | 2.44        | 0.47     |
| 25:DC:12:ARG:HA    | 25:DC:15:VAL:CG2  | 2.45        | 0.47     |
| 53:D6:178:LYS:HA   | 53:D6:181:GLN:OE1 | 2.14        | 0.47     |
| 23:BB:2270:A:H2'   | 23:BB:2271:G:O4'  | 2.13        | 0.47     |
| 8:CI:33:SER:HB3    | 8:CI:36:GLN:NE2   | 2.30        | 0.47     |
| 1:AA:723:U:O4'     | 21:AU:48:LYS:HD3  | 2.13        | 0.47     |
| 48:DG:148:ARG:HD2  | 48:DG:149:ALA:N   | 2.30        | 0.47     |
| 23:DB:981:A:H4'    | 23:DB:2037:A:H5'  | 1.97        | 0.47     |
| 13:CN:20:PHE:CB    | 13:CN:24:ALA:HB2  | 2.45        | 0.47     |
| 43:BO:26:LEU:HA    | 43:BO:39:VAL:HA   | 1.97        | 0.47     |
| 25:BC:204:LEU:HD23 | 25:BC:209:ALA:CB  | 2.45        | 0.47     |
| 1:AA:465:A:H5'     | 1:AA:465:A:N3     | 2.30        | 0.47     |
| 23:DB:2723:C:O3'   | 42:DN:1:MET:HE1   | 2.14        | 0.47     |
| 26:DD:114:LYS:HG2  | 26:DD:166:GLY:HA2 | 1.96        | 0.47     |
| 22:BA:105:G:O2'    | 22:BA:106:G:H5'   | 2.15        | 0.47     |
| 38:BM:26:VAL:HG23  | 38:BM:104:GLU:OE2 | 2.14        | 0.47     |
| 49:BR:49:ILE:HG22  | 49:BR:54:VAL:HB   | 1.95        | 0.47     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:1197:G:H2'  | 23:DB:1198:U:H6    | 1.80        | 0.47     |
| 20:CB:212:TYR:O   | 20:CB:216:VAL:HG13 | 2.15        | 0.47     |
| 20:CB:110:ILE:O   | 20:CB:113:LEU:HB3  | 2.15        | 0.47     |
| 23:DB:192:C:C2'   | 23:DB:193:U:H5'    | 2.44        | 0.47     |
| 23:DB:2078:C:O2'  | 23:DB:2079:U:H5'   | 2.14        | 0.47     |
| 14:CO:16:GLY:HA2  | 14:CO:27:VAL:CG2   | 2.44        | 0.47     |
| 4:AE:45:VAL:CG1   | 4:AE:116:VAL:HG23  | 2.45        | 0.47     |
| 46:BU:9:GLU:CD    | 46:BU:21:ARG:HD2   | 2.35        | 0.47     |
| 1:CA:238:A:C3'    | 1:CA:239:U:H5''    | 2.45        | 0.47     |
| 23:DB:116:C:O2'   | 23:DB:126:A:C8     | 2.68        | 0.47     |
| 23:BB:1854:A:H2   | 23:BB:2087:G:N3    | 2.12        | 0.47     |
| 30:BY:7:THR:O     | 30:BY:54:VAL:HG12  | 2.14        | 0.47     |
| 3:CD:84:ASN:HD22  | 3:CD:85:THR:N      | 2.12        | 0.47     |
| 40:DH:3:VAL:HG12  | 40:DH:38:PRO:HA    | 1.96        | 0.47     |
| 5:CF:53:LYS:HB3   | 5:CF:54:LEU:HD22   | 1.96        | 0.47     |
| 7:CH:44:PHE:HE2   | 7:CH:100:ILE:HG12  | 1.79        | 0.47     |
| 19:AT:35:TYR:CG   | 19:AT:36:ALA:N     | 2.83        | 0.47     |
| 6:AG:129:ASN:HA   | 6:AG:134:VAL:HG11  | 1.95        | 0.47     |
| 6:CG:91:ARG:HD2   | 6:CG:91:ARG:H      | 1.80        | 0.47     |
| 22:BA:8:C:O2'     | 43:BO:40:ILE:HD13  | 2.14        | 0.47     |
| 1:AA:585:G:H2'    | 1:AA:586:C:C6      | 2.50        | 0.47     |
| 34:B3:38:LYS:HG3  | 34:B3:41:ARG:NH1   | 2.30        | 0.47     |
| 23:DB:902:C:H2'   | 23:DB:903:C:H6     | 1.80        | 0.47     |
| 23:DB:1846:G:H2'  | 23:DB:1847:A:O4'   | 2.14        | 0.47     |
| 23:BB:1275:A:N3   | 23:BB:1275:A:H2'   | 2.29        | 0.47     |
| 23:BB:585:G:H2'   | 23:BB:1251:C:H42   | 1.80        | 0.47     |
| 23:DB:76:C:O2'    | 23:DB:77:G:H5'     | 2.14        | 0.47     |
| 34:B3:14:LYS:O    | 34:B3:21:PHE:O     | 2.32        | 0.47     |
| 23:BB:1747:U:H2'  | 23:BB:1748:C:C6    | 2.49        | 0.47     |
| 24:DI:102:ARG:HG3 | 24:DI:141:ASP:CB   | 2.44        | 0.47     |
| 1:AA:777:A:H2'    | 1:AA:778:G:C8      | 2.49        | 0.47     |
| 29:DE:88:ARG:HG3  | 29:DE:88:ARG:NH2   | 2.29        | 0.47     |
| 17:AR:44:THR:OG1  | 17:AR:46:THR:HG22  | 2.14        | 0.47     |
| 6:AG:15:PRO:HG2   | 6:AG:43:TYR:OH     | 2.14        | 0.47     |
| 1:CA:1437:A:H2'   | 1:CA:1438:G:H8     | 1.78        | 0.47     |
| 23:BB:640:C:H2'   | 23:BB:641:U:C6     | 2.49        | 0.47     |
| 45:BS:4:ILE:CG2   | 45:BS:106:VAL:HG22 | 2.45        | 0.47     |
| 23:DB:167:A:H2'   | 23:DB:168:G:O4'    | 2.15        | 0.47     |
| 1:AA:224:U:H2'    | 1:AA:225:C:H6      | 1.78        | 0.47     |
| 23:BB:757:G:H2'   | 23:BB:758:C:H5'    | 1.97        | 0.47     |
| 23:BB:1479:G:O2'  | 23:BB:1480:C:H5'   | 2.15        | 0.47     |
| 48:DG:125:PRO:HB2 | 48:DG:129:GLU:OE2  | 2.14        | 0.47     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:960:U:O2      | 1:CA:960:U:H5''    | 2.15        | 0.47     |
| 23:DB:1661:G:O2'   | 23:DB:1662:U:H5'   | 2.15        | 0.47     |
| 23:DB:1098:A:O3'   | 24:DI:4:VAL:O      | 2.32        | 0.47     |
| 2:CC:190:THR:CG2   | 2:CC:191:THR:N     | 2.77        | 0.47     |
| 23:BB:921:C:H2'    | 23:BB:922:C:H6     | 1.80        | 0.47     |
| 25:BC:169:ALA:O    | 25:BC:185:ALA:HB3  | 2.15        | 0.47     |
| 23:DB:2336:A:N6    | 52:DW:40:ARG:HD2   | 2.29        | 0.47     |
| 48:BG:42:VAL:HG23  | 48:BG:50:THR:O     | 2.14        | 0.47     |
| 44:DQ:18:LYS:C     | 44:DQ:20:ALA:N     | 2.68        | 0.47     |
| 48:DG:68:ARG:NH1   | 48:DG:72:ASN:HD22  | 2.11        | 0.47     |
| 37:BL:124:GLY:N    | 37:BL:143:GLU:CG   | 2.71        | 0.47     |
| 53:D6:68:VAL:C     | 53:D6:70:SER:H     | 2.17        | 0.47     |
| 53:D6:73:GLN:O     | 53:D6:77:LYS:HE2   | 2.14        | 0.47     |
| 53:B6:28:LEU:HD11  | 53:B6:121:TYR:HE2  | 1.80        | 0.47     |
| 53:B6:68:VAL:CG1   | 53:B6:79:ILE:HD13  | 2.45        | 0.47     |
| 40:BH:82:SER:HB2   | 40:BH:146:VAL:HG13 | 1.97        | 0.47     |
| 8:CI:64:ILE:HD12   | 8:CI:64:ILE:N      | 2.28        | 0.47     |
| 20:CB:164:ASP:OD1  | 20:CB:203:ASP:HB2  | 2.14        | 0.47     |
| 20:CB:209:VAL:HG23 | 20:CB:210:THR:H    | 1.79        | 0.47     |
| 1:AA:1147:C:H2'    | 1:AA:1148:U:C6     | 2.50        | 0.47     |
| 51:DZ:49:LEU:HB2   | 51:DZ:51:VAL:HG23  | 1.97        | 0.47     |
| 25:BC:141:HIS:CG   | 25:BC:142:ASN:H    | 2.32        | 0.47     |
| 37:DL:127:VAL:HG22 | 37:DL:128:THR:N    | 2.29        | 0.47     |
| 2:AC:80:GLY:O      | 2:AC:84:GLU:HB2    | 2.14        | 0.47     |
| 48:DG:15:ASP:OD2   | 48:DG:17:LYS:HB2   | 2.14        | 0.47     |
| 48:DG:33:THR:HA    | 48:DG:34:ARG:NH1   | 2.30        | 0.47     |
| 1:CA:1216:A:H5''   | 13:CN:4:SER:CB     | 2.42        | 0.47     |
| 50:BT:23:ALA:C     | 50:BT:25:GLU:H     | 2.16        | 0.47     |
| 50:BT:54:GLU:HB3   | 50:BT:88:LYS:HB2   | 1.96        | 0.47     |
| 46:DU:86:PHE:HB3   | 46:DU:90:LYS:O     | 2.15        | 0.47     |
| 40:DH:127:GLU:HB2  | 40:DH:143:ILE:HG22 | 1.96        | 0.47     |
| 25:BC:188:ARG:HG2  | 25:BC:188:ARG:HH21 | 1.80        | 0.47     |
| 43:BO:34:HIS:HB3   | 43:BO:36:TYR:CE2   | 2.46        | 0.47     |
| 43:BO:51:ALA:HB3   | 43:BO:78:VAL:CG2   | 2.44        | 0.47     |
| 1:AA:410:G:P       | 3:AD:25:ARG:HE     | 2.38        | 0.47     |
| 24:DI:72:THR:CG2   | 24:DI:112:LYS:HD2  | 2.44        | 0.47     |
| 24:DI:75:ALA:O     | 24:DI:79:LEU:HG    | 2.15        | 0.47     |
| 47:BF:66:ILE:HA    | 47:BF:85:GLY:O     | 2.15        | 0.47     |
| 29:BE:126:VAL:HG21 | 29:BE:133:LEU:HB2  | 1.97        | 0.47     |
| 40:DH:126:GLY:H    | 40:DH:146:VAL:HB   | 1.80        | 0.47     |
| 47:DF:113:PHE:CZ   | 47:DF:175:PRO:HB2  | 2.50        | 0.47     |
| 10:AK:83:VAL:CB    | 10:AK:109:ILE:HG23 | 2.40        | 0.47     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 18:CS:48:ILE:HG22 | 18:CS:49:ALA:N     | 2.27        | 0.47     |
| 12:AM:10:ASP:HA   | 12:AM:44:ILE:CD1   | 2.43        | 0.47     |
| 18:AS:46:LEU:O    | 18:AS:60:PHE:HA    | 2.14        | 0.47     |
| 13:AN:25:GLU:O    | 13:AN:29:ILE:HG13  | 2.15        | 0.47     |
| 18:AS:62:THR:H    | 18:AS:65:MET:HB3   | 1.79        | 0.47     |
| 33:D1:49:LYS:HG3  | 33:D1:50:GLU:N     | 2.19        | 0.47     |
| 23:BB:1025:G:H1'  | 23:BB:1135:C:O5'   | 2.15        | 0.47     |
| 23:BB:2848:G:H1'  | 23:BB:2868:A:N6    | 2.29        | 0.47     |
| 29:BE:58:LYS:N    | 29:BE:58:LYS:HD3   | 2.29        | 0.47     |
| 53:D6:174:GLN:NE2 | 53:D6:178:LYS:HE2  | 2.30        | 0.47     |
| 45:DS:55:ILE:CD1  | 45:DS:107:VAL:HG21 | 2.45        | 0.47     |
| 23:DB:27:G:HO2'   | 23:DB:28:A:H8      | 1.55        | 0.47     |
| 32:D4:16:ILE:HG12 | 32:D4:25:VAL:HG22  | 1.95        | 0.47     |
| 23:DB:2037:A:H2'  | 23:DB:2038:G:C8    | 2.50        | 0.47     |
| 1:AA:1470:U:O2'   | 1:AA:1471:U:H5'    | 2.15        | 0.47     |
| 25:BC:15:VAL:HG22 | 25:BC:204:LEU:O    | 2.15        | 0.47     |
| 27:BK:15:GLY:HA2  | 27:BK:46:ALA:HA    | 1.96        | 0.47     |
| 23:DB:2773:C:H5'' | 26:DD:169:ARG:HB2  | 1.94        | 0.47     |
| 23:DB:2773:C:O2'  | 23:DB:2774:C:H5'   | 2.15        | 0.47     |
| 31:D0:50:GLY:C    | 31:D0:51:ARG:HG2   | 2.35        | 0.47     |
| 23:DB:591:U:O2'   | 23:DB:592:A:H5'    | 2.14        | 0.47     |
| 2:CC:110:LEU:HD21 | 2:CC:140:ALA:O     | 2.14        | 0.47     |
| 44:BQ:105:PHE:HA  | 44:BQ:108:LEU:HG   | 1.97        | 0.47     |
| 27:DK:113:MET:HA  | 27:DK:116:ILE:HD11 | 1.95        | 0.47     |
| 44:BQ:14:LYS:O    | 44:BQ:15:LYS:C     | 2.52        | 0.47     |
| 1:AA:842:U:H2'    | 1:AA:843:U:O3'     | 2.15        | 0.47     |
| 28:DP:6:GLN:O     | 28:DP:10:GLU:HB2   | 2.15        | 0.47     |
| 1:AA:86:G:H1'     | 1:AA:87:C:H5       | 1.78        | 0.47     |
| 20:CB:65:LYS:HA   | 20:CB:89:PHE:HE1   | 1.79        | 0.47     |
| 1:CA:842:U:H2'    | 1:CA:843:U:O3'     | 2.15        | 0.47     |
| 9:AJ:7:ARG:O      | 9:AJ:100:ILE:HA    | 2.14        | 0.47     |
| 20:AB:147:LEU:O   | 20:AB:151:LYS:HB3  | 2.14        | 0.47     |
| 28:BP:6:GLN:HA    | 28:BP:9:GLN:HG2    | 1.95        | 0.47     |
| 4:AE:158:LYS:HZ1  | 7:AH:65:PHE:HA     | 1.80        | 0.47     |
| 10:AK:28:ASN:HD22 | 10:AK:29:THR:H     | 1.63        | 0.47     |
| 10:AK:28:ASN:HD22 | 10:AK:46:ALA:HB3   | 1.78        | 0.47     |
| 34:B3:31:ILE:O    | 34:B3:31:ILE:HG12  | 2.15        | 0.47     |
| 2:CC:113:LYS:HB2  | 2:CC:184:ASN:OD1   | 2.14        | 0.47     |
| 1:CA:1381:U:O2'   | 1:CA:1382:C:H5'    | 2.15        | 0.47     |
| 46:DU:39:ASN:CB   | 46:DU:62:ALA:HB3   | 2.43        | 0.47     |
| 7:CH:58:LEU:O     | 7:CH:60:LEU:N      | 2.48        | 0.47     |
| 2:CC:155:ARG:H    | 2:CC:162:ALA:HA    | 1.79        | 0.47     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 14:AO:25:THR:CB    | 14:AO:70:LEU:HD23  | 2.44        | 0.47     |
| 39:DX:20:ASN:H     | 39:DX:20:ASN:HD22  | 1.60        | 0.47     |
| 23:BB:1776:G:O2'   | 23:BB:1777:U:H5'   | 2.15        | 0.47     |
| 12:CM:89:ARG:HD3   | 12:CM:95:PRO:O     | 2.14        | 0.47     |
| 31:B0:2:VAL:HG12   | 31:B0:3:GLN:H      | 1.80        | 0.47     |
| 39:BX:20:ASN:H     | 39:BX:20:ASN:ND2   | 2.13        | 0.47     |
| 23:BB:2746:U:H5''  | 48:BG:137:LYS:HD2  | 1.97        | 0.47     |
| 1:AA:1096:C:H2'    | 1:AA:1097:C:C6     | 2.49        | 0.47     |
| 46:BU:10:VAL:HG21  | 46:BU:35:VAL:HG21  | 1.96        | 0.47     |
| 40:BH:41:LYS:CA    | 40:BH:44:ILE:HG13  | 2.44        | 0.47     |
| 23:BB:1007:C:H4'   | 41:BJ:110:PRO:HB3  | 1.96        | 0.47     |
| 23:BB:1811:G:O2'   | 23:BB:1812:U:H5'   | 2.15        | 0.47     |
| 3:CD:192:ALA:C     | 3:CD:194:ILE:H     | 2.18        | 0.47     |
| 23:BB:704:G:C2'    | 23:BB:726:G:H22    | 2.26        | 0.47     |
| 45:BS:50:VAL:HA    | 45:BS:53:SER:HB3   | 1.96        | 0.47     |
| 23:DB:21:A:H2'     | 23:DB:22:C:H6      | 1.76        | 0.47     |
| 23:DB:1175:A:H2'   | 23:DB:1175:A:N3    | 2.29        | 0.47     |
| 23:DB:705:A:N6     | 23:DB:726:G:H1'    | 2.29        | 0.47     |
| 23:DB:2028:U:O2'   | 23:DB:2029:G:H5'   | 2.14        | 0.47     |
| 23:BB:1592:C:H2'   | 23:BB:1593:A:C8    | 2.48        | 0.47     |
| 23:DB:1805:A:N3    | 25:DC:49:THR:HG23  | 2.29        | 0.47     |
| 23:DB:1810:A:H2'   | 23:DB:1811:G:O4'   | 2.15        | 0.47     |
| 1:AA:769:G:H4'     | 1:AA:1513:A:H4'    | 1.96        | 0.47     |
| 23:DB:2462:C:H2'   | 23:DB:2463:C:C6    | 2.50        | 0.47     |
| 23:DB:1356:G:O2'   | 23:DB:1357:C:H5'   | 2.15        | 0.47     |
| 23:DB:1573:G:H2'   | 23:DB:1574:C:H5'   | 1.97        | 0.47     |
| 26:DD:16:THR:HG22  | 26:DD:17:GLU:H     | 1.80        | 0.47     |
| 42:DN:12:ARG:HG2   | 42:DN:16:HIS:HB2   | 1.97        | 0.47     |
| 20:AB:172:ILE:HG23 | 20:AB:182:VAL:HG11 | 1.96        | 0.47     |
| 23:DB:1637:A:H2'   | 23:DB:1638:C:H6    | 1.78        | 0.47     |
| 1:AA:1460:C:H2'    | 1:AA:1461:G:C8     | 2.49        | 0.47     |
| 23:BB:1063:G:H4'   | 24:BI:135:MET:HB3  | 1.96        | 0.47     |
| 50:DT:14:PRO:HA    | 50:DT:32:LEU:CB    | 2.45        | 0.47     |
| 23:DB:962:G:H21    | 23:DB:2250:G:H1    | 1.60        | 0.47     |
| 16:AQ:30:HIS:ND1   | 16:AQ:32:ILE:HG22  | 2.30        | 0.47     |
| 23:BB:231:A:H3'    | 23:BB:232:G:C8     | 2.50        | 0.47     |
| 23:DB:832:U:OP1    | 37:DL:38:GLN:N     | 2.48        | 0.47     |
| 48:BG:39:ALA:HB1   | 48:BG:57:TYR:CG    | 2.50        | 0.47     |
| 37:BL:129:LYS:HA   | 37:BL:132:ARG:HG2  | 1.95        | 0.47     |
| 50:DT:45:ALA:HA    | 50:DT:48:GLN:CG    | 2.45        | 0.47     |
| 23:BB:832:U:OP1    | 37:BL:38:GLN:N     | 2.48        | 0.47     |
| 1:AA:91:U:H6       | 1:AA:91:U:O5'      | 1.96        | 0.47     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 28:DP:103:THR:HG22 | 28:DP:104:GLY:N   | 2.28        | 0.47     |
| 23:BB:269:C:H2'    | 23:BB:270:A:C8    | 2.47        | 0.47     |
| 37:DL:131:ALA:C    | 37:DL:133:ALA:N   | 2.68        | 0.47     |
| 1:AA:546:A:P       | 3:AD:68:GLU:HB3   | 2.54        | 0.47     |
| 22:BA:11:C:H5''    | 52:BW:71:LYS:HE3  | 1.96        | 0.47     |
| 23:DB:1252:G:H1'   | 44:DQ:32:ARG:NH2  | 2.29        | 0.47     |
| 23:BB:2543:G:H2'   | 23:BB:2544:G:H8   | 1.80        | 0.47     |
| 2:CC:176:THR:HB    | 2:CC:179:ALA:HB2  | 1.96        | 0.47     |
| 23:BB:2636:C:H2'   | 23:BB:2637:U:H6   | 1.80        | 0.47     |
| 23:BB:2324:U:H3'   | 23:BB:2325:G:C5'  | 2.45        | 0.47     |
| 1:CA:1367:C:O2'    | 1:CA:1368:A:H5'   | 2.15        | 0.47     |
| 40:BH:59:ALA:CA    | 40:BH:62:LEU:HG   | 2.45        | 0.47     |
| 6:CG:38:ALA:O      | 6:CG:42:VAL:HG23  | 2.14        | 0.47     |
| 23:DB:1712:U:H2'   | 23:DB:1713:A:C8   | 2.49        | 0.47     |
| 23:BB:659:G:H4'    | 29:BE:95:LYS:HD2  | 1.96        | 0.47     |
| 29:BE:88:ARG:NH2   | 29:BE:88:ARG:HG3  | 2.30        | 0.47     |
| 23:DB:736:C:H2'    | 23:DB:737:C:H6    | 1.80        | 0.47     |
| 23:BB:607:U:O4     | 23:BB:620:G:H5''  | 2.15        | 0.47     |
| 1:AA:201:G:H2'     | 1:AA:202:G:O4'    | 2.14        | 0.47     |
| 23:BB:796:C:H2'    | 23:BB:797:G:H8    | 1.78        | 0.47     |
| 27:BK:11:ALA:O     | 27:BK:100:PHE:N   | 2.48        | 0.47     |
| 23:DB:1878:G:H2'   | 23:DB:1879:C:C6   | 2.49        | 0.47     |
| 39:DX:45:GLN:O     | 39:DX:46:VAL:HB   | 2.14        | 0.47     |
| 25:BC:20:ASN:OD1   | 25:BC:22:GLU:HG2  | 2.14        | 0.47     |
| 1:CA:555:U:H2'     | 1:CA:556:C:H6     | 1.80        | 0.47     |
| 25:BC:4:LYS:HD2    | 25:BC:5:CYS:H     | 1.79        | 0.47     |
| 1:AA:1435:G:H2'    | 1:AA:1436:U:C6    | 2.50        | 0.47     |
| 23:BB:200:U:H5''   | 51:BZ:22:LEU:O    | 2.15        | 0.47     |
| 5:CF:11:HIS:CG     | 5:CF:12:PRO:HD2   | 2.49        | 0.47     |
| 30:DY:26:LEU:HB2   | 30:DY:28:LEU:HG   | 1.96        | 0.47     |
| 12:AM:72:ILE:O     | 12:AM:76:ILE:HG13 | 2.14        | 0.47     |
| 1:AA:1294:G:H2'    | 1:AA:1295:U:C6    | 2.49        | 0.47     |
| 1:CA:631:C:H5''    | 1:CA:632:U:O4'    | 2.15        | 0.47     |
| 49:BR:29:THR:HG23  | 49:BR:65:ALA:HA   | 1.97        | 0.47     |
| 23:DB:438:G:H2'    | 23:DB:439:A:H8    | 1.79        | 0.47     |
| 34:B3:9:ALA:HA     | 37:BL:58:TYR:HB2  | 1.97        | 0.47     |
| 11:CL:2:THR:OG1    | 11:CL:5:GLN:HG3   | 2.15        | 0.47     |
| 53:B6:134:ARG:NH1  | 53:B6:135:GLU:HG3 | 2.29        | 0.47     |
| 49:DR:64:VAL:O     | 49:DR:65:ALA:HB3  | 2.14        | 0.47     |
| 7:AH:72:GLU:H      | 7:AH:72:GLU:CD    | 2.18        | 0.47     |
| 47:DF:68:LYS:HD2   | 47:DF:68:LYS:N    | 2.30        | 0.47     |
| 2:AC:54:ILE:HG23   | 2:AC:54:ILE:O     | 2.15        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:BD:61:THR:O    | 26:BD:64:GLU:HB2  | 2.14        | 0.47     |
| 1:AA:991:U:H2'    | 1:AA:1212:U:O2    | 2.15        | 0.47     |
| 1:CA:93:U:O5'     | 1:CA:93:U:H6      | 1.97        | 0.47     |
| 23:DB:1587:G:H2'  | 23:DB:1588:G:H8   | 1.80        | 0.47     |
| 23:DB:1098:A:O5'  | 24:DI:3:LYS:HG2   | 2.15        | 0.47     |
| 48:DG:103:ASN:HA  | 48:DG:113:ASP:OD1 | 2.15        | 0.47     |
| 53:B6:83:ILE:HG22 | 53:B6:90:LEU:N    | 2.30        | 0.47     |
| 44:DQ:91:ARG:NH2  | 49:DR:11:GLN:O    | 2.48        | 0.47     |
| 29:BE:105:LEU:HA  | 29:BE:108:ILE:CG2 | 2.44        | 0.47     |
| 39:BX:23:ARG:O    | 39:BX:27:ASN:N    | 2.44        | 0.47     |
| 44:BQ:91:ARG:HH21 | 44:BQ:94:LEU:HD21 | 1.79        | 0.47     |
| 3:AD:164:ARG:HG2  | 3:AD:164:ARG:HH11 | 1.80        | 0.47     |
| 47:BF:78:ILE:N    | 47:BF:79:ARG:NH1  | 2.62        | 0.47     |
| 9:AJ:53:ILE:HG23  | 9:AJ:54:SER:N     | 2.30        | 0.47     |
| 47:DF:1:ALA:O     | 47:DF:4:HIS:HB3   | 2.15        | 0.47     |
| 11:AL:42:LYS:HB3  | 11:AL:43:LYS:H    | 1.48        | 0.47     |
| 23:DB:483:A:H5'   | 46:DU:44:HIS:O    | 2.15        | 0.47     |
| 41:BJ:82:GLY:O    | 41:BJ:84:ILE:HG22 | 2.15        | 0.47     |
| 38:DM:63:ILE:HA   | 38:DM:104:GLU:O   | 2.15        | 0.47     |
| 23:BB:2886:A:N6   | 31:B0:39:ARG:CZ   | 2.78        | 0.47     |
| 48:DG:144:ALA:HB1 | 48:DG:163:TYR:HE1 | 1.80        | 0.47     |
| 13:CN:50:LEU:HB3  | 13:CN:51:PRO:HD3  | 1.96        | 0.47     |
| 8:CI:94:ARG:HH11  | 8:CI:94:ARG:CB    | 2.21        | 0.47     |
| 1:CA:332:G:P      | 19:CT:2:ASN:HB3   | 2.55        | 0.47     |
| 40:BH:14:SER:CB   | 40:BH:17:ASP:HB2  | 2.41        | 0.47     |
| 31:D0:43:THR:HG23 | 31:D0:47:TYR:C    | 2.35        | 0.47     |
| 44:DQ:111:LYS:HE3 | 49:DR:48:LYS:NZ   | 2.30        | 0.47     |
| 1:AA:1299:A:H2'   | 1:AA:1301:U:C1'   | 2.42        | 0.47     |
| 26:DD:69:ALA:N    | 26:DD:73:VAL:HB   | 2.30        | 0.47     |
| 36:D2:21:ARG:HG2  | 36:D2:31:LEU:CG   | 2.40        | 0.47     |
| 16:AQ:58:VAL:HG12 | 16:AQ:77:VAL:HG13 | 1.97        | 0.47     |
| 1:AA:1342:C:O2'   | 1:AA:1343:G:H5'   | 2.14        | 0.47     |
| 5:CF:98:GLU:HG2   | 5:CF:99:ALA:H     | 1.80        | 0.47     |
| 3:CD:197:HIS:O    | 3:CD:201:GLU:HG3  | 2.15        | 0.47     |
| 23:BB:1210:G:H1'  | 23:BB:1212:G:C2   | 2.50        | 0.47     |
| 23:BB:582:A:H2'   | 23:BB:583:G:H8    | 1.80        | 0.47     |
| 1:CA:191:G:H2'    | 1:CA:192:A:H8     | 1.80        | 0.47     |
| 35:DV:42:LEU:N    | 35:DV:42:LEU:HD23 | 2.26        | 0.47     |
| 39:DX:56:LEU:O    | 39:DX:58:ASN:N    | 2.47        | 0.47     |
| 1:AA:401:C:H1'    | 1:AA:622:A:H1'    | 1.96        | 0.47     |
| 23:BB:705:A:N6    | 23:BB:726:G:H1'   | 2.29        | 0.47     |
| 39:BX:55:THR:O    | 39:BX:58:ASN:HB3  | 2.14        | 0.47     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:AA:170:U:O2'     | 1:AA:171:A:H5'    | 2.15        | 0.47     |
| 23:BB:754:U:H2'    | 23:BB:755:U:C6    | 2.50        | 0.47     |
| 43:DO:9:ARG:HG3    | 43:DO:10:ARG:H    | 1.80        | 0.47     |
| 23:BB:1939:U:O2    | 23:BB:1967:C:H4'  | 2.14        | 0.47     |
| 23:DB:834:G:O2'    | 23:DB:835:C:H5'   | 2.15        | 0.47     |
| 20:AB:94:ARG:HD2   | 20:AB:142:LYS:HE2 | 1.96        | 0.47     |
| 23:DB:754:U:H2'    | 23:DB:755:U:C6    | 2.49        | 0.47     |
| 1:AA:182:A:O2'     | 1:AA:183:C:H3'    | 2.14        | 0.47     |
| 1:AA:470:C:H2'     | 1:AA:471:U:H6     | 1.80        | 0.47     |
| 41:DJ:100:VAL:O    | 41:DJ:104:ALA:HB2 | 2.15        | 0.47     |
| 23:DB:1093:G:O2'   | 23:DB:1094:U:H5'  | 2.15        | 0.47     |
| 23:BB:2803:G:O2'   | 23:BB:2804:U:H5'  | 2.14        | 0.47     |
| 23:DB:459:U:C2'    | 23:DB:460:A:H5'   | 2.45        | 0.47     |
| 4:AE:103:GLY:O     | 4:AE:121:ASN:HA   | 2.15        | 0.47     |
| 23:BB:2686:G:H2'   | 23:BB:2687:U:C6   | 2.50        | 0.47     |
| 23:BB:2360:G:H4'   | 37:BL:61:LEU:HD11 | 1.96        | 0.47     |
| 1:CA:1486:G:H2'    | 1:CA:1487:G:C8    | 2.50        | 0.47     |
| 23:BB:1633:G:O2'   | 23:BB:1634:A:H5'' | 2.15        | 0.47     |
| 23:DB:2098:U:H2'   | 23:DB:2099:U:C6   | 2.49        | 0.47     |
| 1:CA:825:A:H2'     | 1:CA:826:C:C6     | 2.50        | 0.47     |
| 53:B6:156:ARG:NH2  | 53:B6:160:GLU:HB2 | 2.30        | 0.47     |
| 3:CD:145:ARG:HH21  | 3:CD:147:LYS:HE2  | 1.79        | 0.47     |
| 23:DB:2880:C:O4'   | 42:DN:91:ALA:HB3  | 2.15        | 0.47     |
| 46:DU:18:LYS:HD2   | 46:DU:19:GLY:N    | 2.30        | 0.47     |
| 1:AA:201:G:O2'     | 1:AA:202:G:H5'    | 2.15        | 0.47     |
| 23:BB:243:U:P      | 34:B3:5:THR:HG1   | 2.38        | 0.47     |
| 52:BW:47:GLY:HA3   | 52:BW:80:SER:CB   | 2.44        | 0.47     |
| 23:DB:1833:C:O2'   | 23:DB:1834:U:H5'  | 2.15        | 0.47     |
| 2:AC:40:GLN:HG3    | 2:AC:41:TYR:H     | 1.78        | 0.47     |
| 20:CB:35:ASN:HD22  | 20:CB:35:ASN:HA   | 1.54        | 0.47     |
| 1:CA:770:C:O2'     | 1:CA:771:G:H5'    | 2.15        | 0.47     |
| 28:BP:114:ASN:HD22 | 28:BP:114:ASN:HA  | 1.50        | 0.47     |
| 23:BB:1799:G:H4'   | 23:BB:1800:C:O5'  | 2.15        | 0.47     |
| 48:BG:9:VAL:HA     | 48:BG:48:THR:CG2  | 2.43        | 0.47     |
| 48:BG:90:GLY:HA3   | 48:BG:93:TYR:CZ   | 2.50        | 0.47     |
| 26:BD:31:ALA:O     | 26:BD:52:THR:HG23 | 2.13        | 0.47     |
| 53:D6:80:GLU:CG    | 53:D6:92:PRO:HB3  | 2.45        | 0.47     |
| 52:DW:23:LYS:H     | 52:DW:68:PHE:HE2  | 1.62        | 0.47     |
| 51:DZ:33:LEU:HA    | 51:DZ:51:VAL:O    | 2.14        | 0.47     |
| 23:DB:496:G:H4'    | 45:DS:61:ASN:HD21 | 1.80        | 0.47     |
| 25:DC:93:VAL:HG12  | 25:DC:101:ARG:O   | 2.15        | 0.47     |
| 41:BJ:38:GLY:HA3   | 41:BJ:50:THR:O    | 2.15        | 0.47     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 51:BZ:6:GLN:HE22   | 51:BZ:77:LYS:CE    | 2.28        | 0.47     |
| 24:DI:57:VAL:HG23  | 24:DI:71:LYS:HZ1   | 1.80        | 0.47     |
| 46:DU:81:ARG:HB2   | 46:DU:96:LYS:HG2   | 1.97        | 0.47     |
| 47:BF:29:ARG:HD3   | 47:BF:29:ARG:H     | 1.79        | 0.47     |
| 37:BL:79:LEU:HB2   | 37:BL:113:ALA:N    | 2.25        | 0.47     |
| 38:BM:21:ALA:CB    | 38:BM:100:LYS:HG2  | 2.45        | 0.47     |
| 12:CM:103:THR:HG22 | 12:CM:104:ASN:OD1  | 2.14        | 0.47     |
| 8:AI:87:MET:HB2    | 8:AI:94:ARG:HD3    | 1.97        | 0.47     |
| 46:BU:81:ARG:CD    | 46:BU:96:LYS:HG3   | 2.44        | 0.47     |
| 23:DB:2267:A:C8    | 23:DB:2267:A:O5'   | 2.65        | 0.47     |
| 10:CK:90:PRO:C     | 10:CK:92:ARG:H     | 2.18        | 0.47     |
| 53:D6:106:LEU:HG   | 53:D6:111:ARG:HE   | 1.79        | 0.47     |
| 23:BB:545:U:C5     | 23:BB:547:A:H5'    | 2.50        | 0.47     |
| 23:BB:2733:A:H3'   | 23:BB:2733:A:C8    | 2.50        | 0.47     |
| 27:DK:79:PHE:HZ    | 27:DK:104:THR:HG23 | 1.80        | 0.47     |
| 49:BR:59:ILE:HA    | 49:BR:101:ILE:H    | 1.79        | 0.47     |
| 40:BH:141:LYS:N    | 40:BH:141:LYS:HD3  | 2.30        | 0.47     |
| 7:AH:48:PHE:HA     | 7:AH:59:GLU:O      | 2.14        | 0.47     |
| 26:DD:90:PHE:O     | 26:DD:91:THR:C     | 2.53        | 0.47     |
| 28:DP:6:GLN:HA     | 28:DP:9:GLN:HG2    | 1.96        | 0.47     |
| 23:BB:1439:A:H1'   | 23:BB:1553:A:N6    | 2.30        | 0.47     |
| 23:BB:1441:G:H4'   | 23:BB:1628:G:OP1   | 2.15        | 0.47     |
| 25:BC:159:THR:H    | 25:BC:194:VAL:CG1  | 2.27        | 0.47     |
| 9:AJ:8:ILE:HD12    | 9:AJ:8:ILE:N       | 2.29        | 0.47     |
| 20:AB:101:THR:HG23 | 20:AB:102:ASN:H    | 1.80        | 0.47     |
| 2:AC:155:ARG:H     | 2:AC:162:ALA:CB    | 2.28        | 0.47     |
| 1:CA:34:C:H2'      | 1:CA:35:G:H8       | 1.80        | 0.47     |
| 11:CL:66:ILE:N     | 11:CL:66:ILE:HD12  | 2.30        | 0.47     |
| 49:BR:23:GLU:O     | 49:BR:25:LEU:HD22  | 2.15        | 0.47     |
| 41:BJ:96:ARG:NE    | 41:BJ:99:ARG:HD2   | 2.29        | 0.47     |
| 41:BJ:96:ARG:O     | 41:BJ:99:ARG:HG3   | 2.15        | 0.47     |
| 23:BB:2590:A:O2'   | 23:BB:2591:C:H5'   | 2.15        | 0.47     |
| 3:CD:100:VAL:HG21  | 3:CD:136:VAL:HG21  | 1.97        | 0.47     |
| 23:DB:1854:A:H2    | 23:DB:2087:G:N3    | 2.13        | 0.47     |
| 23:DB:1175:A:C3'   | 23:DB:1176:U:H5'   | 2.45        | 0.47     |
| 53:B6:140:LEU:O    | 53:B6:143:LEU:HB2  | 2.15        | 0.47     |
| 23:BB:2217:G:O2'   | 23:BB:2218:G:H5'   | 2.14        | 0.47     |
| 1:AA:954:G:H2'     | 1:AA:955:U:C6      | 2.49        | 0.47     |
| 2:AC:70:ALA:HA     | 2:AC:105:VAL:CG2   | 2.45        | 0.47     |
| 23:BB:2799:A:O3'   | 23:BB:2800:A:O4'   | 2.32        | 0.47     |
| 23:BB:1902:C:H4'   | 25:BC:241:LYS:O    | 2.15        | 0.47     |
| 14:AO:5:THR:O      | 14:AO:8:THR:HB     | 2.15        | 0.47     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:1386:G:H2'    | 1:CA:1387:G:H8     | 1.80        | 0.47     |
| 23:BB:1946:U:H2'   | 23:BB:1947:C:H6    | 1.80        | 0.47     |
| 1:CA:1278:G:H4'    | 1:CA:1279:G:O4'    | 2.15        | 0.47     |
| 43:BO:7:ARG:HA     | 43:BO:10:ARG:HD2   | 1.96        | 0.47     |
| 1:CA:1180:A:OP1    | 8:CI:104:THR:HG22  | 2.13        | 0.47     |
| 11:AL:7:VAL:HG22   | 16:AQ:33:TYR:CD1   | 2.49        | 0.47     |
| 1:AA:415:A:H3'     | 1:AA:416:G:H8      | 1.80        | 0.47     |
| 23:DB:2636:C:H2'   | 23:DB:2637:U:H6    | 1.80        | 0.47     |
| 1:CA:153:C:O2'     | 1:CA:154:U:H5'     | 2.15        | 0.47     |
| 1:CA:1132:C:H2'    | 1:CA:1133:G:H8     | 1.79        | 0.47     |
| 23:DB:1275:A:N3    | 23:DB:1275:A:H2'   | 2.29        | 0.47     |
| 25:DC:177:SER:O    | 25:DC:270:ARG:HG3  | 2.14        | 0.47     |
| 23:DB:1159:U:O2'   | 23:DB:1160:G:H5'   | 2.15        | 0.47     |
| 33:D1:29:LYS:HE2   | 33:D1:31:GLU:OE1   | 2.15        | 0.47     |
| 23:BB:516:C:H2'    | 23:BB:517:C:H6     | 1.80        | 0.47     |
| 25:DC:73:ILE:HG21  | 25:DC:97:ASP:HB2   | 1.97        | 0.47     |
| 1:CA:160:A:H2'     | 1:CA:161:A:O4'     | 2.14        | 0.47     |
| 23:BB:2011:U:H2'   | 23:BB:2012:G:O4'   | 2.14        | 0.47     |
| 6:CG:125:ASP:HA    | 6:CG:128:GLU:OE1   | 2.15        | 0.47     |
| 23:DB:621:A:H2'    | 23:DB:622:G:O4'    | 2.14        | 0.47     |
| 1:CA:1109:C:H2'    | 1:CA:1110:A:O4'    | 2.14        | 0.47     |
| 45:DS:57:ASN:HD22  | 45:DS:57:ASN:HA    | 1.53        | 0.47     |
| 50:BT:7:LEU:O      | 50:BT:7:LEU:HD13   | 2.15        | 0.47     |
| 16:AQ:25:GLU:HA    | 16:AQ:39:ARG:O     | 2.14        | 0.47     |
| 25:DC:4:LYS:HD2    | 25:DC:5:CYS:H      | 1.79        | 0.47     |
| 40:BH:27:ARG:H     | 40:BH:31:VAL:HG23  | 1.79        | 0.47     |
| 48:BG:9:VAL:HG12   | 48:BG:11:PRO:CD    | 2.41        | 0.47     |
| 25:DC:171:VAL:HG23 | 25:DC:185:ALA:HB2  | 1.97        | 0.47     |
| 47:BF:57:ALA:HB2   | 47:BF:64:PRO:CG    | 2.45        | 0.47     |
| 8:CI:24:ASN:HD22   | 8:CI:25:GLY:H      | 1.59        | 0.47     |
| 47:DF:79:ARG:NE    | 47:DF:82:TYR:HD2   | 2.13        | 0.47     |
| 22:DA:28:C:N4      | 22:DA:56:G:C6      | 2.82        | 0.47     |
| 22:DA:28:C:O2'     | 22:DA:29:A:H5'     | 2.15        | 0.47     |
| 44:BQ:94:LEU:CD1   | 49:BR:13:ARG:HB2   | 2.44        | 0.47     |
| 47:BF:101:ARG:NH1  | 47:BF:138:PRO:HB2  | 2.29        | 0.47     |
| 29:BE:142:ALA:O    | 29:BE:143:LEU:HD23 | 2.15        | 0.47     |
| 42:DN:102:PHE:N    | 42:DN:109:PRO:HA   | 2.26        | 0.47     |
| 18:AS:2:ARG:O      | 18:AS:3:SER:C      | 2.54        | 0.47     |
| 50:DT:58:VAL:O     | 50:DT:58:VAL:HG13  | 2.15        | 0.47     |
| 39:DX:7:ARG:O      | 39:DX:7:ARG:HG3    | 2.15        | 0.47     |
| 32:B4:7:VAL:HG11   | 32:B4:23:ILE:O     | 2.14        | 0.47     |
| 13:AN:52:ARG:C     | 13:AN:54:SER:H     | 2.19        | 0.47     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 21:CU:24:LYS:HB3  | 21:CU:24:LYS:NZ    | 2.30        | 0.47     |
| 45:BS:29:VAL:CA   | 45:BS:32:ALA:HB3   | 2.44        | 0.47     |
| 23:DB:2345:G:H4'  | 23:DB:2346:A:O5'   | 2.15        | 0.47     |
| 23:DB:559:G:H2'   | 23:DB:560:C:O4'    | 2.15        | 0.47     |
| 51:DZ:14:THR:HA   | 51:DZ:28:ARG:HB2   | 1.96        | 0.47     |
| 4:AE:38:VAL:O     | 4:AE:45:VAL:HA     | 2.15        | 0.47     |
| 39:DX:20:ASN:H    | 39:DX:20:ASN:ND2   | 2.11        | 0.47     |
| 19:AT:66:ILE:CG2  | 19:AT:70:LYS:HB3   | 2.44        | 0.47     |
| 23:DB:718:A:H2'   | 23:DB:719:C:H5'    | 1.96        | 0.47     |
| 9:CJ:35:GLN:HG2   | 9:CJ:78:GLU:OE1    | 2.15        | 0.47     |
| 3:CD:96:ARG:HB3   | 3:CD:98:ASP:OD2    | 2.15        | 0.47     |
| 28:DP:20:ARG:CG   | 28:DP:21:PRO:HD2   | 2.45        | 0.47     |
| 23:BB:705:A:O2'   | 25:BC:6:LYS:HG3    | 2.15        | 0.47     |
| 40:BH:57:LYS:HZ3  | 40:BH:58:LEU:HD13  | 1.78        | 0.47     |
| 23:BB:755:U:H2'   | 23:BB:756:A:C8     | 2.50        | 0.47     |
| 43:DO:7:ARG:HA    | 43:DO:10:ARG:CD    | 2.45        | 0.47     |
| 7:CH:74:ILE:O     | 7:CH:74:ILE:HG23   | 2.15        | 0.47     |
| 23:BB:1041:G:H2'  | 23:BB:1042:G:H8    | 1.79        | 0.47     |
| 28:DP:25:VAL:HA   | 28:DP:85:VAL:CA    | 2.45        | 0.47     |
| 6:CG:135:LYS:HE2  | 6:CG:139:ASP:OD2   | 2.15        | 0.47     |
| 30:BY:29:ARG:HB2  | 30:BY:33:HIS:HD2   | 1.80        | 0.47     |
| 23:BB:1509:A:H5'' | 23:BB:1509:A:C8    | 2.50        | 0.47     |
| 23:DB:122:G:O2'   | 23:DB:123:G:H5'    | 2.15        | 0.47     |
| 1:AA:548:G:H2'    | 1:AA:549:C:C6      | 2.49        | 0.47     |
| 51:BZ:68:LEU:O    | 51:BZ:72:ARG:HG2   | 2.15        | 0.47     |
| 23:DB:316:C:O2'   | 23:DB:317:G:H5'    | 2.15        | 0.47     |
| 15:AP:34:GLU:CD   | 15:AP:60:TRP:HE1   | 2.19        | 0.47     |
| 2:AC:16:PRO:CG    | 2:AC:53:ARG:HH22   | 2.28        | 0.47     |
| 12:AM:23:GLY:HA3  | 12:AM:68:LEU:CD1   | 2.44        | 0.47     |
| 23:DB:1707:G:O2'  | 23:DB:1708:C:H5'   | 2.14        | 0.47     |
| 23:DB:2649:C:H2'  | 23:DB:2650:U:H6    | 1.79        | 0.47     |
| 25:BC:270:ARG:HB3 | 25:BC:270:ARG:CZ   | 2.45        | 0.47     |
| 23:BB:2649:C:H2'  | 23:BB:2650:U:H6    | 1.80        | 0.47     |
| 29:DE:122:GLU:O   | 29:DE:123:LYS:CB   | 2.63        | 0.47     |
| 1:AA:1477:U:O2'   | 1:AA:1478:U:H5'    | 2.15        | 0.47     |
| 1:AA:160:A:H2'    | 1:AA:161:A:O4'     | 2.15        | 0.47     |
| 40:BH:25:TYR:CD2  | 40:BH:30:LEU:HD11  | 2.49        | 0.47     |
| 10:CK:67:GLU:HG3  | 10:CK:68:ARG:N     | 2.30        | 0.47     |
| 47:BF:13:LYS:HZ2  | 47:BF:13:LYS:C     | 2.18        | 0.47     |
| 28:BP:13:LYS:HD2  | 28:BP:76:HIS:HA    | 1.97        | 0.47     |
| 11:AL:30:ARG:O    | 11:AL:57:THR:HG23  | 2.15        | 0.47     |
| 45:BS:4:ILE:HG22  | 45:BS:106:VAL:HG22 | 1.96        | 0.47     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:555:U:H2'     | 1:CA:556:C:C6      | 2.50        | 0.47     |
| 1:AA:656:G:O2'     | 1:AA:657:U:H5'     | 2.14        | 0.47     |
| 23:DB:2519:U:C6    | 23:DB:2542:A:N6    | 2.83        | 0.47     |
| 23:DB:431:U:O2'    | 23:DB:432:A:H5'    | 2.15        | 0.47     |
| 23:BB:838:C:O2'    | 23:BB:839:U:H5'    | 2.15        | 0.47     |
| 40:DH:54:LEU:HD22  | 40:DH:58:LEU:HD12  | 1.96        | 0.47     |
| 1:AA:509:A:H3'     | 57:AA:1771:HOH:O   | 2.15        | 0.47     |
| 5:AF:45:ARG:HH22   | 17:AR:25:ILE:HD13  | 1.80        | 0.47     |
| 50:BT:76:ARG:NH1   | 50:BT:76:ARG:HB3   | 2.30        | 0.47     |
| 49:DR:70:GLU:N     | 49:DR:70:GLU:CD    | 2.68        | 0.47     |
| 23:DB:2903:U:O2    | 23:DB:2903:U:C2'   | 2.62        | 0.47     |
| 1:AA:624:C:H2'     | 1:AA:625:U:C6      | 2.50        | 0.47     |
| 1:CA:144:G:H2'     | 1:CA:145:G:O4'     | 2.15        | 0.47     |
| 3:AD:106:PHE:CD1   | 3:AD:144:ILE:HD11  | 2.49        | 0.47     |
| 52:BW:19:ARG:HD3   | 52:BW:36:ILE:HD11  | 1.97        | 0.46     |
| 52:BW:61:LYS:HB3   | 52:BW:62:ALA:H     | 1.42        | 0.46     |
| 37:BL:89:VAL:O     | 37:BL:89:VAL:HG13  | 2.14        | 0.46     |
| 48:DG:112:VAL:O    | 48:DG:113:ASP:HB2  | 2.14        | 0.46     |
| 8:CI:24:ASN:O      | 8:CI:60:LEU:N      | 2.48        | 0.46     |
| 8:AI:66:VAL:HG22   | 8:AI:67:LYS:N      | 2.29        | 0.46     |
| 13:AN:61:ASN:O     | 13:AN:62:ARG:HB2   | 2.15        | 0.46     |
| 35:BV:1:MET:HG3    | 35:BV:2:PHE:N      | 2.29        | 0.46     |
| 13:CN:9:GLU:O      | 13:CN:13:VAL:HG23  | 2.15        | 0.46     |
| 48:BG:17:LYS:HZ2   | 48:BG:18:ILE:N     | 2.13        | 0.46     |
| 48:BG:18:ILE:HA    | 48:BG:22:VAL:O     | 2.14        | 0.46     |
| 25:BC:90:ILE:HD12  | 25:BC:102:TYR:HB3  | 1.96        | 0.46     |
| 47:BF:79:ARG:NE    | 47:BF:82:TYR:HD2   | 2.13        | 0.46     |
| 47:BF:142:TYR:H    | 47:BF:142:TYR:HD1  | 1.58        | 0.46     |
| 47:BF:21:TYR:HD2   | 47:BF:27:VAL:HG12  | 1.80        | 0.46     |
| 47:DF:111:ARG:HE   | 47:DF:135:ILE:HG22 | 1.79        | 0.46     |
| 53:D6:74:ASN:ND2   | 53:D6:74:ASN:N     | 2.59        | 0.46     |
| 38:BM:135:VAL:O    | 38:BM:136:MET:HG3  | 2.15        | 0.46     |
| 1:CA:1316:G:OP2    | 1:CA:1316:G:H8     | 1.98        | 0.46     |
| 18:CS:35:ARG:HB3   | 18:CS:50:VAL:HG13  | 1.96        | 0.46     |
| 18:CS:52:ASN:O     | 18:CS:76:THR:HG23  | 2.14        | 0.46     |
| 53:B6:111:ARG:HD2  | 53:B6:111:ARG:HA   | 1.84        | 0.46     |
| 53:B6:115:VAL:HG22 | 53:B6:184:LEU:HD12 | 1.96        | 0.46     |
| 13:AN:53:ASP:HA    | 13:AN:58:ARG:HD2   | 1.97        | 0.46     |
| 2:AC:106:ARG:HG2   | 2:AC:106:ARG:O     | 2.15        | 0.46     |
| 23:DB:2281:A:O2'   | 23:DB:2282:G:H5'   | 2.15        | 0.46     |
| 23:DB:850:U:H2'    | 23:DB:851:C:H6     | 1.81        | 0.46     |
| 1:AA:1326:U:H2'    | 1:AA:1327:C:H6     | 1.77        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BC:11:GLY:O    | 25:BC:206:LYS:HB3  | 2.15        | 0.46     |
| 29:DE:138:LEU:O   | 29:DE:142:ALA:N    | 2.48        | 0.46     |
| 27:DK:5:GLN:HA    | 27:DK:20:MET:SD    | 2.55        | 0.46     |
| 40:DH:47:PHE:O    | 40:DH:51:ARG:HB2   | 2.15        | 0.46     |
| 1:AA:1239:A:H4'   | 1:AA:1240:U:C5'    | 2.46        | 0.46     |
| 23:BB:1737:G:H5'  | 23:BB:1738:G:OP2   | 2.14        | 0.46     |
| 23:DB:2015:A:C2   | 31:D0:2:VAL:HG22   | 2.50        | 0.46     |
| 4:AE:84:VAL:HG11  | 4:AE:146:MET:HB3   | 1.96        | 0.46     |
| 37:BL:93:ASN:HD22 | 37:BL:94:THR:H     | 1.63        | 0.46     |
| 23:BB:1681:G:H2'  | 23:BB:1757:A:N1    | 2.29        | 0.46     |
| 23:DB:2720:U:H2'  | 23:DB:2721:A:C8    | 2.50        | 0.46     |
| 28:DP:56:SER:O    | 28:DP:74:GLN:HA    | 2.14        | 0.46     |
| 3:CD:197:HIS:HA   | 3:CD:200:VAL:HG22  | 1.97        | 0.46     |
| 4:CE:71:ILE:HD11  | 4:CE:144:GLU:HG3   | 1.96        | 0.46     |
| 1:CA:617:G:H4'    | 15:CP:46:LYS:CE    | 2.46        | 0.46     |
| 1:CA:338:A:H2'    | 1:CA:339:C:C6      | 2.50        | 0.46     |
| 39:DX:14:LEU:O    | 39:DX:18:LEU:HB2   | 2.15        | 0.46     |
| 23:DB:96:C:H2'    | 23:DB:97:C:H6      | 1.80        | 0.46     |
| 23:DB:1180:U:H2'  | 23:DB:1181:U:C6    | 2.50        | 0.46     |
| 39:BX:56:LEU:C    | 39:BX:58:ASN:N     | 2.68        | 0.46     |
| 23:DB:2461:A:H1'  | 23:DB:2492:U:C2    | 2.50        | 0.46     |
| 1:AA:955:U:H1'    | 1:AA:1227:A:N6     | 2.30        | 0.46     |
| 23:DB:2626:C:H2'  | 23:DB:2627:G:C8    | 2.50        | 0.46     |
| 1:CA:1144:G:N2    | 1:CA:1146:A:H62    | 2.12        | 0.46     |
| 1:CA:373:A:OP2    | 1:CA:373:A:H3'     | 2.14        | 0.46     |
| 1:AA:502:A:H4'    | 1:AA:550:G:H4'     | 1.97        | 0.46     |
| 20:AB:23:ASN:OD1  | 20:AB:25:LYS:HB2   | 2.14        | 0.46     |
| 40:DH:65:ALA:HB1  | 40:DH:138:VAL:HG11 | 1.97        | 0.46     |
| 23:DB:2623:G:H4'  | 23:DB:2825:G:C8    | 2.50        | 0.46     |
| 1:CA:1042:A:H2'   | 1:CA:1043:G:O4'    | 2.15        | 0.46     |
| 1:CA:590:U:H2'    | 1:CA:591:U:H6      | 1.80        | 0.46     |
| 19:AT:27:MET:CE   | 19:AT:28:ARG:HG2   | 2.45        | 0.46     |
| 23:DB:443:A:H1'   | 23:DB:1201:U:O4'   | 2.15        | 0.46     |
| 23:BB:1719:G:O2'  | 23:BB:1720:U:H5'   | 2.14        | 0.46     |
| 23:BB:2105:U:H2'  | 23:BB:2106:U:C6    | 2.49        | 0.46     |
| 6:AG:45:ALA:HB3   | 6:AG:119:LEU:HD23  | 1.96        | 0.46     |
| 25:BC:226:PRO:HG3 | 25:BC:233:GLY:N    | 2.30        | 0.46     |
| 5:CF:10:VAL:HG12  | 5:CF:11:HIS:N      | 2.31        | 0.46     |
| 5:CF:45:ARG:HG2   | 5:CF:46:GLN:N      | 2.30        | 0.46     |
| 10:AK:27:ASN:O    | 10:AK:56:LYS:HD2   | 2.14        | 0.46     |
| 5:CF:42:TRP:HB2   | 5:CF:59:TYR:HB2    | 1.96        | 0.46     |
| 53:D6:28:LEU:HD21 | 53:D6:121:TYR:HE2  | 1.80        | 0.46     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:114:U:H2'     | 1:AA:115:G:C8      | 2.50        | 0.46     |
| 23:DB:997:G:O2'    | 23:DB:998:C:H5'    | 2.16        | 0.46     |
| 11:AL:2:THR:OG1    | 11:AL:5:GLN:HG3    | 2.15        | 0.46     |
| 30:BY:26:LEU:HB2   | 30:BY:28:LEU:HG    | 1.97        | 0.46     |
| 15:CP:12:LYS:C     | 15:CP:14:ARG:H     | 2.17        | 0.46     |
| 23:BB:1501:G:O2'   | 23:BB:1502:A:H5'   | 2.15        | 0.46     |
| 10:AK:126:ARG:HA   | 10:AK:126:ARG:NE   | 2.30        | 0.46     |
| 21:AU:36:PHE:CZ    | 21:AU:44:ARG:NH2   | 2.83        | 0.46     |
| 48:DG:106:LEU:O    | 48:DG:108:PHE:HD1  | 1.97        | 0.46     |
| 48:DG:108:PHE:C    | 48:DG:110:HIS:H    | 2.18        | 0.46     |
| 26:BD:3:GLY:C      | 26:BD:4:LEU:HD22   | 2.36        | 0.46     |
| 53:B6:67:VAL:HA    | 53:B6:99:LEU:O     | 2.15        | 0.46     |
| 41:DJ:3:THR:HG21   | 44:DQ:60:TRP:NE1   | 2.29        | 0.46     |
| 22:DA:27:C:C2'     | 22:DA:28:C:H5'     | 2.45        | 0.46     |
| 23:BB:997:G:O2'    | 23:BB:998:C:H5'    | 2.15        | 0.46     |
| 44:BQ:59:LEU:C     | 44:BQ:59:LEU:HD13  | 2.36        | 0.46     |
| 46:DU:86:PHE:HD1   | 46:DU:88:ASP:N     | 2.14        | 0.46     |
| 40:DH:127:GLU:CA   | 40:DH:145:ASN:HA   | 2.40        | 0.46     |
| 43:BO:31:THR:HG23  | 43:BO:34:HIS:O     | 2.15        | 0.46     |
| 23:BB:1059:G:H2'   | 23:BB:1060:U:C5    | 2.50        | 0.46     |
| 47:BF:103:ILE:HD11 | 47:BF:174:PHE:CD1  | 2.50        | 0.46     |
| 47:DF:108:PRO:O    | 47:DF:110:ILE:HG23 | 2.14        | 0.46     |
| 47:DF:106:ALA:HA   | 47:DF:135:ILE:CD1  | 2.45        | 0.46     |
| 1:AA:1361:G:N2     | 1:AA:1362:A:N7     | 2.63        | 0.46     |
| 13:AN:26:LEU:C     | 13:AN:26:LEU:HD23  | 2.36        | 0.46     |
| 24:DI:27:LEU:HB2   | 24:DI:32:VAL:HG21  | 1.96        | 0.46     |
| 23:BB:1028:A:N6    | 23:BB:1125:G:H2'   | 2.30        | 0.46     |
| 13:AN:52:ARG:HG3   | 13:AN:53:ASP:N     | 2.30        | 0.46     |
| 48:DG:86:LEU:HD23  | 48:DG:162:ARG:O    | 2.16        | 0.46     |
| 23:BB:1082:U:C2    | 23:BB:1086:A:N1    | 2.84        | 0.46     |
| 13:CN:26:LEU:C     | 13:CN:26:LEU:HD23  | 2.35        | 0.46     |
| 23:BB:1189:A:H2'   | 23:BB:1190:G:O4'   | 2.15        | 0.46     |
| 15:CP:67:ILE:HD11  | 15:CP:71:VAL:HG22  | 1.97        | 0.46     |
| 27:DK:19:VAL:C     | 27:DK:41:ILE:HD11  | 2.36        | 0.46     |
| 20:CB:16:GLY:HA2   | 20:CB:40:ILE:HD12  | 1.98        | 0.46     |
| 49:BR:16:GLU:HG2   | 49:BR:101:ILE:HB   | 1.96        | 0.46     |
| 45:DS:74:ILE:HD12  | 45:DS:104:THR:O    | 2.16        | 0.46     |
| 29:DE:152:GLU:O    | 29:DE:153:LEU:HB3  | 2.16        | 0.46     |
| 46:DU:9:GLU:CD     | 46:DU:21:ARG:HD2   | 2.36        | 0.46     |
| 22:BA:74:U:H2'     | 22:BA:75:G:O4'     | 2.15        | 0.46     |
| 1:CA:925:G:O2'     | 1:CA:926:G:H5''    | 2.14        | 0.46     |
| 22:BA:113:C:H2'    | 22:BA:114:C:H6     | 1.79        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 35:DV:78:GLN:HB2  | 35:DV:88:HIS:O    | 2.14        | 0.46     |
| 3:CD:185:PRO:HB2  | 3:CD:190:LEU:HG   | 1.96        | 0.46     |
| 23:DB:48:G:HO2'   | 23:DB:49:A:H2     | 1.62        | 0.46     |
| 39:DX:9:LYS:NZ    | 39:DX:60:LYS:HE3  | 2.30        | 0.46     |
| 2:AC:129:PHE:CE2  | 2:AC:165:GLU:HG2  | 2.44        | 0.46     |
| 23:DB:2340:A:H2'  | 23:DB:2341:G:C8   | 2.50        | 0.46     |
| 49:DR:2:TYR:CB    | 49:DR:42:ALA:HB2  | 2.44        | 0.46     |
| 23:DB:1350:C:O2   | 23:DB:1350:C:H2'  | 2.15        | 0.46     |
| 1:AA:366:A:O2'    | 1:AA:394:G:N2     | 2.48        | 0.46     |
| 7:CH:101:ALA:O    | 7:CH:103:VAL:HG23 | 2.16        | 0.46     |
| 1:CA:1511:G:O2'   | 1:CA:1512:U:H5'   | 2.14        | 0.46     |
| 23:BB:630:G:H22   | 23:BB:632:A:H3'   | 1.79        | 0.46     |
| 23:BB:2699:C:H2'  | 23:BB:2700:A:C8   | 2.50        | 0.46     |
| 28:BP:25:VAL:HA   | 28:BP:85:VAL:CA   | 2.46        | 0.46     |
| 1:CA:376:G:O3'    | 15:CP:5:ARG:HD3   | 2.15        | 0.46     |
| 1:CA:1464:U:H2'   | 1:CA:1465:A:H8    | 1.79        | 0.46     |
| 43:BO:28:VAL:HG11 | 43:BO:92:PHE:CZ   | 2.51        | 0.46     |
| 41:DJ:28:LEU:HG   | 41:DJ:32:LEU:CD1  | 2.46        | 0.46     |
| 23:BB:1350:C:H2'  | 23:BB:1350:C:O2   | 2.16        | 0.46     |
| 22:DA:60:C:O2'    | 22:DA:61:G:H5'    | 2.14        | 0.46     |
| 1:AA:128:G:H2'    | 1:AA:129:A:H8     | 1.80        | 0.46     |
| 23:BB:2527:C:O2'  | 23:BB:2528:U:H5'  | 2.14        | 0.46     |
| 23:BB:354:A:H2'   | 23:BB:355:U:O4'   | 2.14        | 0.46     |
| 23:DB:1118:C:H2'  | 23:DB:1119:U:C6   | 2.50        | 0.46     |
| 23:BB:1849:G:H2'  | 23:BB:1850:G:C8   | 2.50        | 0.46     |
| 23:BB:1201:U:H2'  | 23:BB:1202:G:C8   | 2.51        | 0.46     |
| 46:BU:14:THR:HG21 | 46:BU:64:ILE:HD13 | 1.97        | 0.46     |
| 28:DP:61:ARG:HD3  | 28:DP:70:GLU:HG3  | 1.97        | 0.46     |
| 23:DB:1843:C:H2'  | 23:DB:1844:C:H6   | 1.80        | 0.46     |
| 1:CA:631:C:H3'    | 1:CA:632:U:H5'    | 1.97        | 0.46     |
| 5:AF:45:ARG:HG2   | 5:AF:46:GLN:N     | 2.29        | 0.46     |
| 28:DP:13:LYS:HD2  | 28:DP:76:HIS:HA   | 1.97        | 0.46     |
| 4:AE:79:THR:OG1   | 4:AE:97:PRO:HA    | 2.16        | 0.46     |
| 23:BB:2508:G:O2'  | 23:BB:2509:G:H5'  | 2.15        | 0.46     |
| 1:AA:1387:G:H2'   | 1:AA:1388:C:H6    | 1.79        | 0.46     |
| 5:AF:49:TYR:CE1   | 17:AR:65:SER:HA   | 2.50        | 0.46     |
| 23:BB:1936:A:H2   | 23:BB:1943:U:O4   | 1.99        | 0.46     |
| 1:AA:787:A:O2'    | 1:AA:788:U:H5'    | 2.16        | 0.46     |
| 23:DB:1130:U:C2   | 23:DB:2025:C:H5'' | 2.49        | 0.46     |
| 24:DI:69:VAL:HG23 | 24:DI:69:VAL:O    | 2.14        | 0.46     |
| 1:CA:230:G:O2'    | 1:CA:231:U:H5'    | 2.15        | 0.46     |
| 23:BB:919:U:H2'   | 23:BB:920:A:H8    | 1.73        | 0.46     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 52:BW:35:ILE:CG1   | 52:BW:35:ILE:O    | 2.64        | 0.46     |
| 52:BW:65:LYS:HG3   | 52:BW:84:GLU:CB   | 2.40        | 0.46     |
| 48:BG:72:ASN:O     | 48:BG:76:ILE:HG12 | 2.16        | 0.46     |
| 20:AB:163:ILE:CG2  | 20:AB:164:ASP:H   | 2.09        | 0.46     |
| 48:DG:89:VAL:CB    | 48:DG:159:LYS:HA  | 2.28        | 0.46     |
| 23:DB:2365:G:O2'   | 52:DW:59:PHE:CE1  | 2.68        | 0.46     |
| 40:BH:124:THR:HG22 | 40:BH:126:GLY:H   | 1.80        | 0.46     |
| 53:B6:84:ARG:O     | 53:B6:85:ASP:HB2  | 2.14        | 0.46     |
| 5:AF:3:HIS:ND1     | 5:AF:95:ALA:HB2   | 2.31        | 0.46     |
| 51:DZ:5:CYS:SG     | 51:DZ:8:THR:HG23  | 2.55        | 0.46     |
| 41:DJ:36:LEU:HD21  | 41:DJ:122:LEU:CD1 | 2.45        | 0.46     |
| 50:BT:29:THR:CG2   | 50:BT:86:THR:HG22 | 2.45        | 0.46     |
| 3:AD:25:ARG:HB2    | 3:AD:25:ARG:NH1   | 2.30        | 0.46     |
| 30:BY:15:ARG:HD2   | 30:BY:15:ARG:N    | 2.30        | 0.46     |
| 12:CM:33:LEU:HD13  | 12:CM:39:ALA:O    | 2.16        | 0.46     |
| 47:BF:113:PHE:HZ   | 47:BF:175:PRO:HB2 | 1.80        | 0.46     |
| 47:DF:107:VAL:HB   | 47:DF:108:PRO:HD3 | 1.97        | 0.46     |
| 7:AH:31:LEU:O      | 7:AH:35:ILE:HG13  | 2.16        | 0.46     |
| 13:AN:30:ILE:CG2   | 13:AN:44:VAL:HG11 | 2.45        | 0.46     |
| 23:BB:1174:U:H2'   | 23:BB:1175:A:H5'' | 1.97        | 0.46     |
| 38:DM:53:MET:SD    | 38:DM:63:ILE:HG21 | 2.55        | 0.46     |
| 25:BC:18:VAL:CG1   | 25:BC:202:ARG:HD2 | 2.45        | 0.46     |
| 27:DK:15:GLY:HA2   | 27:DK:46:ALA:HA   | 1.97        | 0.46     |
| 23:BB:30:G:H2'     | 23:BB:31:C:H6     | 1.73        | 0.46     |
| 26:DD:26:VAL:HG13  | 26:DD:188:LEU:CD2 | 2.45        | 0.46     |
| 26:DD:148:GLN:HG3  | 26:DD:152:PRO:CG  | 2.44        | 0.46     |
| 23:DB:1438:U:O2'   | 23:DB:1439:A:H5'  | 2.15        | 0.46     |
| 28:DP:9:GLN:HA     | 28:DP:12:MET:CG   | 2.45        | 0.46     |
| 4:AE:82:HIS:CE1    | 4:AE:146:MET:HA   | 2.51        | 0.46     |
| 23:DB:1804:C:P     | 25:DC:256:THR:HB  | 2.55        | 0.46     |
| 29:DE:153:LEU:HG   | 29:DE:154:ASP:N   | 2.29        | 0.46     |
| 23:DB:1680:U:H2'   | 23:DB:1681:G:O4'  | 2.15        | 0.46     |
| 1:AA:338:A:H2'     | 1:AA:339:C:H6     | 1.80        | 0.46     |
| 14:AO:16:GLY:HA2   | 14:AO:27:VAL:CG2  | 2.45        | 0.46     |
| 38:BM:110:GLU:HG2  | 38:BM:111:GLU:N   | 2.30        | 0.46     |
| 1:CA:490:C:H2'     | 1:CA:491:G:C8     | 2.51        | 0.46     |
| 23:DB:2528:U:O2'   | 23:DB:2529:G:H3'  | 2.16        | 0.46     |
| 1:CA:474:G:H2'     | 1:CA:475:C:H6     | 1.75        | 0.46     |
| 23:BB:718:A:H2'    | 23:BB:719:C:H5'   | 1.97        | 0.46     |
| 2:AC:156:LEU:HD12  | 2:AC:163:ARG:HG3  | 1.98        | 0.46     |
| 1:AA:925:G:O2'     | 1:AA:926:G:H5''   | 2.15        | 0.46     |
| 7:AH:54:THR:HG23   | 7:AH:55:LYS:N     | 2.30        | 0.46     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:67:C:H4'      | 1:AA:172:A:H4'     | 1.97        | 0.46     |
| 23:BB:379:G:O4'    | 23:BB:2232:C:H5''  | 2.15        | 0.46     |
| 23:BB:1902:C:H2'   | 23:BB:1903:G:O4'   | 2.15        | 0.46     |
| 23:BB:2511:U:H2'   | 23:BB:2512:C:C6    | 2.50        | 0.46     |
| 23:BB:1258:U:O4'   | 29:BE:79:ARG:HD2   | 2.14        | 0.46     |
| 23:DB:1946:U:H2'   | 23:DB:1947:C:H6    | 1.80        | 0.46     |
| 23:BB:350:G:H2'    | 23:BB:351:C:O4'    | 2.15        | 0.46     |
| 1:AA:373:A:OP2     | 1:AA:373:A:H3'     | 2.15        | 0.46     |
| 23:BB:1913:A:H4'   | 23:BB:1914:C:C5'   | 2.45        | 0.46     |
| 1:CA:1432:G:H5'    | 28:DP:105:LYS:HG2  | 1.97        | 0.46     |
| 23:DB:378:C:O2'    | 23:DB:379:G:H5'    | 2.14        | 0.46     |
| 23:BB:2498:C:H3'   | 57:BB:3587:HOH:O   | 2.15        | 0.46     |
| 14:CO:43:PHE:CD1   | 14:CO:56:LEU:HD22  | 2.50        | 0.46     |
| 1:AA:1385:G:O2'    | 1:AA:1386:G:H5'    | 2.15        | 0.46     |
| 29:DE:18:THR:HG22  | 29:DE:106:LYS:NZ   | 2.31        | 0.46     |
| 48:DG:87:GLN:H     | 48:DG:164:ALA:HB2  | 1.81        | 0.46     |
| 23:DB:1047:G:C3'   | 23:DB:1048:A:H5'   | 2.44        | 0.46     |
| 23:DB:1837:C:O2    | 23:DB:1927:A:H2    | 1.99        | 0.46     |
| 23:DB:235:U:H2'    | 23:DB:236:C:C6     | 2.49        | 0.46     |
| 28:BP:103:THR:HG22 | 28:BP:104:GLY:N    | 2.29        | 0.46     |
| 1:CA:766:A:H2'     | 1:CA:767:A:C8      | 2.50        | 0.46     |
| 1:AA:478:A:H2'     | 1:AA:479:U:O4'     | 2.15        | 0.46     |
| 23:DB:1118:C:H2'   | 23:DB:1119:U:H6    | 1.79        | 0.46     |
| 26:DD:45:TYR:CD2   | 26:DD:83:ARG:HD3   | 2.49        | 0.46     |
| 1:CA:560:A:H5'     | 1:CA:566:G:N2      | 2.29        | 0.46     |
| 7:CH:118:ALA:HB3   | 7:CH:120:LEU:CD2   | 2.44        | 0.46     |
| 23:DB:1704:C:H2'   | 23:DB:1705:A:C8    | 2.51        | 0.46     |
| 7:CH:79:ARG:HB2    | 7:CH:80:PRO:HD2    | 1.96        | 0.46     |
| 23:BB:736:C:H2'    | 23:BB:737:C:H6     | 1.81        | 0.46     |
| 23:BB:2856:A:H2'   | 23:BB:2857:G:H8    | 1.79        | 0.46     |
| 23:BB:2181:U:H2'   | 23:BB:2182:U:H6    | 1.80        | 0.46     |
| 1:AA:935:A:O2'     | 1:AA:936:C:H5'     | 2.14        | 0.46     |
| 38:BM:12:MET:HB2   | 38:BM:72:PRO:HG2   | 1.95        | 0.46     |
| 1:CA:1019:A:H2'    | 1:CA:1020:G:C8     | 2.51        | 0.46     |
| 23:DB:822:G:H2'    | 23:DB:823:C:C6     | 2.50        | 0.46     |
| 23:DB:477:A:H2'    | 23:DB:478:A:C8     | 2.50        | 0.46     |
| 13:CN:42:ASN:O     | 13:CN:45:LEU:HB3   | 2.16        | 0.46     |
| 23:DB:677:A:O2'    | 23:DB:678:C:H5'    | 2.15        | 0.46     |
| 21:CU:36:PHE:CZ    | 21:CU:44:ARG:NH2   | 2.83        | 0.46     |
| 21:CU:35:GLU:HB3   | 21:CU:36:PHE:H     | 1.53        | 0.46     |
| 10:CK:70:ALA:O     | 10:CK:74:LYS:HB2   | 2.15        | 0.46     |
| 20:AB:205:ALA:O    | 20:AB:209:VAL:HG22 | 2.16        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 40:BH:133:GLN:HG2 | 40:BH:139:PHE:HB3  | 1.97        | 0.46     |
| 53:D6:41:LEU:O    | 53:D6:43:VAL:N     | 2.44        | 0.46     |
| 47:DF:90:LEU:C    | 47:DF:91:ARG:HD3   | 2.35        | 0.46     |
| 40:BH:89:LYS:NZ   | 40:BH:123:ARG:HB3  | 2.31        | 0.46     |
| 41:DJ:45:THR:OG1  | 41:DJ:48:VAL:HB    | 2.16        | 0.46     |
| 27:DK:47:ILE:HG23 | 27:DK:48:PRO:CD    | 2.46        | 0.46     |
| 51:DZ:77:LYS:CG   | 51:DZ:78:TYR:H     | 2.27        | 0.46     |
| 27:BK:47:ILE:HG23 | 27:BK:48:PRO:CD    | 2.45        | 0.46     |
| 47:DF:39:VAL:CG2  | 47:DF:48:LEU:HG    | 2.45        | 0.46     |
| 7:AH:87:ARG:H     | 7:AH:90:GLU:CB     | 2.29        | 0.46     |
| 30:DY:16:LEU:O    | 30:DY:20:LYS:HG3   | 2.15        | 0.46     |
| 50:BT:50:LEU:C    | 50:BT:52:GLU:H     | 2.16        | 0.46     |
| 50:BT:58:VAL:O    | 50:BT:58:VAL:HG13  | 2.16        | 0.46     |
| 39:BX:23:ARG:HD3  | 50:BT:50:LEU:HD12  | 1.97        | 0.46     |
| 46:BU:86:PHE:HD1  | 46:BU:88:ASP:N     | 2.14        | 0.46     |
| 24:BI:79:LEU:HD23 | 24:BI:108:ILE:CD1  | 2.46        | 0.46     |
| 47:BF:106:ALA:HA  | 47:BF:135:ILE:CD1  | 2.46        | 0.46     |
| 38:BM:24:THR:HG23 | 38:BM:34:LYS:HE3   | 1.97        | 0.46     |
| 23:DB:518:G:H4'   | 45:DS:18:ARG:CZ    | 2.46        | 0.46     |
| 1:AA:865:A:C2     | 1:AA:918:A:H4'     | 2.51        | 0.46     |
| 23:DB:1018:U:O2'  | 23:DB:1019:U:H5'   | 2.15        | 0.46     |
| 18:CS:61:VAL:HA   | 18:CS:65:MET:SD    | 2.56        | 0.46     |
| 37:DL:42:SER:C    | 37:DL:44:GLY:N     | 2.68        | 0.46     |
| 28:BP:99:LEU:HD13 | 28:BP:99:LEU:O     | 2.15        | 0.46     |
| 50:DT:40:LYS:HD3  | 50:DT:58:VAL:O     | 2.15        | 0.46     |
| 53:D6:18:LEU:HD22 | 53:D6:168:PHE:CE2  | 2.51        | 0.46     |
| 53:D6:22:GLU:HG2  | 53:D6:175:LEU:HD21 | 1.96        | 0.46     |
| 24:DI:23:VAL:HG12 | 24:DI:24:GLY:N     | 2.30        | 0.46     |
| 32:B4:7:VAL:HG13  | 32:B4:8:LYS:N      | 2.29        | 0.46     |
| 21:CU:16:ARG:HG3  | 21:CU:19:LYS:HD2   | 1.97        | 0.46     |
| 23:BB:1942:C:C1'  | 53:B6:133:ARG:HH22 | 2.27        | 0.46     |
| 23:DB:1124:G:H1'  | 32:D4:38:GLY:OXT   | 2.15        | 0.46     |
| 1:CA:980:C:H4'    | 13:CN:58:ARG:HH12  | 1.81        | 0.46     |
| 5:CF:70:VAL:HG23  | 5:CF:71:ILE:H      | 1.81        | 0.46     |
| 1:AA:116:A:H2'    | 1:AA:117:G:O4'     | 2.14        | 0.46     |
| 38:BM:96:ILE:HD11 | 38:BM:126:ILE:HG12 | 1.97        | 0.46     |
| 44:BQ:97:ILE:HD11 | 44:BQ:108:LEU:HD11 | 1.97        | 0.46     |
| 49:BR:4:VAL:HB    | 49:BR:39:LEU:HG    | 1.96        | 0.46     |
| 49:DR:39:LEU:HA   | 49:DR:49:ILE:HG21  | 1.98        | 0.46     |
| 49:DR:40:MET:O    | 49:DR:41:ILE:HD13  | 2.16        | 0.46     |
| 46:BU:40:LEU:HB3  | 46:BU:59:GLU:HG2   | 1.96        | 0.46     |
| 23:BB:2896:C:H2'  | 23:BB:2897:U:C6    | 2.50        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1723:G:N7   | 23:BB:1737:G:N2    | 2.60        | 0.46     |
| 25:DC:159:THR:N   | 25:DC:194:VAL:CG1  | 2.79        | 0.46     |
| 23:BB:2186:G:H2'  | 23:BB:2187:U:H6    | 1.79        | 0.46     |
| 38:BM:2:LEU:HD23  | 38:BM:46:ILE:HD11  | 1.97        | 0.46     |
| 4:AE:81:GLN:CD    | 4:AE:148:SER:HA    | 2.35        | 0.46     |
| 14:CO:25:THR:CB   | 14:CO:70:LEU:HD23  | 2.44        | 0.46     |
| 23:BB:2135:A:H61  | 23:BB:2156:G:C2'   | 2.28        | 0.46     |
| 3:CD:89:LEU:CD2   | 3:CD:199:ILE:HD11  | 2.46        | 0.46     |
| 2:CC:155:ARG:H    | 2:CC:162:ALA:CB    | 2.28        | 0.46     |
| 3:AD:96:ARG:HB3   | 3:AD:98:ASP:OD2    | 2.15        | 0.46     |
| 1:AA:555:U:H2'    | 1:AA:556:C:H6      | 1.79        | 0.46     |
| 4:CE:38:VAL:O     | 4:CE:45:VAL:HA     | 2.15        | 0.46     |
| 46:BU:35:VAL:HB   | 46:BU:38:ILE:HB    | 1.98        | 0.46     |
| 40:BH:44:ILE:CG1  | 40:BH:45:GLU:H     | 2.28        | 0.46     |
| 40:BH:44:ILE:O    | 40:BH:48:GLU:HB3   | 2.16        | 0.46     |
| 3:AD:84:ASN:HD22  | 3:AD:85:THR:N      | 2.13        | 0.46     |
| 38:DM:69:PRO:HA   | 38:DM:94:ALA:HB2   | 1.97        | 0.46     |
| 23:DB:1248:G:OP1  | 29:DE:44:ARG:NH1   | 2.48        | 0.46     |
| 8:AI:9:GLY:HA2    | 8:AI:80:HIS:HD2    | 1.77        | 0.46     |
| 23:DB:1584:U:H3'  | 23:DB:1585:C:H5'   | 1.96        | 0.46     |
| 1:AA:1330:U:C2'   | 1:AA:1331:G:H5'    | 2.45        | 0.46     |
| 3:AD:2:ARG:HB3    | 3:AD:114:ARG:NH2   | 2.30        | 0.46     |
| 1:AA:801:U:O2'    | 1:AA:802:A:H5'     | 2.14        | 0.46     |
| 23:DB:2492:U:O2'  | 23:DB:2493:U:H5'   | 2.16        | 0.46     |
| 12:AM:112:ARG:HB3 | 12:AM:114:PRO:HD3  | 1.98        | 0.46     |
| 38:BM:4:PRO:HG2   | 38:BM:70:ASP:HA    | 1.97        | 0.46     |
| 23:BB:2064:C:H1'  | 23:BB:2450:A:C6    | 2.50        | 0.46     |
| 23:BB:2853:C:O2'  | 23:BB:2854:G:H5'   | 2.15        | 0.46     |
| 1:AA:1308:U:H2'   | 1:AA:1309:G:H8     | 1.81        | 0.46     |
| 23:DB:2070:A:H2'  | 23:DB:2071:A:H8    | 1.77        | 0.46     |
| 40:DH:65:ALA:C    | 40:DH:138:VAL:HG11 | 2.35        | 0.46     |
| 23:BB:1708:C:H2'  | 23:BB:1709:U:C6    | 2.51        | 0.46     |
| 41:DJ:99:ARG:HA   | 41:DJ:102:GLU:HB2  | 1.98        | 0.46     |
| 23:DB:325:G:H2'   | 23:DB:326:G:H8     | 1.80        | 0.46     |
| 23:BB:251:A:H2'   | 23:BB:252:G:O4'    | 2.15        | 0.46     |
| 26:BD:45:TYR:CD2  | 26:BD:83:ARG:HD3   | 2.50        | 0.46     |
| 23:BB:1313:U:O2   | 23:BB:1313:U:H2'   | 2.15        | 0.46     |
| 23:DB:685:A:H1'   | 23:DB:688:U:O4     | 2.15        | 0.46     |
| 1:CA:1436:U:H2'   | 1:CA:1437:A:H8     | 1.81        | 0.46     |
| 25:BC:73:ILE:HG21 | 25:BC:97:ASP:HB2   | 1.97        | 0.46     |
| 2:CC:91:ALA:O     | 2:CC:95:GLY:N      | 2.49        | 0.46     |
| 23:BB:2838:G:H2'  | 23:BB:2839:G:H8    | 1.81        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:2771:C:H1'  | 26:DD:208:LYS:HZ1 | 1.80        | 0.46     |
| 14:CO:62:GLN:O    | 14:CO:66:LEU:HD23 | 2.15        | 0.46     |
| 23:DB:332:A:O2'   | 23:DB:334:C:OP2   | 2.33        | 0.46     |
| 52:BW:25:PHE:HD1  | 52:BW:26:GLY:H    | 1.64        | 0.46     |
| 48:DG:66:THR:O    | 48:DG:70:LEU:HB2  | 2.15        | 0.46     |
| 23:BB:69:C:O2'    | 23:BB:70:G:H5'    | 2.14        | 0.46     |
| 15:AP:22:ALA:HA   | 15:AP:33:ILE:HG13 | 1.97        | 0.46     |
| 1:AA:144:G:H2'    | 1:AA:145:G:O4'    | 2.16        | 0.46     |
| 28:BP:101:GLU:OE2 | 28:BP:101:GLU:N   | 2.49        | 0.46     |
| 23:DB:2408:U:H2'  | 23:DB:2409:G:C8   | 2.51        | 0.46     |
| 23:DB:2696:U:O2'  | 23:DB:2697:G:H5'  | 2.16        | 0.46     |
| 37:DL:124:GLY:O   | 37:DL:125:LEU:HG  | 2.16        | 0.46     |
| 41:BJ:36:LEU:HD21 | 41:BJ:122:LEU:CD1 | 2.45        | 0.46     |
| 23:DB:996:A:H4'   | 44:DQ:91:ARG:CG   | 2.46        | 0.46     |
| 13:CN:60:ARG:HE   | 13:CN:62:ARG:HG2  | 1.81        | 0.46     |
| 51:BZ:49:LEU:HB2  | 51:BZ:51:VAL:HG23 | 1.96        | 0.46     |
| 46:BU:86:PHE:HD1  | 46:BU:88:ASP:H    | 1.59        | 0.46     |
| 23:BB:320:A:H2'   | 29:BE:131:THR:OG1 | 2.16        | 0.46     |
| 23:BB:1462:C:O2'  | 23:BB:1463:C:H5'  | 2.16        | 0.46     |
| 18:AS:50:VAL:HG23 | 18:AS:59:VAL:HG21 | 1.96        | 0.46     |
| 28:BP:92:ARG:NH1  | 28:BP:92:ARG:HG3  | 2.31        | 0.46     |
| 50:DT:11:LEU:CD2  | 50:DT:46:ALA:HB1  | 2.46        | 0.46     |
| 50:DT:29:THR:CG2  | 50:DT:86:THR:HG22 | 2.46        | 0.46     |
| 23:BB:165:A:H2'   | 23:BB:166:U:H6    | 1.79        | 0.46     |
| 1:AA:332:G:P      | 19:AT:2:ASN:HB3   | 2.55        | 0.46     |
| 31:B0:43:THR:HG23 | 31:B0:47:TYR:C    | 2.35        | 0.46     |
| 38:DM:2:LEU:HD23  | 38:DM:46:ILE:HD11 | 1.97        | 0.46     |
| 27:BK:104:THR:HB  | 27:BK:106:GLU:OE1 | 2.16        | 0.46     |
| 1:CA:312:C:H2'    | 1:CA:313:A:H8     | 1.80        | 0.46     |
| 27:BK:58:LEU:H    | 27:BK:58:LEU:HD23 | 1.80        | 0.46     |
| 1:AA:1299:A:C2'   | 1:AA:1301:U:H1'   | 2.41        | 0.46     |
| 23:BB:1427:A:H4'  | 23:BB:1428:C:O5'  | 2.15        | 0.46     |
| 23:BB:1724:G:H2'  | 23:BB:1725:U:H6   | 1.80        | 0.46     |
| 20:CB:75:ALA:O    | 20:CB:79:VAL:HG23 | 2.15        | 0.46     |
| 11:AL:28:GLN:HG3  | 11:AL:80:LEU:HD21 | 1.98        | 0.46     |
| 4:AE:158:LYS:HZ3  | 7:AH:65:PHE:HA    | 1.80        | 0.46     |
| 1:AA:109:A:H2'    | 1:AA:326:G:N2     | 2.30        | 0.46     |
| 23:DB:321:U:OP2   | 29:DE:130:LYS:HA  | 2.16        | 0.46     |
| 2:AC:112:ALA:HB1  | 2:AC:184:ASN:HB2  | 1.97        | 0.46     |
| 15:CP:43:ALA:HA   | 15:CP:46:LYS:HE3  | 1.95        | 0.46     |
| 2:CC:26:LYS:HG3   | 2:CC:27:GLU:HG3   | 1.98        | 0.46     |
| 23:DB:2602:A:H3'  | 23:DB:2602:A:OP1  | 2.15        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:560:C:H2'   | 23:BB:561:G:O4'    | 2.16        | 0.46     |
| 11:AL:33:CYS:H    | 11:AL:54:VAL:HG13  | 1.80        | 0.46     |
| 1:AA:238:A:C3'    | 1:AA:239:U:H5''    | 2.46        | 0.46     |
| 1:AA:490:C:H2'    | 1:AA:491:G:C8      | 2.50        | 0.46     |
| 1:CA:807:A:H2'    | 1:CA:808:C:C6      | 2.50        | 0.46     |
| 45:BS:42:LYS:O    | 45:BS:46:LEU:HG    | 2.16        | 0.46     |
| 1:AA:1226:C:H4'   | 1:AA:1227:A:OP1    | 2.15        | 0.46     |
| 1:CA:212:G:H2'    | 1:CA:213:G:H8      | 1.80        | 0.46     |
| 20:CB:23:ASN:OD1  | 20:CB:25:LYS:HB2   | 2.16        | 0.46     |
| 20:CB:22:TRP:CZ3  | 20:CB:24:PRO:HA    | 2.51        | 0.46     |
| 16:CQ:80:LYS:O    | 16:CQ:83:LEU:HD13  | 2.15        | 0.46     |
| 23:DB:876:C:H2'   | 23:DB:877:A:O4'    | 2.15        | 0.46     |
| 23:BB:1867:G:O2'  | 23:BB:1868:C:H5'   | 2.15        | 0.46     |
| 22:BA:8:C:H4'     | 43:BO:27:VAL:HG21  | 1.98        | 0.46     |
| 23:BB:139:U:H3'   | 23:BB:140:C:C4'    | 2.43        | 0.46     |
| 23:BB:2093:G:O2'  | 23:BB:2094:A:H5'   | 2.15        | 0.46     |
| 1:CA:1258:G:O2'   | 1:CA:1259:C:H5'    | 2.16        | 0.46     |
| 43:DO:110:ALA:O   | 43:DO:115:LEU:HB2  | 2.15        | 0.46     |
| 3:CD:77:GLU:OE1   | 3:CD:80:ARG:HD3    | 2.15        | 0.46     |
| 1:CA:539:A:H2'    | 1:CA:540:G:H8      | 1.77        | 0.46     |
| 23:BB:708:G:H2'   | 23:BB:709:U:C6     | 2.50        | 0.46     |
| 1:AA:586:C:C5'    | 7:AH:81:GLY:HA2    | 2.46        | 0.46     |
| 1:CA:591:U:H2'    | 1:CA:592:G:C8      | 2.50        | 0.46     |
| 43:DO:28:VAL:HG11 | 43:DO:92:PHE:CZ    | 2.49        | 0.46     |
| 23:DB:2730:C:H4'  | 26:DD:174:SER:HB3  | 1.96        | 0.46     |
| 46:BU:66:VAL:C    | 46:BU:68:ASN:H     | 2.19        | 0.46     |
| 26:BD:38:LYS:HD3  | 26:BD:45:TYR:OH    | 2.15        | 0.46     |
| 8:AI:71:ILE:N     | 8:AI:71:ILE:HD12   | 2.31        | 0.46     |
| 1:AA:821:G:O2'    | 1:AA:822:U:H5'     | 2.16        | 0.46     |
| 25:DC:226:PRO:HG3 | 25:DC:233:GLY:H    | 1.81        | 0.46     |
| 1:CA:1246:A:H2'   | 1:CA:1247:U:C6     | 2.50        | 0.46     |
| 48:BG:29:ASN:ND2  | 48:BG:77:GLY:O     | 2.49        | 0.46     |
| 23:BB:1435:G:H2'  | 23:BB:1436:G:H8    | 1.80        | 0.46     |
| 23:DB:1136:G:H2'  | 23:DB:1137:G:H8    | 1.80        | 0.46     |
| 23:BB:1711:A:O2'  | 23:BB:1712:U:H5'   | 2.16        | 0.46     |
| 51:BZ:2:SER:HB3   | 51:BZ:4:VAL:HG23   | 1.98        | 0.46     |
| 23:BB:730:A:H3'   | 57:BB:3597:HOH:O   | 2.15        | 0.46     |
| 45:DS:4:ILE:HG22  | 45:DS:106:VAL:HG22 | 1.98        | 0.46     |
| 23:BB:915:C:H3'   | 23:BB:916:G:H8     | 1.81        | 0.46     |
| 49:BR:62:GLU:O    | 49:BR:96:VAL:HA    | 2.16        | 0.46     |
| 23:BB:285:G:H2'   | 23:BB:286:U:C6     | 2.50        | 0.46     |
| 25:BC:35:LYS:HD2  | 25:BC:36:ASN:H     | 1.80        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:483:A:O2'   | 46:BU:56:GLY:HA2  | 2.15        | 0.46     |
| 23:BB:2047:C:H2'  | 23:BB:2048:G:H8   | 1.80        | 0.46     |
| 23:DB:2109:U:N3   | 23:DB:2180:U:O4   | 2.47        | 0.46     |
| 10:AK:36:ARG:HG3  | 10:AK:36:ARG:HH11 | 1.81        | 0.46     |
| 7:CH:72:GLU:CD    | 7:CH:72:GLU:H     | 2.19        | 0.46     |
| 23:DB:56:A:H2'    | 23:DB:57:C:C6     | 2.49        | 0.46     |
| 22:DA:57:A:OP2    | 22:DA:58:A:OP2    | 2.33        | 0.46     |
| 25:BC:146:LYS:HB2 | 25:BC:149:LYS:HB2 | 1.97        | 0.46     |
| 23:DB:2269:G:H4'  | 52:DW:19:ARG:HH11 | 1.80        | 0.46     |
| 40:DH:133:GLN:CB  | 40:DH:139:PHE:HB3 | 2.26        | 0.46     |
| 48:DG:83:THR:C    | 48:DG:84:LYS:HD3  | 2.36        | 0.46     |
| 48:DG:90:GLY:HA3  | 48:DG:93:TYR:CZ   | 2.50        | 0.46     |
| 53:D6:60:ALA:HA   | 53:D6:66:LEU:HD12 | 1.98        | 0.46     |
| 40:BH:77:THR:HG22 | 40:BH:79:THR:HG23 | 1.97        | 0.46     |
| 1:CA:1148:U:H5'   | 8:CI:6:TYR:OH     | 2.16        | 0.46     |
| 23:DB:996:A:H4'   | 44:DQ:91:ARG:HD2  | 1.98        | 0.46     |
| 47:DF:66:ILE:HA   | 47:DF:85:GLY:O    | 2.15        | 0.46     |
| 48:DG:26:LYS:HB2  | 48:DG:32:LEU:HG   | 1.98        | 0.46     |
| 48:DG:34:ARG:HH11 | 48:DG:34:ARG:N    | 1.99        | 0.46     |
| 23:DB:674:G:H2'   | 23:DB:804:A:H61   | 1.81        | 0.46     |
| 41:BJ:3:THR:HG21  | 44:BQ:60:TRP:NE1  | 2.27        | 0.46     |
| 41:BJ:45:THR:HG23 | 41:BJ:45:THR:O    | 2.15        | 0.46     |
| 48:BG:32:LEU:HB3  | 48:BG:34:ARG:CZ   | 2.45        | 0.46     |
| 30:BY:16:LEU:O    | 30:BY:20:LYS:HG3  | 2.16        | 0.46     |
| 34:B3:28:LEU:HD22 | 34:B3:43:LEU:HB2  | 1.97        | 0.46     |
| 47:DF:100:GLU:O   | 47:DF:104:THR:HB  | 2.15        | 0.46     |
| 47:DF:7:TYR:HA    | 47:DF:11:VAL:HB   | 1.97        | 0.46     |
| 47:DF:169:LEU:HA  | 47:DF:172:PHE:HD2 | 1.80        | 0.46     |
| 18:AS:35:ARG:HB3  | 18:AS:50:VAL:HG13 | 1.97        | 0.46     |
| 18:AS:39:ILE:HG21 | 18:AS:61:VAL:HG13 | 1.97        | 0.46     |
| 23:DB:483:A:C8    | 46:DU:44:HIS:HB3  | 2.50        | 0.46     |
| 53:D6:22:GLU:HG2  | 53:D6:175:LEU:CD2 | 2.45        | 0.46     |
| 40:BH:5:LEU:C     | 40:BH:6:LEU:HD12  | 2.36        | 0.46     |
| 32:B4:15:LYS:O    | 32:B4:15:LYS:HE2  | 2.16        | 0.46     |
| 32:B4:22:VAL:O    | 32:B4:24:ARG:HG3  | 2.16        | 0.46     |
| 15:AP:66:THR:HG22 | 15:AP:67:ILE:H    | 1.81        | 0.46     |
| 32:D4:7:VAL:HG11  | 32:D4:23:ILE:O    | 2.15        | 0.46     |
| 23:DB:2038:G:H2'  | 23:DB:2039:U:C6   | 2.51        | 0.46     |
| 23:DB:1654:A:O2'  | 26:DD:118:PHE:CB  | 2.57        | 0.46     |
| 2:CC:140:ALA:HB3  | 2:CC:148:ILE:HD12 | 1.96        | 0.46     |
| 48:DG:30:GLY:O    | 48:DG:78:VAL:HG12 | 2.16        | 0.46     |
| 1:CA:279:A:C5'    | 1:CA:280:C:H3'    | 2.43        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:1776:G:O2'  | 23:DB:1777:U:H5'   | 2.16        | 0.46     |
| 1:AA:906:A:O2'    | 1:AA:907:A:H5''    | 2.16        | 0.46     |
| 24:DI:96:LYS:HD3  | 24:DI:138:VAL:HG21 | 1.97        | 0.46     |
| 36:D2:21:ARG:C    | 36:D2:23:ALA:H     | 2.18        | 0.46     |
| 20:AB:95:TRP:HZ2  | 20:AB:100:LEU:HD13 | 1.79        | 0.46     |
| 33:B1:7:LYS:CD    | 34:B3:33:THR:HG21  | 2.43        | 0.46     |
| 2:CC:117:ASP:OD2  | 2:CC:186:SER:HB3   | 2.16        | 0.46     |
| 23:BB:1210:G:H5'  | 23:BB:1212:G:H5'   | 1.98        | 0.46     |
| 1:AA:957:U:H2'    | 1:AA:959:A:OP2     | 2.16        | 0.46     |
| 43:BO:47:VAL:O    | 43:BO:48:LEU:HD23  | 2.16        | 0.46     |
| 1:CA:856:C:O2'    | 1:CA:857:C:H5'     | 2.16        | 0.46     |
| 39:DX:56:LEU:C    | 39:DX:58:ASN:N     | 2.67        | 0.46     |
| 4:AE:106:ALA:HB1  | 4:AE:110:MET:CB    | 2.45        | 0.46     |
| 23:BB:72:U:H1'    | 39:BX:51:ALA:HA    | 1.97        | 0.46     |
| 50:DT:69:ARG:HB3  | 50:DT:74:ILE:HA    | 1.97        | 0.46     |
| 1:AA:212:G:H2'    | 1:AA:213:G:C8      | 2.51        | 0.46     |
| 23:DB:1924:C:H2'  | 23:DB:1925:C:H6    | 1.81        | 0.46     |
| 23:DB:899:A:C5    | 23:DB:900:A:H1'    | 2.51        | 0.46     |
| 1:CA:1035:A:H2'   | 1:CA:1036:A:C8     | 2.48        | 0.46     |
| 23:DB:828:U:H2'   | 23:DB:829:A:C8     | 2.51        | 0.46     |
| 23:DB:826:U:O2'   | 37:DL:53:GLY:HA3   | 2.15        | 0.46     |
| 3:CD:16:THR:HG22  | 3:CD:17:ASP:H      | 1.78        | 0.46     |
| 50:DT:45:ALA:HA   | 50:DT:48:GLN:HB2   | 1.96        | 0.46     |
| 50:DT:48:GLN:HA   | 50:DT:48:GLN:NE2   | 2.29        | 0.46     |
| 23:DB:1535:A:O2'  | 23:DB:1536:C:H5'   | 2.15        | 0.46     |
| 23:DB:2804:U:H2'  | 23:DB:2805:C:H6    | 1.78        | 0.46     |
| 1:AA:1039:G:H2'   | 1:AA:1040:U:H6     | 1.79        | 0.46     |
| 19:CT:49:ALA:HA   | 19:CT:52:GLU:CD    | 2.36        | 0.46     |
| 23:DB:1708:C:H2'  | 23:DB:1709:U:H6    | 1.79        | 0.46     |
| 23:BB:2322:A:C6   | 23:BB:2333:A:N6    | 2.84        | 0.46     |
| 23:BB:2825:G:H5'' | 23:BB:2825:G:N3    | 2.31        | 0.46     |
| 23:BB:443:A:H1'   | 23:BB:1201:U:O4'   | 2.16        | 0.46     |
| 23:DB:1676:A:C2   | 23:DB:1677:A:H1'   | 2.50        | 0.46     |
| 23:BB:660:C:H2'   | 23:BB:661:A:C8     | 2.49        | 0.46     |
| 1:CA:207:C:O2'    | 1:CA:208:U:H5'     | 2.15        | 0.46     |
| 48:BG:4:ALA:HB3   | 48:BG:61:TRP:HZ3   | 1.81        | 0.46     |
| 23:DB:927:A:O2'   | 23:DB:928:A:H5'    | 2.16        | 0.46     |
| 23:DB:2836:U:H2'  | 23:DB:2837:A:C8    | 2.51        | 0.46     |
| 1:AA:558:G:H8     | 1:AA:559:A:H2'     | 1.80        | 0.46     |
| 1:CA:80:A:H2'     | 1:CA:81:A:H8       | 1.79        | 0.46     |
| 48:DG:28:LYS:O    | 48:DG:29:ASN:HB3   | 2.15        | 0.46     |
| 1:CA:160:A:H1'    | 1:CA:344:A:N7      | 2.29        | 0.46     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:1354:U:H2'    | 1:CA:1355:G:H8     | 1.81        | 0.46     |
| 22:BA:54:G:H21     | 47:BF:25:MET:CE    | 2.29        | 0.46     |
| 30:DY:3:THR:HB     | 30:DY:36:GLU:HG2   | 1.98        | 0.46     |
| 25:DC:11:GLY:O     | 25:DC:206:LYS:HB3  | 2.16        | 0.46     |
| 2:CC:40:GLN:HG3    | 2:CC:41:TYR:H      | 1.81        | 0.46     |
| 1:CA:1409:C:H2'    | 1:CA:1410:A:H8     | 1.81        | 0.46     |
| 23:DB:1949:G:H2'   | 23:DB:1950:G:C8    | 2.51        | 0.46     |
| 20:CB:134:LEU:HD11 | 20:CB:138:ARG:HH12 | 1.79        | 0.46     |
| 49:BR:34:GLU:OE1   | 49:BR:60:LYS:HE2   | 2.14        | 0.46     |
| 23:BB:2331:G:H4'   | 52:BW:39:GLN:HA    | 1.98        | 0.46     |
| 10:AK:12:ARG:HD3   | 10:AK:76:TYR:CE1   | 2.50        | 0.46     |
| 48:BG:94:ARG:NH2   | 48:BG:104:LEU:HA   | 2.30        | 0.46     |
| 41:DJ:16:TYR:O     | 41:DJ:55:ILE:HG12  | 2.16        | 0.46     |
| 30:DY:15:ARG:N     | 30:DY:15:ARG:HD2   | 2.31        | 0.46     |
| 42:DN:38:LEU:CB    | 42:DN:39:PRO:HD3   | 2.41        | 0.46     |
| 43:BO:35:ILE:HG21  | 43:BO:71:ALA:HA    | 1.96        | 0.46     |
| 42:BN:79:LEU:C     | 42:BN:81:ASN:H     | 2.19        | 0.46     |
| 1:AA:1258:G:O2'    | 1:AA:1259:C:H5'    | 2.15        | 0.46     |
| 29:DE:108:ILE:HD11 | 29:DE:181:ILE:CB   | 2.37        | 0.46     |
| 18:CS:42:ASN:HD21  | 18:CS:43:MET:HG2   | 1.78        | 0.46     |
| 12:AM:79:LEU:HD22  | 12:AM:86:ARG:HE    | 1.80        | 0.46     |
| 18:AS:6:LYS:N      | 18:AS:6:LYS:HD2    | 2.30        | 0.46     |
| 11:AL:42:LYS:HB2   | 11:AL:88:ASP:HA    | 1.98        | 0.46     |
| 29:BE:77:ILE:HG13  | 29:BE:77:ILE:H     | 1.57        | 0.46     |
| 35:DV:14:LYS:HE3   | 35:DV:18:ARG:NH2   | 2.31        | 0.46     |
| 11:CL:49:ARG:HH12  | 11:CL:88:ASP:HB2   | 1.81        | 0.46     |
| 1:CA:1325:C:O2'    | 1:CA:1326:U:H5'    | 2.16        | 0.46     |
| 43:BO:26:LEU:HD13  | 43:BO:39:VAL:CG2   | 2.45        | 0.46     |
| 35:DV:44:HIS:O     | 35:DV:45:ASP:C     | 2.54        | 0.46     |
| 45:BS:28:LYS:O     | 45:BS:71:VAL:HG12  | 2.16        | 0.46     |
| 25:BC:16:VAL:CB    | 25:BC:203:VAL:HB   | 2.40        | 0.46     |
| 29:DE:142:ALA:O    | 29:DE:143:LEU:HD23 | 2.16        | 0.46     |
| 29:DE:115:GLN:NE2  | 37:DL:2:ARG:HD3    | 2.31        | 0.46     |
| 46:DU:12:VAL:HG22  | 46:DU:69:VAL:CG1   | 2.41        | 0.46     |
| 5:CF:62:MET:O      | 5:CF:63:ASN:HB2    | 2.16        | 0.46     |
| 20:CB:16:GLY:HA2   | 20:CB:40:ILE:HG13  | 1.97        | 0.46     |
| 20:CB:186:VAL:O    | 20:CB:200:PRO:HA   | 2.16        | 0.46     |
| 38:BM:65:ILE:HG23  | 38:BM:103:TYR:CE2  | 2.51        | 0.46     |
| 3:CD:122:ILE:HG22  | 3:CD:123:MET:N     | 2.31        | 0.46     |
| 1:CA:1411:C:H2'    | 1:CA:1412:C:C6     | 2.51        | 0.46     |
| 44:BQ:108:LEU:O    | 44:BQ:111:LYS:HB3  | 2.16        | 0.46     |
| 37:DL:95:LEU:HB3   | 37:DL:100:ILE:CG2  | 2.45        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:2896:C:H2'  | 23:DB:2897:U:C6   | 2.50        | 0.46     |
| 23:DB:1441:G:O2'  | 23:DB:1442:U:H5'  | 2.16        | 0.46     |
| 23:BB:1446:C:H2'  | 23:BB:1447:C:C6   | 2.50        | 0.46     |
| 31:D0:2:VAL:HG12  | 31:D0:3:GLN:H     | 1.81        | 0.46     |
| 49:DR:25:LEU:H    | 49:DR:94:THR:HG21 | 1.81        | 0.46     |
| 12:AM:89:ARG:CB   | 12:AM:96:VAL:HG22 | 2.46        | 0.46     |
| 23:BB:1139:G:O2'  | 23:BB:1143:A:N1   | 2.42        | 0.46     |
| 23:BB:1138:G:H21  | 41:BJ:108:MET:CE  | 2.29        | 0.46     |
| 1:AA:1049:U:O4'   | 1:AA:1201:A:N7    | 2.49        | 0.46     |
| 23:DB:1213:A:C6   | 23:DB:1237:A:H1'  | 2.50        | 0.46     |
| 22:BA:13:G:H1     | 22:BA:69:G:HO2'   | 1.64        | 0.46     |
| 23:DB:52:A:C5     | 23:DB:118:A:C2    | 3.04        | 0.46     |
| 23:DB:1248:G:C4   | 44:DQ:2:ARG:HD2   | 2.50        | 0.46     |
| 23:DB:1180:U:H2'  | 23:DB:1181:U:O4'  | 2.15        | 0.46     |
| 34:D3:60:CYS:C    | 34:D3:62:PRO:HD3  | 2.36        | 0.46     |
| 37:DL:47:ARG:HH21 | 37:DL:47:ARG:HB3  | 1.80        | 0.46     |
| 20:AB:83:ALA:CB   | 20:AB:90:PHE:HB3  | 2.45        | 0.46     |
| 1:AA:858:G:O6     | 1:AA:869:G:H3'    | 2.16        | 0.46     |
| 23:DB:1590:A:H2'  | 23:DB:1591:A:H8   | 1.81        | 0.46     |
| 1:AA:1123:U:C2'   | 1:AA:1124:G:H5'   | 2.46        | 0.46     |
| 23:DB:2853:C:O2'  | 23:DB:2854:G:H5'  | 2.16        | 0.46     |
| 19:CT:35:TYR:CG   | 19:CT:36:ALA:N    | 2.82        | 0.46     |
| 1:AA:1054:C:O2'   | 1:AA:1055:A:H5''  | 2.16        | 0.46     |
| 1:AA:1143:G:O2'   | 1:AA:1144:G:H5'   | 2.16        | 0.46     |
| 8:AI:99:LYS:HE3   | 9:CJ:80:THR:HA    | 1.97        | 0.46     |
| 16:CQ:30:HIS:ND1  | 16:CQ:32:ILE:HG22 | 2.30        | 0.46     |
| 23:DB:2699:C:H2'  | 23:DB:2700:A:C8   | 2.50        | 0.46     |
| 51:DZ:63:GLY:HA3  | 51:DZ:66:THR:OG1  | 2.16        | 0.46     |
| 22:DA:49:C:O2'    | 22:DA:50:A:H5'    | 2.16        | 0.46     |
| 21:AU:31:VAL:O    | 21:AU:31:VAL:HG12 | 2.15        | 0.46     |
| 23:BB:2730:C:H2'  | 23:BB:2731:G:H8   | 1.79        | 0.46     |
| 5:AF:7:VAL:O      | 5:AF:7:VAL:HG13   | 2.16        | 0.46     |
| 23:DB:1640:A:H2'  | 23:DB:1641:A:H8   | 1.80        | 0.46     |
| 1:CA:170:U:O2'    | 1:CA:171:A:H5'    | 2.16        | 0.46     |
| 1:CA:975:A:H5''   | 1:CA:976:G:O5'    | 2.15        | 0.46     |
| 1:AA:317:U:H2'    | 1:AA:318:G:C8     | 2.50        | 0.46     |
| 49:BR:20:VAL:HG12 | 49:BR:21:ARG:N    | 2.30        | 0.46     |
| 23:DB:686:U:H2'   | 23:DB:788:A:N1    | 2.31        | 0.46     |
| 7:AH:79:ARG:HB2   | 7:AH:80:PRO:HD2   | 1.96        | 0.46     |
| 1:CA:178:C:O2'    | 1:CA:179:A:H5'    | 2.16        | 0.46     |
| 1:AA:26:A:N6      | 1:AA:558:G:H1'    | 2.31        | 0.46     |
| 18:AS:11:ASP:H    | 18:AS:14:LEU:HD21 | 1.81        | 0.46     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:DB:2297:A:H61   | 23:DB:2319:G:H1'  | 1.79        | 0.46     |
| 1:CA:961:U:OP1     | 1:CA:1223:C:H4'   | 2.15        | 0.46     |
| 53:D6:156:ARG:O    | 53:D6:159:ALA:HB3 | 2.16        | 0.46     |
| 25:DC:35:LYS:HD2   | 25:DC:36:ASN:H    | 1.80        | 0.46     |
| 23:BB:1366:A:H2'   | 23:BB:1367:A:O4'  | 2.15        | 0.46     |
| 1:AA:1125:U:O2'    | 1:AA:1126:U:H2'   | 2.16        | 0.46     |
| 50:DT:15:HIS:O     | 50:DT:16:VAL:C    | 2.53        | 0.46     |
| 23:BB:1568:G:H4'   | 25:BC:58:LYS:HB3  | 1.98        | 0.46     |
| 23:BB:2745:C:H4'   | 48:BG:141:GLY:O   | 2.16        | 0.46     |
| 4:AE:17:VAL:HG23   | 4:AE:33:THR:O     | 2.16        | 0.46     |
| 37:BL:142:ILE:HD12 | 37:BL:142:ILE:N   | 2.31        | 0.46     |
| 23:BB:303:G:H2'    | 23:BB:304:U:C6    | 2.51        | 0.46     |
| 1:AA:998:C:H2'     | 1:AA:999:C:C6     | 2.51        | 0.46     |
| 38:BM:33:LEU:HD22  | 38:BM:128:THR:OG1 | 2.16        | 0.46     |
| 23:BB:1664:A:H1'   | 23:BB:2726:A:N1   | 2.31        | 0.46     |
| 10:AK:125:LYS:O    | 21:AU:33:ARG:NH2  | 2.49        | 0.46     |
| 23:BB:2331:G:O2'   | 23:BB:2332:C:H5'  | 2.16        | 0.46     |
| 52:BW:49:ASN:CB    | 52:BW:60:ALA:HA   | 2.45        | 0.46     |
| 23:DB:2330:G:N2    | 52:DW:38:ARG:O    | 2.49        | 0.46     |
| 25:DC:146:LYS:HB2  | 25:DC:149:LYS:HB2 | 1.97        | 0.46     |
| 53:B6:70:SER:N     | 53:B6:97:ASP:O    | 2.47        | 0.46     |
| 53:B6:68:VAL:HG11  | 53:B6:79:ILE:CB   | 2.46        | 0.46     |
| 40:BH:79:THR:HA    | 40:BH:145:ASN:CB  | 2.44        | 0.46     |
| 1:CA:1147:C:H2'    | 1:CA:1148:U:C6    | 2.51        | 0.46     |
| 8:CI:25:GLY:HA3    | 8:CI:57:VAL:HA    | 1.98        | 0.46     |
| 47:DF:115:GLY:CA   | 47:DF:177:ARG:HD2 | 2.30        | 0.46     |
| 41:BJ:18:VAL:HG22  | 41:BJ:19:ASP:N    | 2.31        | 0.46     |
| 23:DB:994:C:O2     | 49:DR:10:LYS:HE3  | 2.16        | 0.46     |
| 13:AN:5:MET:O      | 13:AN:8:ARG:HB3   | 2.16        | 0.46     |
| 37:DL:115:GLU:N    | 37:DL:115:GLU:OE1 | 2.48        | 0.46     |
| 13:CN:78:LEU:HD23  | 13:CN:82:LYS:CB   | 2.45        | 0.46     |
| 38:DM:35:ALA:C     | 38:DM:37:GLY:H    | 2.19        | 0.46     |
| 1:CA:982:U:OP2     | 13:CN:60:ARG:NH1  | 2.48        | 0.46     |
| 13:CN:5:MET:HE2    | 13:CN:60:ARG:NH1  | 2.31        | 0.46     |
| 1:CA:430:A:P       | 3:CD:6:PRO:HA     | 2.56        | 0.46     |
| 51:BZ:71:LEU:CD1   | 51:BZ:76:GLU:HB3  | 2.44        | 0.46     |
| 46:DU:86:PHE:HD1   | 46:DU:88:ASP:H    | 1.60        | 0.46     |
| 22:BA:28:C:C5      | 22:BA:56:G:C2     | 3.04        | 0.46     |
| 37:BL:42:SER:O     | 37:BL:44:GLY:N    | 2.49        | 0.46     |
| 37:BL:80:SER:HB3   | 37:BL:115:GLU:OE2 | 2.16        | 0.46     |
| 35:BV:44:HIS:O     | 35:BV:45:ASP:C    | 2.54        | 0.46     |
| 4:CE:131:ASN:ND2   | 4:CE:134:ASN:H    | 2.14        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:AI:87:MET:HB2   | 8:AI:94:ARG:CD    | 2.46        | 0.46     |
| 9:AJ:57:VAL:HG22  | 9:AJ:58:ASN:N     | 2.20        | 0.46     |
| 50:DT:38:ALA:HB1  | 50:DT:43:ILE:CD1  | 2.45        | 0.46     |
| 23:DB:2893:A:H4'  | 23:DB:2894:G:O5'  | 2.15        | 0.46     |
| 16:AQ:74:LEU:HD22 | 16:AQ:75:VAL:H    | 1.81        | 0.46     |
| 23:BB:2751:G:H4'  | 23:BB:2752:C:OP1  | 2.15        | 0.46     |
| 53:B6:108:GLU:O   | 53:B6:112:LYS:HG3 | 2.16        | 0.46     |
| 32:B4:15:LYS:O    | 32:B4:16:ILE:HB   | 2.16        | 0.46     |
| 1:CA:244:U:O4     | 1:CA:906:A:H1'    | 2.16        | 0.46     |
| 28:DP:92:ARG:NH1  | 28:DP:92:ARG:HG3  | 2.31        | 0.46     |
| 22:DA:76:G:P      | 35:DV:13:GLY:H    | 2.38        | 0.46     |
| 15:CP:72:ALA:HA   | 15:CP:75:ILE:CD1  | 2.45        | 0.46     |
| 26:DD:116:LYS:HB3 | 26:DD:118:PHE:CE2 | 2.50        | 0.46     |
| 23:BB:2443:C:O2'  | 23:BB:2444:G:H5'  | 2.16        | 0.46     |
| 23:DB:970:U:H1'   | 23:DB:985:C:P     | 2.56        | 0.46     |
| 23:DB:1439:A:H1'  | 23:DB:1553:A:N6   | 2.30        | 0.46     |
| 1:CA:842:U:H4'    | 1:CA:846:G:C2     | 2.51        | 0.46     |
| 36:B2:9:VAL:CG1   | 36:B2:10:LEU:N    | 2.79        | 0.46     |
| 23:DB:2244:U:H2'  | 23:DB:2245:U:O4'  | 2.15        | 0.46     |
| 28:BP:6:GLN:O     | 28:BP:10:GLU:HB2  | 2.15        | 0.46     |
| 28:BP:4:ILE:HG22  | 28:BP:5:LYS:N     | 2.27        | 0.46     |
| 4:AE:80:LEU:CD1   | 4:AE:95:MET:HB3   | 2.45        | 0.46     |
| 10:AK:80:ASN:HD22 | 10:AK:80:ASN:H    | 1.63        | 0.46     |
| 49:DR:23:GLU:O    | 49:DR:25:LEU:HD22 | 2.16        | 0.46     |
| 1:CA:440:C:O2'    | 1:CA:441:A:H5'    | 2.16        | 0.46     |
| 3:AD:197:HIS:HA   | 3:AD:200:VAL:HG22 | 1.98        | 0.46     |
| 1:CA:552:U:H2'    | 1:CA:553:A:H8     | 1.79        | 0.46     |
| 35:DV:29:ILE:HD13 | 35:DV:31:TYR:HE2  | 1.81        | 0.46     |
| 23:DB:646:U:H3'   | 23:DB:647:G:H8    | 1.81        | 0.46     |
| 23:DB:154:U:H2'   | 23:DB:155:A:C8    | 2.51        | 0.46     |
| 23:DB:17:G:H2'    | 23:DB:18:U:H6     | 1.81        | 0.46     |
| 23:BB:2626:C:O2'  | 23:BB:2627:G:H5'  | 2.15        | 0.46     |
| 23:BB:1590:A:H2'  | 23:BB:1591:A:H8   | 1.79        | 0.46     |
| 23:BB:1591:A:H2'  | 23:BB:1592:C:C6   | 2.51        | 0.46     |
| 20:AB:63:LYS:HB3  | 20:AB:87:ASP:OD2  | 2.16        | 0.46     |
| 23:DB:2626:C:O2'  | 23:DB:2627:G:H5'  | 2.15        | 0.46     |
| 53:D6:64:ARG:N    | 53:D6:64:ARG:HD2  | 2.31        | 0.46     |
| 1:AA:1461:G:O2'   | 1:AA:1462:C:H5'   | 2.15        | 0.46     |
| 6:CG:91:ARG:HD2   | 6:CG:91:ARG:N     | 2.31        | 0.46     |
| 23:DB:1316:U:H2'  | 23:DB:1317:G:H8   | 1.81        | 0.46     |
| 23:DB:779:U:H2'   | 23:DB:780:G:C8    | 2.51        | 0.46     |
| 23:BB:741:U:H2'   | 23:BB:742:A:H8    | 1.80        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:1278:G:H4'   | 1:CA:1279:G:H5'   | 1.97        | 0.46     |
| 42:DN:58:ASP:OD2  | 42:DN:63:ARG:NH2  | 2.49        | 0.46     |
| 30:DY:29:ARG:HB2  | 30:DY:33:HIS:HD2  | 1.81        | 0.46     |
| 27:DK:76:VAL:HG12 | 27:DK:77:ILE:N    | 2.31        | 0.46     |
| 1:AA:513:C:H2'    | 1:AA:514:C:C6     | 2.50        | 0.46     |
| 23:BB:528:A:C2    | 23:BB:2043:C:H4'  | 2.51        | 0.46     |
| 28:DP:77:SER:O    | 28:DP:80:VAL:HG12 | 2.15        | 0.46     |
| 2:AC:13:ILE:C     | 2:AC:15:LYS:H     | 2.18        | 0.46     |
| 23:DB:236:C:O2'   | 23:DB:237:C:H5'   | 2.16        | 0.46     |
| 23:BB:2648:G:H2'  | 23:BB:2649:C:H6   | 1.79        | 0.46     |
| 23:DB:2730:C:H2'  | 23:DB:2731:G:H8   | 1.81        | 0.46     |
| 37:BL:131:ALA:C   | 37:BL:133:ALA:N   | 2.69        | 0.46     |
| 5:AF:18:VAL:HG21  | 5:AF:58:HIS:CE1   | 2.50        | 0.46     |
| 23:DB:370:G:O2'   | 23:DB:423:A:H3'   | 2.15        | 0.46     |
| 27:DK:25:LEU:HD11 | 27:DK:40:LYS:N    | 2.30        | 0.46     |
| 46:DU:18:LYS:O    | 46:DU:20:LYS:N    | 2.48        | 0.46     |
| 1:CA:624:C:H2'    | 1:CA:625:U:H6     | 1.81        | 0.46     |
| 1:AA:224:U:H2'    | 1:AA:225:C:C6     | 2.51        | 0.46     |
| 25:BC:20:ASN:O    | 25:BC:23:LEU:HD13 | 2.16        | 0.46     |
| 5:AF:46:GLN:NE2   | 5:AF:46:GLN:HA    | 2.31        | 0.46     |
| 23:DB:729:G:C5    | 25:DC:206:LYS:HB2 | 2.51        | 0.46     |
| 1:CA:1409:C:H2'   | 1:CA:1410:A:C8    | 2.51        | 0.46     |
| 46:BU:98:ASN:OD1  | 46:BU:100:GLU:HB2 | 2.15        | 0.46     |
| 23:DB:2515:C:O2'  | 23:DB:2516:A:H5'  | 2.15        | 0.46     |
| 23:DB:1956:U:O2   | 23:DB:1985:C:H4'  | 2.16        | 0.46     |
| 23:BB:1035:U:H2'  | 23:BB:1036:G:H8   | 1.81        | 0.46     |
| 23:DB:1228:G:H2'  | 23:DB:1229:C:H6   | 1.81        | 0.46     |
| 26:BD:16:THR:O    | 28:BP:78:PRO:HG2  | 2.16        | 0.46     |
| 23:DB:1892:C:O2'  | 23:DB:1893:C:H5'  | 2.16        | 0.46     |
| 40:DH:40:THR:O    | 40:DH:42:LYS:N    | 2.48        | 0.46     |
| 23:DB:1435:G:H2'  | 23:DB:1436:G:H8   | 1.81        | 0.46     |
| 23:BB:1924:C:O2'  | 23:BB:1925:C:H5'  | 2.15        | 0.46     |
| 24:BI:72:THR:HG21 | 24:BI:111:THR:O   | 2.16        | 0.46     |
| 25:DC:24:HIS:CE1  | 25:DC:26:GLY:H    | 2.34        | 0.46     |
| 1:CA:610:U:O4'    | 1:CA:610:U:O2     | 2.33        | 0.46     |
| 23:DB:1385:A:O2'  | 23:DB:1396:U:H6   | 1.99        | 0.46     |
| 25:DC:9:SER:HB2   | 25:DC:10:PRO:HD2  | 1.98        | 0.46     |
| 29:BE:200:LEU:O   | 29:BE:201:ALA:HB3 | 2.15        | 0.46     |
| 52:BW:23:LYS:HD2  | 52:BW:24:ARG:H    | 1.81        | 0.46     |
| 48:BG:112:VAL:O   | 48:BG:113:ASP:HB2 | 2.15        | 0.46     |
| 37:DL:141:LYS:HZ3 | 37:DL:143:GLU:HA  | 1.81        | 0.46     |
| 48:DG:88:LEU:O    | 48:DG:88:LEU:HD12 | 2.16        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 53:B6:52:LEU:HA   | 53:B6:55:ILE:CG2   | 2.46        | 0.46     |
| 40:BH:132:PHE:HB2 | 40:BH:142:VAL:CG2  | 2.45        | 0.46     |
| 8:CI:75:ALA:HA    | 8:CI:78:ILE:HD12   | 1.98        | 0.46     |
| 47:DF:43:ILE:HB   | 47:DF:82:TYR:CZ    | 2.51        | 0.46     |
| 23:DB:673:C:H4'   | 29:DE:77:ILE:HD11  | 1.96        | 0.46     |
| 27:DK:29:HIS:O    | 27:DK:30:ARG:C     | 2.54        | 0.46     |
| 46:BU:3:LYS:NZ    | 46:BU:82:VAL:HB    | 2.30        | 0.46     |
| 22:BA:27:C:C2'    | 22:BA:28:C:H5'     | 2.46        | 0.46     |
| 24:DI:78:LEU:HD23 | 24:DI:81:LYS:HE2   | 1.97        | 0.46     |
| 9:CJ:53:ILE:HG23  | 9:CJ:54:SER:N      | 2.31        | 0.46     |
| 47:BF:111:ARG:HE  | 47:BF:135:ILE:HG22 | 1.81        | 0.46     |
| 47:BF:138:PRO:HA  | 47:BF:142:TYR:CE2  | 2.51        | 0.46     |
| 47:BF:113:PHE:CZ  | 47:BF:175:PRO:HB2  | 2.51        | 0.46     |
| 2:CC:80:GLY:O     | 2:CC:84:GLU:HB2    | 2.16        | 0.46     |
| 24:BI:32:VAL:HG13 | 24:BI:66:PHE:CD2   | 2.50        | 0.46     |
| 18:CS:44:ILE:HA   | 18:CS:61:VAL:CG1   | 2.46        | 0.46     |
| 23:DB:138:U:H2'   | 23:DB:140:C:O4'    | 2.16        | 0.46     |
| 23:BB:2466:C:OP1  | 32:B4:4:ARG:HB3    | 2.15        | 0.46     |
| 32:B4:16:ILE:HG12 | 32:B4:25:VAL:HG22  | 1.97        | 0.46     |
| 23:DB:26:G:H1'    | 23:DB:514:A:H61    | 1.81        | 0.46     |
| 38:DM:65:ILE:HG23 | 38:DM:103:TYR:CE2  | 2.51        | 0.46     |
| 2:AC:11:LEU:HD11  | 13:AN:87:ALA:O     | 2.16        | 0.46     |
| 23:DB:2848:G:H1'  | 23:DB:2868:A:N6    | 2.31        | 0.46     |
| 35:DV:83:LYS:O    | 35:DV:85:LYS:N     | 2.49        | 0.46     |
| 48:BG:163:TYR:O   | 48:BG:165:ASP:N    | 2.49        | 0.46     |
| 24:BI:126:ARG:HA  | 24:BI:129:GLU:OE2  | 2.16        | 0.46     |
| 9:CJ:76:ILE:HD12  | 9:CJ:76:ILE:O      | 2.16        | 0.46     |
| 5:CF:5:GLU:HA     | 5:CF:63:ASN:HA     | 1.98        | 0.46     |
| 1:AA:311:C:O2'    | 1:AA:312:C:H5'     | 2.16        | 0.46     |
| 40:BH:69:ALA:HA   | 40:BH:141:LYS:HZ2  | 1.81        | 0.46     |
| 49:DR:39:LEU:CA   | 49:DR:53:PHE:HA    | 2.43        | 0.46     |
| 1:CA:116:A:H2'    | 1:CA:117:G:O4'     | 2.16        | 0.46     |
| 23:BB:1309:G:OP1  | 36:B2:9:VAL:N      | 2.48        | 0.46     |
| 9:CJ:12:ALA:HB3   | 9:CJ:18:ILE:HB     | 1.97        | 0.46     |
| 1:AA:1074:G:C1'   | 20:AB:102:ASN:HB2  | 2.46        | 0.46     |
| 2:AC:155:ARG:H    | 2:AC:162:ALA:HA    | 1.81        | 0.46     |
| 12:CM:89:ARG:CB   | 12:CM:96:VAL:HG22  | 2.46        | 0.46     |
| 23:DB:858:G:H21   | 23:DB:2268:A:H3'   | 1.81        | 0.46     |
| 1:CA:236:A:H2'    | 1:CA:237:G:C8      | 2.50        | 0.46     |
| 7:CH:65:PHE:CE2   | 7:CH:66:GLN:HG3    | 2.51        | 0.46     |
| 7:AH:7:ALA:O      | 7:AH:11:THR:HG23   | 2.16        | 0.46     |
| 23:BB:558:U:O3'   | 41:BJ:111:LYS:HD3  | 2.15        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:646:U:H3'   | 23:BB:647:G:H8     | 1.81        | 0.46     |
| 23:DB:1597:A:C5'  | 23:DB:1598:A:H5'   | 2.42        | 0.46     |
| 1:CA:803:G:H2'    | 1:CA:804:U:H6      | 1.80        | 0.46     |
| 23:BB:1386:C:H1'  | 23:BB:1470:A:H1'   | 1.97        | 0.46     |
| 23:DB:2840:C:O2'  | 23:DB:2841:C:H5'   | 2.15        | 0.46     |
| 1:AA:803:G:H2'    | 1:AA:804:U:C6      | 2.51        | 0.46     |
| 23:DB:1685:C:O2'  | 23:DB:1686:C:H5'   | 2.15        | 0.46     |
| 23:DB:1404:C:O2'  | 23:DB:1405:U:H5'   | 2.16        | 0.46     |
| 1:CA:828:U:O2'    | 20:CB:24:PRO:HB3   | 2.16        | 0.46     |
| 23:BB:2415:G:C4'  | 37:BL:66:PHE:HB2   | 2.45        | 0.46     |
| 22:DA:6:G:H2'     | 22:DA:7:G:C8       | 2.51        | 0.46     |
| 1:AA:505:G:H2'    | 1:AA:506:G:C8      | 2.50        | 0.46     |
| 39:DX:33:ALA:CB   | 50:DT:14:PRO:HD2   | 2.46        | 0.46     |
| 20:AB:22:TRP:CG   | 20:AB:23:ASN:N     | 2.82        | 0.46     |
| 43:BO:6:ALA:HB1   | 43:BO:10:ARG:HH11  | 1.81        | 0.46     |
| 23:DB:2606:C:O2'  | 23:DB:2607:G:H5'   | 2.16        | 0.46     |
| 28:DP:101:GLU:OE2 | 28:DP:101:GLU:N    | 2.48        | 0.46     |
| 23:BB:1918:A:O2'  | 23:BB:1920:C:C4    | 2.68        | 0.46     |
| 23:DB:480:A:H3'   | 23:DB:481:G:H5''   | 1.98        | 0.46     |
| 23:DB:2785:C:H2'  | 23:DB:2786:U:C6    | 2.51        | 0.46     |
| 25:DC:221:GLY:O   | 25:DC:223:ALA:N    | 2.49        | 0.46     |
| 1:CA:205:A:H2'    | 1:CA:206:C:O4'     | 2.16        | 0.46     |
| 27:DK:107:LEU:C   | 27:DK:109:SER:H    | 2.18        | 0.46     |
| 29:BE:102:ARG:HG3 | 29:BE:102:ARG:HH21 | 1.81        | 0.46     |
| 1:CA:728:A:H2'    | 1:CA:729:A:C8      | 2.51        | 0.46     |
| 23:BB:1640:A:H2'  | 23:BB:1641:A:H8    | 1.79        | 0.46     |
| 1:CA:448:A:H2'    | 1:CA:449:G:H8      | 1.80        | 0.46     |
| 23:BB:2677:G:H2'  | 23:BB:2678:C:H6    | 1.79        | 0.46     |
| 6:AG:72:VAL:HA    | 6:AG:89:GLU:HA     | 1.98        | 0.46     |
| 23:DB:1031:G:C4'  | 32:D4:6:SER:HB3    | 2.45        | 0.46     |
| 41:DJ:88:THR:HG22 | 41:DJ:91:GLU:OE1   | 2.16        | 0.46     |
| 2:AC:176:THR:HB   | 2:AC:179:ALA:HB2   | 1.96        | 0.46     |
| 23:BB:2213:U:O2   | 23:BB:2213:U:H2'   | 2.15        | 0.46     |
| 46:DU:66:VAL:C    | 46:DU:68:ASN:H     | 2.19        | 0.46     |
| 28:BP:64:SER:O    | 28:BP:66:GLY:N     | 2.48        | 0.46     |
| 23:DB:1693:U:O2'  | 25:DC:13:ARG:NH2   | 2.49        | 0.46     |
| 1:AA:960:U:O2'    | 1:AA:1223:C:H4'    | 2.16        | 0.46     |
| 1:AA:223:A:H2'    | 1:AA:224:U:C6      | 2.51        | 0.46     |
| 1:AA:624:C:H2'    | 1:AA:625:U:H6      | 1.79        | 0.46     |
| 52:DW:47:GLY:HA3  | 52:DW:80:SER:CB    | 2.46        | 0.46     |
| 50:BT:15:HIS:O    | 50:BT:16:VAL:C     | 2.53        | 0.46     |
| 26:DD:61:THR:O    | 26:DD:64:GLU:HB2   | 2.15        | 0.46     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:BB:685:A:H1'    | 23:BB:688:U:O4    | 2.16        | 0.46     |
| 23:DB:802:A:H4'    | 57:DB:3287:HOH:O  | 2.15        | 0.46     |
| 40:BH:11:ASN:O     | 40:BH:12:LEU:HB3  | 2.15        | 0.46     |
| 20:AB:131:LYS:O    | 20:AB:135:MET:HB2 | 2.16        | 0.46     |
| 7:AH:74:ILE:O      | 7:AH:74:ILE:HG23  | 2.16        | 0.46     |
| 1:AA:95:C:H2'      | 1:AA:95:C:O2      | 2.16        | 0.46     |
| 23:DB:2693:G:H2'   | 23:DB:2694:G:H8   | 1.80        | 0.46     |
| 2:CC:57:GLU:HB2    | 2:CC:64:ARG:HB2   | 1.97        | 0.46     |
| 23:BB:2545:G:O2'   | 23:BB:2546:U:H5'  | 2.15        | 0.46     |
| 38:BM:54:THR:C     | 38:BM:56:ALA:H    | 2.20        | 0.46     |
| 24:DI:2:LYS:O      | 24:DI:3:LYS:HG3   | 2.16        | 0.46     |
| 2:AC:190:THR:CG2   | 2:AC:191:THR:N    | 2.78        | 0.46     |
| 10:CK:126:ARG:NE   | 10:CK:126:ARG:HA  | 2.30        | 0.46     |
| 52:DW:19:ARG:HD3   | 52:DW:36:ILE:HD11 | 1.98        | 0.46     |
| 25:DC:131:MET:CE   | 25:DC:189:ALA:HB2 | 2.46        | 0.46     |
| 37:DL:124:GLY:H    | 37:DL:143:GLU:HG3 | 1.75        | 0.46     |
| 40:BH:133:GLN:NE2  | 40:BH:135:HIS:O   | 2.49        | 0.46     |
| 23:DB:2313:C:H4'   | 47:DF:87:LYS:HB3  | 1.98        | 0.46     |
| 8:CI:22:PRO:HA     | 8:CI:60:LEU:HB2   | 1.97        | 0.46     |
| 41:DJ:44:TYR:CD2   | 41:DJ:44:TYR:C    | 2.88        | 0.46     |
| 41:DJ:24:THR:O     | 41:DJ:25:LEU:HB3  | 2.16        | 0.46     |
| 13:CN:13:VAL:HG22  | 13:CN:59:GLN:HG2  | 1.97        | 0.46     |
| 46:DU:5:ARG:NH2    | 46:DU:93:ARG:HD3  | 2.31        | 0.46     |
| 40:DH:127:GLU:HA   | 40:DH:144:VAL:O   | 2.16        | 0.46     |
| 23:BB:78:U:H2'     | 23:BB:79:C:C6     | 2.50        | 0.46     |
| 47:BF:100:GLU:O    | 47:BF:104:THR:HB  | 2.15        | 0.46     |
| 29:BE:126:VAL:HG22 | 29:BE:127:GLU:H   | 1.80        | 0.46     |
| 1:AA:764:C:H2'     | 1:AA:765:G:C5'    | 2.46        | 0.46     |
| 47:DF:137:PHE:CD2  | 47:DF:137:PHE:N   | 2.84        | 0.46     |
| 1:CA:1361:G:N2     | 1:CA:1362:A:N7    | 2.64        | 0.46     |
| 23:DB:670:A:H4'    | 23:DB:671:C:C5'   | 2.37        | 0.46     |
| 18:AS:44:ILE:O     | 18:AS:44:ILE:HG23 | 2.16        | 0.46     |
| 50:DT:57:VAL:HG22  | 50:DT:58:VAL:N    | 2.21        | 0.46     |
| 22:DA:97:C:H2'     | 22:DA:98:G:H5'    | 1.98        | 0.46     |
| 46:BU:47:PRO:HB3   | 46:BU:55:GLY:CA   | 2.46        | 0.46     |
| 38:DM:103:TYR:HB2  | 38:DM:117:PHE:CE1 | 2.51        | 0.46     |
| 23:BB:2886:A:H3'   | 23:BB:2887:A:C8   | 2.46        | 0.46     |
| 1:AA:1269:A:H2     | 1:AA:1312:G:N3    | 2.13        | 0.46     |
| 43:BO:58:ILE:HG22  | 43:BO:62:LEU:CD2  | 2.40        | 0.46     |
| 20:CB:57:ASN:HD22  | 20:CB:223:GLY:CA  | 2.29        | 0.46     |
| 1:AA:1001:C:H2'    | 1:AA:1002:G:H8    | 1.79        | 0.46     |
| 27:DK:58:LEU:H     | 27:DK:58:LEU:HD23 | 1.81        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 26:BD:113:SER:HB3 | 26:BD:167:ASN:H    | 1.78        | 0.46     |
| 26:BD:113:SER:HB3 | 26:BD:167:ASN:HA   | 1.97        | 0.46     |
| 23:DB:322:A:C2    | 23:DB:340:A:C6     | 3.03        | 0.46     |
| 46:BU:11:ILE:O    | 46:BU:11:ILE:HD13  | 2.16        | 0.46     |
| 3:AD:196:GLU:O    | 3:AD:200:VAL:HG13  | 2.16        | 0.46     |
| 4:CE:80:LEU:CD1   | 4:CE:95:MET:HB3    | 2.46        | 0.46     |
| 11:AL:33:CYS:N    | 11:AL:54:VAL:HG13  | 2.30        | 0.46     |
| 35:DV:42:LEU:H    | 35:DV:42:LEU:CD2   | 2.21        | 0.46     |
| 9:CJ:37:ARG:CZ    | 9:CJ:37:ARG:HA     | 2.46        | 0.46     |
| 23:BB:2345:G:H4'  | 23:BB:2346:A:O5'   | 2.16        | 0.46     |
| 34:B3:60:CYS:C    | 34:B3:62:PRO:HD3   | 2.36        | 0.46     |
| 1:AA:926:G:H3'    | 1:AA:1505:G:H21    | 1.80        | 0.46     |
| 23:BB:2000:C:O2'  | 23:BB:2001:C:H5'   | 2.16        | 0.46     |
| 23:DB:2460:U:O2'  | 23:DB:2461:A:H5'   | 2.15        | 0.46     |
| 23:BB:2028:U:O2'  | 23:BB:2029:G:H5'   | 2.15        | 0.46     |
| 25:BC:244:VAL:HA  | 25:BC:249:VAL:O    | 2.16        | 0.46     |
| 23:DB:876:C:N3    | 23:DB:901:C:N4     | 2.63        | 0.46     |
| 1:CA:378:G:H2'    | 1:CA:379:C:C6      | 2.51        | 0.46     |
| 16:CQ:31:PRO:O    | 16:CQ:32:ILE:HB    | 2.16        | 0.46     |
| 1:CA:1037:C:H2'   | 1:CA:1038:C:H6     | 1.81        | 0.46     |
| 48:BG:38:ASP:CG   | 48:BG:39:ALA:N     | 2.68        | 0.46     |
| 23:DB:314:C:O2'   | 23:DB:315:G:H5'    | 2.16        | 0.46     |
| 23:BB:1535:A:O2'  | 23:BB:1536:C:H5'   | 2.16        | 0.46     |
| 29:BE:122:GLU:O   | 29:BE:123:LYS:CB   | 2.62        | 0.46     |
| 23:DB:2543:G:H2'  | 23:DB:2544:G:H8    | 1.79        | 0.46     |
| 1:AA:386:C:C2'    | 1:AA:387:U:H5'     | 2.46        | 0.46     |
| 47:DF:120:SER:OG  | 47:DF:129:MET:HB3  | 2.16        | 0.46     |
| 2:AC:179:ALA:HB3  | 2:AC:181:ILE:HD11  | 1.97        | 0.46     |
| 1:CA:912:C:O2'    | 1:CA:913:A:H5'     | 2.16        | 0.46     |
| 23:DB:335:C:O2'   | 23:DB:336:C:H5'    | 2.16        | 0.46     |
| 8:CI:11:ARG:CZ    | 8:CI:106:ASP:OD1   | 2.64        | 0.46     |
| 23:BB:437:U:H2'   | 23:BB:438:G:C8     | 2.50        | 0.46     |
| 23:DB:2420:C:O2'  | 23:DB:2421:G:H5'   | 2.16        | 0.46     |
| 23:BB:902:C:H2'   | 23:BB:903:C:H6     | 1.81        | 0.46     |
| 1:AA:559:A:H5'    | 57:AA:1807:HOH:O   | 2.16        | 0.46     |
| 48:BG:77:GLY:HA3  | 48:BG:135:ALA:O    | 2.16        | 0.46     |
| 53:D6:24:ASN:HB3  | 53:D6:121:TYR:CE1  | 2.51        | 0.46     |
| 45:DS:4:ILE:CG2   | 45:DS:106:VAL:HG22 | 2.46        | 0.46     |
| 23:BB:1344:U:H4'  | 23:BB:1384:A:C5    | 2.51        | 0.46     |
| 23:BB:2563:U:H2'  | 23:BB:2565:A:OP2   | 2.16        | 0.46     |
| 5:AF:10:VAL:HG12  | 5:AF:11:HIS:N      | 2.31        | 0.46     |
| 23:BB:2611:C:O2'  | 23:BB:2612:C:H5'   | 2.15        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:656:G:O2'    | 1:CA:657:U:H5'     | 2.16        | 0.46     |
| 23:DB:1908:C:O2'  | 23:DB:1909:C:H5'   | 2.16        | 0.46     |
| 3:CD:43:ARG:HH11  | 3:CD:43:ARG:HB3    | 1.80        | 0.46     |
| 5:CF:17:GLN:O     | 5:CF:21:MET:HG3    | 2.16        | 0.46     |
| 23:DB:1098:A:H2'  | 24:DI:3:LYS:C      | 2.37        | 0.45     |
| 25:DC:141:HIS:CG  | 25:DC:142:ASN:H    | 2.32        | 0.45     |
| 25:DC:52:HIS:O    | 25:DC:53:ILE:HB    | 2.16        | 0.45     |
| 48:BG:94:ARG:HH21 | 48:BG:104:LEU:HA   | 1.81        | 0.45     |
| 5:CF:3:HIS:ND1    | 5:CF:95:ALA:HB2    | 2.31        | 0.45     |
| 23:DB:921:C:H2'   | 23:DB:922:C:H6     | 1.80        | 0.45     |
| 35:DV:1:MET:CE    | 35:DV:2:PHE:H      | 2.29        | 0.45     |
| 25:BC:115:ILE:HA  | 25:BC:127:ASN:OD1  | 2.15        | 0.45     |
| 25:BC:75:ALA:CB   | 25:BC:93:VAL:HG22  | 2.46        | 0.45     |
| 35:BV:1:MET:HE2   | 35:BV:2:PHE:H      | 1.80        | 0.45     |
| 35:BV:62:THR:CB   | 35:BV:71:LYS:HG2   | 2.44        | 0.45     |
| 41:DJ:25:LEU:HB2  | 41:DJ:62:VAL:CG2   | 2.46        | 0.45     |
| 47:DF:74:ALA:HB3  | 47:DF:77:LYS:O     | 2.16        | 0.45     |
| 13:CN:70:HIS:O    | 13:CN:71:GLY:C     | 2.54        | 0.45     |
| 38:BM:24:THR:HG23 | 38:BM:34:LYS:CE    | 2.46        | 0.45     |
| 47:DF:3:LEU:HD11  | 47:DF:172:PHE:CD1  | 2.51        | 0.45     |
| 53:D6:46:TYR:OH   | 53:D6:74:ASN:HB3   | 2.15        | 0.45     |
| 1:CA:17:U:H4'     | 1:CA:1079:G:O2'    | 2.16        | 0.45     |
| 23:BB:1018:U:O2'  | 23:BB:1019:U:H5'   | 2.16        | 0.45     |
| 33:D1:33:LEU:HD12 | 33:D1:34:GLU:N     | 2.32        | 0.45     |
| 29:DE:33:VAL:O    | 29:DE:36:ALA:HB3   | 2.16        | 0.45     |
| 23:BB:2886:A:H62  | 31:B0:39:ARG:CD    | 2.29        | 0.45     |
| 9:CJ:51:VAL:HG22  | 13:CN:80:ARG:HB2   | 1.98        | 0.45     |
| 53:D6:111:ARG:O   | 53:D6:115:VAL:HG22 | 2.15        | 0.45     |
| 53:B6:17:SER:O    | 53:B6:20:VAL:HB    | 2.16        | 0.45     |
| 27:DK:79:PHE:CD2  | 28:DP:69:VAL:HG12  | 2.51        | 0.45     |
| 23:BB:970:U:H1'   | 23:BB:985:C:P      | 2.56        | 0.45     |
| 23:BB:589:U:H2'   | 23:BB:590:A:H8     | 1.80        | 0.45     |
| 23:BB:591:U:O2'   | 23:BB:592:A:H5'    | 2.16        | 0.45     |
| 20:AB:216:VAL:O   | 20:AB:220:VAL:HG23 | 2.16        | 0.45     |
| 5:CF:4:TYR:CE2    | 5:CF:71:ILE:HG21   | 2.51        | 0.45     |
| 23:DB:2886:A:H62  | 31:D0:39:ARG:CZ    | 2.28        | 0.45     |
| 49:DR:1:MET:HG3   | 49:DR:101:ILE:HG21 | 1.98        | 0.45     |
| 7:AH:58:LEU:O     | 7:AH:60:LEU:N      | 2.48        | 0.45     |
| 23:DB:30:G:OP1    | 44:DQ:4:LYS:HG2    | 2.15        | 0.45     |
| 11:AL:51:VAL:HG12 | 11:AL:52:CYS:N     | 2.25        | 0.45     |
| 20:AB:148:GLY:C   | 20:AB:150:ILE:H    | 2.19        | 0.45     |
| 1:CA:1239:A:H4'   | 1:CA:1240:U:C5'    | 2.47        | 0.45     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:173:A:H2'   | 23:DB:174:U:H6     | 1.81        | 0.45     |
| 46:DU:26:ASN:ND2  | 46:DU:34:ILE:HD12  | 2.30        | 0.45     |
| 5:AF:98:GLU:CG    | 5:AF:99:ALA:N      | 2.74        | 0.45     |
| 39:BX:20:ASN:H    | 39:BX:20:ASN:HD22  | 1.63        | 0.45     |
| 27:BK:87:LEU:HB2  | 27:BK:93:GLN:C     | 2.36        | 0.45     |
| 23:BB:720:U:O2'   | 23:BB:721:A:H5'    | 2.16        | 0.45     |
| 3:CD:169:TRP:CD1  | 3:CD:170:LEU:HD23  | 2.50        | 0.45     |
| 38:BM:40:ARG:HB2  | 38:BM:93:VAL:HG21  | 1.99        | 0.45     |
| 23:BB:1597:A:C5'  | 23:BB:1598:A:H5'   | 2.45        | 0.45     |
| 1:CA:1270:G:H2'   | 1:CA:1271:A:C8     | 2.51        | 0.45     |
| 49:BR:2:TYR:HB2   | 49:BR:42:ALA:CB    | 2.46        | 0.45     |
| 23:DB:2843:G:O2'  | 23:DB:2844:G:H5'   | 2.15        | 0.45     |
| 1:CA:1330:U:C2'   | 1:CA:1331:G:H5'    | 2.46        | 0.45     |
| 23:DB:2449:U:H4'  | 23:DB:2450:A:OP1   | 2.16        | 0.45     |
| 3:AD:77:GLU:O     | 3:AD:81:LEU:HG     | 2.16        | 0.45     |
| 41:DJ:96:ARG:CZ   | 41:DJ:99:ARG:HD2   | 2.45        | 0.45     |
| 26:BD:15:PHE:N    | 26:BD:15:PHE:CD1   | 2.81        | 0.45     |
| 37:DL:129:LYS:HA  | 37:DL:132:ARG:CD   | 2.46        | 0.45     |
| 1:CA:821:G:O2'    | 1:CA:822:U:H5'     | 2.15        | 0.45     |
| 1:AA:159:G:H5'    | 1:AA:160:A:OP2     | 2.16        | 0.45     |
| 29:BE:3:LEU:O     | 29:BE:12:LEU:HD23  | 2.16        | 0.45     |
| 23:DB:728:G:O2'   | 23:DB:730:A:H8     | 1.98        | 0.45     |
| 33:B1:28:THR:O    | 33:B1:29:LYS:HD2   | 2.16        | 0.45     |
| 26:BD:16:THR:HG22 | 26:BD:17:GLU:H     | 1.80        | 0.45     |
| 23:DB:2256:G:H2'  | 23:DB:2257:U:H6    | 1.81        | 0.45     |
| 29:DE:4:VAL:HG12  | 29:DE:6:LYS:H      | 1.81        | 0.45     |
| 23:DB:2081:U:H2'  | 23:DB:2082:A:C8    | 2.51        | 0.45     |
| 48:DG:60:GLY:O    | 48:DG:62:ALA:N     | 2.49        | 0.45     |
| 23:DB:1568:G:H4'  | 25:DC:58:LYS:HB3   | 1.97        | 0.45     |
| 23:DB:1360:G:H2'  | 23:DB:1361:G:O4'   | 2.17        | 0.45     |
| 23:DB:1733:G:H2'  | 23:DB:1734:G:C8    | 2.51        | 0.45     |
| 41:DJ:98:GLU:CD   | 41:DJ:98:GLU:H     | 2.19        | 0.45     |
| 29:DE:73:ILE:HG12 | 29:DE:73:ILE:O     | 2.16        | 0.45     |
| 26:BD:27:ILE:HG23 | 26:BD:201:LEU:HD12 | 1.98        | 0.45     |
| 23:BB:1956:U:O2   | 23:BB:1985:C:H4'   | 2.16        | 0.45     |
| 15:CP:22:ALA:HA   | 15:CP:33:ILE:HG13  | 1.97        | 0.45     |
| 23:BB:1123:C:O2'  | 23:BB:1124:G:H5'   | 2.16        | 0.45     |
| 23:DB:1099:G:C8   | 24:DI:3:LYS:CB     | 2.99        | 0.45     |
| 52:BW:49:ASN:HB2  | 52:BW:61:LYS:N     | 2.26        | 0.45     |
| 25:DC:151:GLY:C   | 25:DC:152:GLN:HG3  | 2.37        | 0.45     |
| 44:DQ:23:TYR:HB2  | 44:DQ:27:ARG:HB3   | 1.99        | 0.45     |
| 37:BL:141:LYS:HD3 | 37:BL:141:LYS:C    | 2.36        | 0.45     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 16:CQ:60:ILE:HG12  | 16:CQ:72:TRP:HE3   | 1.80        | 0.45     |
| 8:AI:20:ILE:HD13   | 8:AI:85:ALA:CB     | 2.44        | 0.45     |
| 8:AI:83:THR:OG1    | 8:AI:97:LEU:HD13   | 2.14        | 0.45     |
| 35:DV:32:GLY:C     | 35:DV:93:ARG:HG3   | 2.36        | 0.45     |
| 37:DL:77:ILE:HB    | 37:DL:109:LYS:O    | 2.17        | 0.45     |
| 22:DA:28:C:C5      | 22:DA:56:G:C2      | 3.04        | 0.45     |
| 30:DY:6:ILE:HG21   | 30:DY:47:ILE:HD12  | 1.97        | 0.45     |
| 50:BT:40:LYS:HD3   | 50:BT:58:VAL:O     | 2.16        | 0.45     |
| 1:CA:429:U:H3'     | 3:CD:8:LEU:CD2     | 2.41        | 0.45     |
| 12:AM:109:LYS:HG3  | 12:AM:110:GLY:N    | 2.30        | 0.45     |
| 23:DB:1059:G:H2'   | 23:DB:1060:U:C5    | 2.51        | 0.45     |
| 23:BB:2308:G:O6    | 23:BB:2311:A:N7    | 2.49        | 0.45     |
| 38:BM:35:ALA:C     | 38:BM:37:GLY:H     | 2.20        | 0.45     |
| 1:CA:978:A:H5'     | 1:CA:1362:A:H61    | 1.77        | 0.45     |
| 18:CS:39:ILE:HG13  | 18:CS:68:HIS:O     | 2.16        | 0.45     |
| 23:DB:137:U:H1'    | 50:DT:1:MET:H2     | 1.80        | 0.45     |
| 50:DT:10:VAL:O     | 50:DT:11:LEU:C     | 2.54        | 0.45     |
| 53:D6:181:GLN:O    | 53:D6:184:LEU:N    | 2.49        | 0.45     |
| 45:DS:27:LYS:CD    | 45:DS:27:LYS:H     | 2.28        | 0.45     |
| 53:B6:184:LEU:O    | 53:B6:184:LEU:HD23 | 2.16        | 0.45     |
| 11:CL:42:LYS:HB2   | 11:CL:88:ASP:HA    | 1.98        | 0.45     |
| 11:CL:86:VAL:CG1   | 11:CL:89:LEU:HD23  | 2.46        | 0.45     |
| 13:CN:52:ARG:HD2   | 13:CN:58:ARG:HH21  | 1.80        | 0.45     |
| 23:DB:1082:U:C2    | 23:DB:1086:A:N1    | 2.84        | 0.45     |
| 27:BK:29:HIS:O     | 27:BK:30:ARG:C     | 2.53        | 0.45     |
| 23:DB:2105:U:H2'   | 23:DB:2106:U:C6    | 2.50        | 0.45     |
| 45:DS:66:ILE:HG12  | 45:DS:67:ASP:N     | 2.31        | 0.45     |
| 44:BQ:9:ALA:C      | 44:BQ:11:ALA:N     | 2.69        | 0.45     |
| 27:BK:99:ILE:HG12  | 27:BK:115:ILE:HG13 | 1.97        | 0.45     |
| 37:DL:96:LYS:HE2   | 37:DL:102:GLY:O    | 2.16        | 0.45     |
| 34:B3:16:THR:HG21  | 34:B3:48:MET:CE    | 2.46        | 0.45     |
| 24:DI:100:ILE:HG23 | 24:DI:104:GLN:OE1  | 2.16        | 0.45     |
| 24:DI:138:VAL:HG12 | 24:DI:139:VAL:N    | 2.31        | 0.45     |
| 26:DD:9:VAL:O      | 26:DD:9:VAL:HG22   | 2.16        | 0.45     |
| 26:BD:9:VAL:HG22   | 26:BD:9:VAL:O      | 2.16        | 0.45     |
| 1:CA:1299:A:C2'    | 1:CA:1301:U:H1'    | 2.43        | 0.45     |
| 20:AB:27:LYS:C     | 20:AB:27:LYS:HD2   | 2.37        | 0.45     |
| 2:AC:184:ASN:HD22  | 2:AC:185:THR:H     | 1.64        | 0.45     |
| 1:AA:264:C:H2'     | 1:AA:265:G:O4'     | 2.16        | 0.45     |
| 4:CE:82:HIS:CE1    | 4:CE:146:MET:HA    | 2.51        | 0.45     |
| 50:DT:31:VAL:HA    | 50:DT:84:TYR:H     | 1.80        | 0.45     |
| 5:CF:16:GLU:CD     | 5:CF:16:GLU:N      | 2.68        | 0.45     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1248:G:C5    | 29:DE:46:GLN:NE2   | 2.78        | 0.45     |
| 53:B6:140:LEU:HD23 | 53:B6:158:GLU:HG2  | 1.98        | 0.45     |
| 23:BB:2626:C:H2'   | 23:BB:2627:G:C8    | 2.51        | 0.45     |
| 39:BX:8:GLU:O      | 39:BX:12:GLU:HB2   | 2.16        | 0.45     |
| 1:CA:366:A:O2'     | 1:CA:394:G:N2      | 2.48        | 0.45     |
| 23:DB:1902:C:H2'   | 23:DB:1903:G:O4'   | 2.16        | 0.45     |
| 9:CJ:21:ALA:O      | 9:CJ:25:ILE:HG13   | 2.15        | 0.45     |
| 11:CL:33:CYS:N     | 11:CL:54:VAL:HG13  | 2.32        | 0.45     |
| 19:AT:85:LEU:HD23  | 19:AT:86:ALA:H     | 1.81        | 0.45     |
| 1:CA:1499:A:H2'    | 1:CA:1500:A:H8     | 1.81        | 0.45     |
| 37:BL:111:ILE:HD13 | 37:BL:128:THR:HG23 | 1.97        | 0.45     |
| 23:BB:1041:G:H2'   | 23:BB:1042:G:C8    | 2.51        | 0.45     |
| 53:D6:33:ALA:HB2   | 53:D6:63:PRO:HA    | 1.97        | 0.45     |
| 1:AA:389:A:H3'     | 1:AA:390:U:H6      | 1.81        | 0.45     |
| 23:DB:506:G:H1'    | 23:DB:507:A:C8     | 2.50        | 0.45     |
| 20:CB:129:THR:O    | 20:CB:131:LYS:N    | 2.48        | 0.45     |
| 1:AA:784:A:N6      | 1:AA:799:G:C6      | 2.84        | 0.45     |
| 23:BB:2813:A:H2'   | 23:BB:2814:A:H8    | 1.81        | 0.45     |
| 23:DB:707:G:O2'    | 23:DB:708:G:H5'    | 2.16        | 0.45     |
| 29:DE:18:THR:HG22  | 29:DE:106:LYS:HE2  | 1.97        | 0.45     |
| 23:BB:528:A:H3'    | 23:BB:528:A:H8     | 1.81        | 0.45     |
| 27:BK:109:SER:C    | 27:BK:111:LYS:H    | 2.19        | 0.45     |
| 23:DB:131:A:H2'    | 23:DB:132:G:C8     | 2.52        | 0.45     |
| 23:BB:1704:C:H2'   | 23:BB:1705:A:C8    | 2.52        | 0.45     |
| 10:CK:60:PHE:O     | 10:CK:63:GLN:HB3   | 2.16        | 0.45     |
| 23:DB:2300:C:H2'   | 23:DB:2301:C:H6    | 1.81        | 0.45     |
| 40:DH:30:LEU:O     | 40:DH:35:LYS:HB2   | 2.16        | 0.45     |
| 48:DG:4:ALA:HB3    | 48:DG:61:TRP:HZ3   | 1.80        | 0.45     |
| 23:DB:437:U:H2'    | 23:DB:438:G:C8     | 2.52        | 0.45     |
| 23:DB:2408:U:O2'   | 23:DB:2409:G:H5'   | 2.16        | 0.45     |
| 23:DB:2523:G:O2'   | 23:DB:2524:G:H5'   | 2.15        | 0.45     |
| 3:AD:12:ARG:O      | 3:AD:37:PRO:HG3    | 2.16        | 0.45     |
| 48:BG:66:THR:O     | 48:BG:70:LEU:HB2   | 2.16        | 0.45     |
| 9:AJ:67:ILE:HA     | 13:AN:94:GLY:O     | 2.16        | 0.45     |
| 23:DB:1987:A:O2'   | 23:DB:1988:G:H5'   | 2.16        | 0.45     |
| 23:BB:1733:G:H2'   | 23:BB:1734:G:C8    | 2.51        | 0.45     |
| 7:CH:62:LEU:HB3    | 7:CH:64:TYR:CE1    | 2.52        | 0.45     |
| 1:AA:1120:C:O2'    | 1:AA:1121:U:H5'    | 2.16        | 0.45     |
| 40:DH:9:VAL:HB     | 40:DH:12:LEU:O     | 2.16        | 0.45     |
| 23:DB:1544:A:H2'   | 23:DB:1545:A:C8    | 2.52        | 0.45     |
| 3:AD:57:LYS:C      | 3:AD:57:LYS:HD3    | 2.37        | 0.45     |
| 19:CT:77:ASN:O     | 19:CT:81:GLN:HG3   | 2.16        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:1426:G:O2'   | 1:AA:1427:C:H5'   | 2.16        | 0.45     |
| 42:BN:64:ARG:O    | 42:BN:67:PHE:HB3  | 2.16        | 0.45     |
| 23:DB:2049:G:O2'  | 23:DB:2050:C:H5'  | 2.15        | 0.45     |
| 23:DB:1799:G:N2   | 23:DB:1818:U:O2'  | 2.49        | 0.45     |
| 1:CA:1091:U:H5''  | 6:CG:3:ARG:NH2    | 2.32        | 0.45     |
| 20:AB:166:ASP:OD2 | 20:AB:190:SER:HA  | 2.17        | 0.45     |
| 52:DW:65:LYS:HG3  | 52:DW:84:GLU:CB   | 2.42        | 0.45     |
| 8:CI:38:PHE:HB3   | 8:CI:43:ALA:HB3   | 1.98        | 0.45     |
| 1:CA:1250:A:H2    | 1:CA:1370:G:H1'   | 1.81        | 0.45     |
| 8:AI:22:PRO:HA    | 8:AI:60:LEU:HB2   | 1.97        | 0.45     |
| 43:DO:34:HIS:HB3  | 43:DO:36:TYR:CE2  | 2.48        | 0.45     |
| 29:DE:61:ARG:HH12 | 29:DE:64:GLY:HA3  | 1.82        | 0.45     |
| 38:DM:24:THR:HG23 | 38:DM:34:LYS:CE   | 2.45        | 0.45     |
| 1:CA:1216:A:O2'   | 1:CA:1217:C:H5'   | 2.17        | 0.45     |
| 50:BT:11:LEU:CD2  | 50:BT:46:ALA:HB1  | 2.47        | 0.45     |
| 42:BN:38:LEU:HD11 | 42:BN:42:LYS:HD2  | 1.98        | 0.45     |
| 23:DB:1169:A:H2'  | 23:DB:1170:C:C6   | 2.50        | 0.45     |
| 47:DF:113:PHE:CE1 | 47:DF:116:LEU:HB2 | 2.51        | 0.45     |
| 10:AK:89:GLY:O    | 10:AK:92:ARG:HB2  | 2.17        | 0.45     |
| 4:CE:17:VAL:HA    | 4:CE:33:THR:O     | 2.16        | 0.45     |
| 45:BS:13:SER:CB   | 45:BS:16:LYS:HE3  | 2.46        | 0.45     |
| 1:AA:1316:G:OP2   | 1:AA:1316:G:H8    | 2.00        | 0.45     |
| 29:BE:32:VAL:HG23 | 29:BE:33:VAL:N    | 2.32        | 0.45     |
| 23:DB:2867:G:HO2' | 23:DB:2868:A:H8   | 1.63        | 0.45     |
| 5:CF:61:LEU:HD12  | 5:CF:63:ASN:OD1   | 2.17        | 0.45     |
| 11:CL:20:VAL:HB   | 11:CL:94:TYR:CE1  | 2.51        | 0.45     |
| 1:CA:723:U:O4'    | 21:CU:48:LYS:HD3  | 2.16        | 0.45     |
| 20:CB:148:GLY:C   | 20:CB:150:ILE:H   | 2.19        | 0.45     |
| 1:CA:33:A:O2'     | 1:CA:34:C:H5'     | 2.16        | 0.45     |
| 2:CC:112:ALA:HB1  | 2:CC:184:ASN:HB2  | 1.99        | 0.45     |
| 16:AQ:18:LYS:HG2  | 16:AQ:48:GLU:HA   | 1.98        | 0.45     |
| 23:BB:2794:C:O2'  | 23:BB:2795:C:H5'  | 2.16        | 0.45     |
| 1:CA:264:C:H4'    | 16:CQ:64:ARG:HD2  | 1.98        | 0.45     |
| 23:DB:355:U:H2'   | 23:DB:356:G:H8    | 1.80        | 0.45     |
| 1:AA:440:C:O2'    | 1:AA:441:A:H5'    | 2.15        | 0.45     |
| 23:DB:1509:A:C8   | 23:DB:1509:A:H5'' | 2.51        | 0.45     |
| 28:BP:50:ARG:O    | 28:BP:51:ASN:HB2  | 2.16        | 0.45     |
| 11:CL:13:ARG:HB2  | 11:CL:14:LYS:H    | 1.44        | 0.45     |
| 42:DN:97:ILE:HD12 | 42:DN:98:LEU:H    | 1.80        | 0.45     |
| 23:BB:2247:A:H2'  | 23:BB:2248:C:H6   | 1.81        | 0.45     |
| 23:BB:2492:U:O2'  | 23:BB:2493:U:H5'  | 2.15        | 0.45     |
| 40:BH:54:LEU:HA   | 40:BH:58:LEU:HB2  | 1.99        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:1349:C:H2'  | 23:DB:1350:C:C6   | 2.50        | 0.45     |
| 1:CA:1009:U:O2    | 1:CA:1009:U:H2'   | 2.15        | 0.45     |
| 43:DO:52:SER:C    | 43:DO:54:VAL:H    | 2.19        | 0.45     |
| 23:DB:2247:A:H3'  | 57:DB:3578:HOH:O  | 2.16        | 0.45     |
| 3:AD:7:LYS:O      | 3:AD:20:LEU:HD12  | 2.17        | 0.45     |
| 42:DN:12:ARG:HG3  | 42:DN:13:ASN:N    | 2.30        | 0.45     |
| 23:BB:2700:A:O2'  | 23:BB:2701:U:H5'  | 2.16        | 0.45     |
| 23:BB:2538:C:O2'  | 23:BB:2539:C:H5'  | 2.16        | 0.45     |
| 21:AU:11:PHE:O    | 21:AU:11:PHE:CD1  | 2.69        | 0.45     |
| 37:DL:23:ILE:HG13 | 49:DR:82:HIS:CE1  | 2.51        | 0.45     |
| 50:BT:45:ALA:HA   | 50:BT:48:GLN:HB2  | 1.98        | 0.45     |
| 29:DE:18:THR:HG22 | 29:DE:106:LYS:CE  | 2.46        | 0.45     |
| 23:DB:1708:C:H2'  | 23:DB:1709:U:C6   | 2.51        | 0.45     |
| 9:AJ:83:THR:O     | 9:AJ:86:ALA:HB3   | 2.17        | 0.45     |
| 29:BE:18:THR:HG22 | 29:BE:106:LYS:CE  | 2.47        | 0.45     |
| 1:CA:102:G:H2'    | 1:CA:103:U:H6     | 1.81        | 0.45     |
| 1:CA:167:A:O2'    | 1:CA:168:G:H5'    | 2.16        | 0.45     |
| 1:AA:54:C:H2'     | 1:AA:352:C:N4     | 2.32        | 0.45     |
| 4:AE:29:ILE:HG22  | 4:AE:29:ILE:O     | 2.17        | 0.45     |
| 24:BI:44:LYS:O    | 24:BI:48:ILE:HG13 | 2.16        | 0.45     |
| 17:AR:63:TYR:HD2  | 17:AR:63:TYR:N    | 2.14        | 0.45     |
| 9:AJ:10:LEU:HD11  | 9:AJ:25:ILE:CD1   | 2.46        | 0.45     |
| 23:BB:2104:C:H2'  | 23:BB:2105:U:C6   | 2.52        | 0.45     |
| 1:AA:1491:G:N3    | 1:AA:1491:G:H2'   | 2.32        | 0.45     |
| 23:DB:2559:C:O2'  | 23:DB:2560:A:H5'  | 2.17        | 0.45     |
| 1:CA:1426:G:H2'   | 1:CA:1427:C:H6    | 1.80        | 0.45     |
| 23:DB:250:G:H2'   | 23:DB:251:A:C8    | 2.50        | 0.45     |
| 2:CC:180:ASP:OD1  | 2:CC:203:LYS:HB2  | 2.16        | 0.45     |
| 5:AF:11:HIS:CG    | 5:AF:12:PRO:HD2   | 2.52        | 0.45     |
| 23:BB:1892:C:O2'  | 23:BB:1893:C:H5'  | 2.16        | 0.45     |
| 15:CP:45:GLU:C    | 15:CP:47:GLU:H    | 2.20        | 0.45     |
| 20:AB:35:ASN:O    | 20:AB:37:VAL:HG12 | 2.17        | 0.45     |
| 23:BB:823:C:H2'   | 23:BB:824:U:C6    | 2.52        | 0.45     |
| 24:BI:63:ASP:C    | 24:BI:65:SER:H    | 2.19        | 0.45     |
| 1:CA:1294:G:H2'   | 1:CA:1295:U:C6    | 2.51        | 0.45     |
| 1:AA:966:G:H2'    | 1:AA:967:C:C6     | 2.52        | 0.45     |
| 23:DB:2667:C:H2'  | 23:DB:2668:G:O4'  | 2.16        | 0.45     |
| 25:BC:79:ARG:HD2  | 25:BC:81:GLU:HG3  | 1.98        | 0.45     |
| 23:BB:696:G:O2'   | 23:BB:697:G:H5'   | 2.16        | 0.45     |
| 52:BW:54:ARG:C    | 52:BW:56:HIS:H    | 2.20        | 0.45     |
| 52:DW:27:GLY:O    | 52:DW:63:ASP:HA   | 2.16        | 0.45     |
| 23:DB:584:C:H2'   | 23:DB:585:G:C8    | 2.52        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 46:DU:98:ASN:OD1  | 46:DU:100:GLU:HB2 | 2.16        | 0.45     |
| 23:BB:921:C:H2'   | 23:BB:922:C:C6    | 2.51        | 0.45     |
| 52:BW:49:ASN:C    | 52:BW:50:VAL:HG22 | 2.37        | 0.45     |
| 23:DB:853:C:H2'   | 23:DB:854:C:C6    | 2.51        | 0.45     |
| 53:B6:30:THR:H    | 53:B6:37:LEU:HD21 | 1.81        | 0.45     |
| 8:CI:20:ILE:CD1   | 8:CI:85:ALA:HB3   | 2.44        | 0.45     |
| 8:CI:119:LYS:C    | 8:CI:121:ARG:H    | 2.20        | 0.45     |
| 41:DJ:45:THR:HG23 | 41:DJ:45:THR:O    | 2.15        | 0.45     |
| 47:DF:43:ILE:O    | 47:DF:46:LYS:HE2  | 2.16        | 0.45     |
| 7:CH:87:ARG:H     | 7:CH:90:GLU:CB    | 2.29        | 0.45     |
| 39:BX:28:LEU:HB3  | 39:BX:43:LEU:CD2  | 2.47        | 0.45     |
| 48:BG:33:THR:HA   | 48:BG:34:ARG:NH1  | 2.31        | 0.45     |
| 46:BU:5:ARG:NH2   | 46:BU:93:ARG:HD3  | 2.30        | 0.45     |
| 33:B1:33:LEU:HD12 | 33:B1:34:GLU:H    | 1.80        | 0.45     |
| 47:BF:78:ILE:HA   | 47:BF:79:ARG:HE   | 1.80        | 0.45     |
| 47:BF:113:PHE:CE1 | 47:BF:116:LEU:HB2 | 2.51        | 0.45     |
| 1:AA:865:A:H2     | 1:AA:918:A:H4'    | 1.80        | 0.45     |
| 47:DF:11:VAL:O    | 47:DF:12:VAL:HB   | 2.16        | 0.45     |
| 47:DF:29:ARG:HD3  | 47:DF:29:ARG:H    | 1.81        | 0.45     |
| 35:BV:83:LYS:O    | 35:BV:85:LYS:N    | 2.49        | 0.45     |
| 45:BS:12:SER:O    | 45:BS:13:SER:HB3  | 2.17        | 0.45     |
| 31:B0:38:LEU:HD13 | 31:B0:41:HIS:NE2  | 2.31        | 0.45     |
| 23:BB:2502:G:H5'  | 23:BB:2503:A:C5'  | 2.38        | 0.45     |
| 48:BG:144:ALA:O   | 48:BG:147:LEU:HB2 | 2.17        | 0.45     |
| 23:DB:2108:A:H5'  | 23:DB:2150:C:O2'  | 2.17        | 0.45     |
| 23:DB:2150:C:H2'  | 23:DB:2151:U:C6   | 2.51        | 0.45     |
| 23:BB:729:G:H2'   | 23:BB:1775:U:H1'  | 1.98        | 0.45     |
| 27:DK:7:MET:SD    | 27:DK:20:MET:HB2  | 2.56        | 0.45     |
| 40:DH:14:SER:CB   | 40:DH:17:ASP:HB2  | 2.41        | 0.45     |
| 2:CC:148:ILE:HA   | 2:CC:200:TRP:O    | 2.16        | 0.45     |
| 1:AA:714:G:H2'    | 1:AA:715:A:C8     | 2.52        | 0.45     |
| 20:CB:212:TYR:HA  | 20:CB:215:ALA:HB3 | 1.98        | 0.45     |
| 20:AB:110:ILE:O   | 20:AB:113:LEU:HB3 | 2.17        | 0.45     |
| 40:DH:46:PHE:HA   | 40:DH:50:ARG:NH2  | 2.26        | 0.45     |
| 16:CQ:58:VAL:HG12 | 16:CQ:77:VAL:HG13 | 1.99        | 0.45     |
| 23:BB:61:C:O2'    | 23:BB:62:U:H5'    | 2.17        | 0.45     |
| 41:DJ:110:PRO:HB2 | 41:DJ:111:LYS:CE  | 2.46        | 0.45     |
| 7:CH:49:LYS:HG3   | 7:CH:50:VAL:N     | 2.31        | 0.45     |
| 23:BB:192:C:C2'   | 23:BB:193:U:H5'   | 2.45        | 0.45     |
| 23:DB:153:U:O2'   | 23:DB:154:U:H5'   | 2.16        | 0.45     |
| 23:DB:742:A:O2'   | 23:DB:743:A:H5'   | 2.17        | 0.45     |
| 2:AC:122:GLN:O    | 2:AC:127:VAL:HG22 | 2.17        | 0.45     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1175:A:C2'   | 23:DB:1175:A:N3    | 2.80        | 0.45     |
| 34:D3:61:LEU:HB2   | 34:D3:64:ALA:HB2   | 1.98        | 0.45     |
| 23:BB:526:A:N6     | 23:BB:2626:C:C4'   | 2.77        | 0.45     |
| 19:CT:43:LYS:HB3   | 19:CT:85:LEU:HD21  | 1.98        | 0.45     |
| 1:CA:1007:U:H2'    | 1:CA:1008:U:H6     | 1.78        | 0.45     |
| 23:BB:2064:C:H2'   | 23:BB:2065:C:H6    | 1.81        | 0.45     |
| 23:DB:900:A:C2'    | 23:DB:901:C:H5'    | 2.46        | 0.45     |
| 18:CS:11:ASP:H     | 18:CS:14:LEU:HD21  | 1.81        | 0.45     |
| 23:DB:2249:U:N3    | 23:DB:2253:G:OP2   | 2.49        | 0.45     |
| 51:DZ:66:THR:O     | 51:DZ:70:GLU:HG3   | 2.17        | 0.45     |
| 20:CB:128:LEU:HD12 | 20:CB:132:GLU:HB2  | 1.98        | 0.45     |
| 12:AM:63:VAL:HB    | 12:AM:68:LEU:HD21  | 1.97        | 0.45     |
| 24:BI:5:GLN:HG2    | 24:BI:6:ALA:H      | 1.79        | 0.45     |
| 2:AC:13:ILE:O      | 2:AC:15:LYS:N      | 2.49        | 0.45     |
| 31:B0:8:THR:HG23   | 31:B0:10:SER:HB3   | 1.99        | 0.45     |
| 42:DN:2:ARG:HH11   | 42:DN:2:ARG:HG2    | 1.81        | 0.45     |
| 23:BB:1301:A:O2'   | 23:BB:1302:A:H2'   | 2.15        | 0.45     |
| 23:BB:1499:C:O2'   | 23:BB:1500:G:H5'   | 2.16        | 0.45     |
| 23:BB:1843:C:H5'   | 25:BC:250:GLN:HE21 | 1.80        | 0.45     |
| 23:BB:1100:C:H2'   | 23:BB:1101:U:C6    | 2.51        | 0.45     |
| 23:DB:1370:C:H2'   | 23:DB:1371:G:C8    | 2.52        | 0.45     |
| 23:BB:2152:G:H2'   | 23:BB:2152:G:N3    | 2.32        | 0.45     |
| 1:CA:1426:G:H2'    | 1:CA:1427:C:C6     | 2.50        | 0.45     |
| 48:BG:29:ASN:HD21  | 48:BG:81:GLY:HA2   | 1.79        | 0.45     |
| 23:DB:1689:A:H2'   | 23:DB:1690:A:H8    | 1.81        | 0.45     |
| 23:BB:2555:U:H2'   | 23:BB:2556:C:O4'   | 2.17        | 0.45     |
| 45:DS:4:ILE:HG22   | 45:DS:106:VAL:HG13 | 1.98        | 0.45     |
| 22:BA:53:A:O2'     | 22:BA:54:G:H5'     | 2.15        | 0.45     |
| 1:CA:538:G:OP2     | 11:CL:111:GLN:HB2  | 2.17        | 0.45     |
| 23:DB:1145:C:O2'   | 23:DB:1146:C:H5'   | 2.16        | 0.45     |
| 1:CA:37:U:H2'      | 1:CA:38:G:C8       | 2.51        | 0.45     |
| 36:B2:22:MET:SD    | 36:B2:28:ARG:HG2   | 2.56        | 0.45     |
| 23:BB:927:A:H2'    | 23:BB:928:A:C8     | 2.51        | 0.45     |
| 1:AA:775:G:O2'     | 1:AA:776:G:H5'     | 2.16        | 0.45     |
| 23:BB:1751:U:H2'   | 23:BB:1752:C:C5    | 2.52        | 0.45     |
| 23:DB:1541:C:H2'   | 23:DB:1542:U:C6    | 2.52        | 0.45     |
| 23:BB:769:U:H2'    | 23:BB:770:G:C8     | 2.51        | 0.45     |
| 24:DI:70:THR:O     | 24:DI:70:THR:HG23  | 2.16        | 0.45     |
| 35:BV:46:LYS:HD2   | 35:BV:46:LYS:N     | 2.31        | 0.45     |
| 1:AA:342:C:O2'     | 1:AA:343:U:H5'     | 2.16        | 0.45     |
| 53:B6:167:GLU:O    | 53:B6:170:ALA:HB3  | 2.16        | 0.45     |
| 49:DR:79:ARG:C     | 49:DR:81:LYS:H     | 2.20        | 0.45     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 47:BF:56:LEU:HD22  | 47:BF:59:ILE:HD12 | 1.98        | 0.45     |
| 23:DB:2057:G:H2'   | 23:DB:2058:A:O4'  | 2.16        | 0.45     |
| 52:BW:39:GLN:CG    | 52:BW:40:ARG:N    | 2.71        | 0.45     |
| 48:BG:47:ASN:CG    | 48:BG:48:THR:N    | 2.70        | 0.45     |
| 25:DC:170:TYR:CE2  | 25:DC:184:GLU:HA  | 2.52        | 0.45     |
| 44:BQ:29:ARG:O     | 44:BQ:30:VAL:HB   | 2.17        | 0.45     |
| 26:BD:92:VAL:O     | 26:BD:94:GLN:N    | 2.49        | 0.45     |
| 47:DF:32:LYS:HA    | 47:DF:95:MET:CG   | 2.44        | 0.45     |
| 23:DB:921:C:H2'    | 23:DB:922:C:C6    | 2.52        | 0.45     |
| 53:B6:32:ARG:NE    | 53:B6:37:LEU:HD23 | 2.09        | 0.45     |
| 44:DQ:59:LEU:C     | 44:DQ:59:LEU:HD13 | 2.37        | 0.45     |
| 8:AI:45:MET:SD     | 8:AI:45:MET:N     | 2.89        | 0.45     |
| 35:DV:93:ARG:HG3   | 35:DV:93:ARG:HH11 | 1.82        | 0.45     |
| 23:BB:142:A:O2'    | 23:BB:143:C:H5'   | 2.16        | 0.45     |
| 35:BV:72:VAL:CG1   | 35:BV:93:ARG:HA   | 2.47        | 0.45     |
| 2:AC:87:ARG:HH21   | 2:AC:88:LYS:HA    | 1.81        | 0.45     |
| 7:AH:86:LYS:HB3    | 7:AH:90:GLU:HG2   | 1.99        | 0.45     |
| 1:CA:600:A:O2'     | 1:CA:601:G:H5'    | 2.17        | 0.45     |
| 38:DM:21:ALA:HB3   | 38:DM:99:GLY:O    | 2.16        | 0.45     |
| 46:BU:85:ARG:NH1   | 46:BU:86:PHE:H    | 2.13        | 0.45     |
| 12:CM:3:ILE:HA     | 12:CM:56:ARG:CG   | 2.41        | 0.45     |
| 40:DH:93:SER:C     | 40:DH:94:ILE:HD12 | 2.37        | 0.45     |
| 1:AA:763:G:H2'     | 1:AA:764:C:H6     | 1.81        | 0.45     |
| 45:DS:13:SER:CB    | 45:DS:16:LYS:HE3  | 2.46        | 0.45     |
| 38:BM:134:THR:HG22 | 38:BM:136:MET:H   | 1.80        | 0.45     |
| 10:AK:95:THR:HG23  | 10:AK:96:ILE:N    | 2.30        | 0.45     |
| 25:DC:207:ALA:O    | 25:DC:208:GLY:C   | 2.55        | 0.45     |
| 15:AP:67:ILE:HD11  | 15:AP:71:VAL:HG22 | 1.99        | 0.45     |
| 1:CA:906:A:C2'     | 1:CA:907:A:H5''   | 2.46        | 0.45     |
| 23:BB:729:G:C8     | 25:BC:206:LYS:HE3 | 2.52        | 0.45     |
| 1:CA:719:C:H2'     | 17:CR:38:ILE:HD13 | 1.98        | 0.45     |
| 23:BB:592:A:H2'    | 23:BB:593:U:H6    | 1.80        | 0.45     |
| 24:DI:21:PRO:HB2   | 24:DI:22:PRO:CD   | 2.42        | 0.45     |
| 20:AB:67:LEU:HA    | 20:AB:89:PHE:O    | 2.15        | 0.45     |
| 43:BO:55:GLU:HB2   | 43:BO:58:ILE:HD12 | 1.99        | 0.45     |
| 23:DB:2344:U:H4'   | 23:DB:2345:G:OP1  | 2.16        | 0.45     |
| 26:DD:10:GLY:O     | 26:DD:11:MET:HB2  | 2.16        | 0.45     |
| 23:BB:459:U:O2'    | 23:BB:460:A:H5'   | 2.17        | 0.45     |
| 36:B2:21:ARG:C     | 36:B2:23:ALA:H    | 2.19        | 0.45     |
| 23:BB:1444:G:H2'   | 23:BB:1445:G:H8   | 1.82        | 0.45     |
| 37:BL:85:VAL:HG22  | 37:BL:94:THR:CG2  | 2.47        | 0.45     |
| 2:AC:26:LYS:HG3    | 2:AC:27:GLU:HG3   | 1.98        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:338:A:H2'    | 1:AA:339:C:C6     | 2.51        | 0.45     |
| 23:DB:1161:C:H4'  | 49:DR:8:GLY:O     | 2.17        | 0.45     |
| 12:AM:95:PRO:HB2  | 12:AM:99:GLN:CD   | 2.37        | 0.45     |
| 6:CG:57:GLU:O     | 6:CG:61:PHE:N     | 2.47        | 0.45     |
| 3:CD:84:ASN:C     | 3:CD:84:ASN:ND2   | 2.69        | 0.45     |
| 1:CA:1270:G:H2'   | 1:CA:1271:A:H8    | 1.80        | 0.45     |
| 23:DB:610:C:O2'   | 23:DB:611:C:H5'   | 2.17        | 0.45     |
| 12:AM:19:THR:HA   | 12:AM:24:VAL:HG23 | 1.99        | 0.45     |
| 23:BB:2247:A:H2'  | 23:BB:2248:C:C6   | 2.51        | 0.45     |
| 48:DG:39:ALA:HB1  | 48:DG:57:TYR:CG   | 2.50        | 0.45     |
| 28:BP:24:THR:C    | 28:BP:25:VAL:HG13 | 2.36        | 0.45     |
| 23:BB:955:U:H5''  | 38:BM:86:LYS:CD   | 2.45        | 0.45     |
| 43:BO:27:VAL:HG12 | 43:BO:28:VAL:N    | 2.32        | 0.45     |
| 1:AA:829:G:H4'    | 20:AB:24:PRO:HG3  | 1.97        | 0.45     |
| 20:AB:62:ARG:HG3  | 20:AB:62:ARG:HH11 | 1.81        | 0.45     |
| 23:BB:828:U:H2'   | 23:BB:829:A:C8    | 2.51        | 0.45     |
| 23:DB:1092:C:C2'  | 23:DB:1093:G:H5'  | 2.46        | 0.45     |
| 27:DK:109:SER:C   | 27:DK:111:LYS:H   | 2.20        | 0.45     |
| 22:DA:8:C:O2'     | 43:DO:40:ILE:HD13 | 2.17        | 0.45     |
| 49:DR:58:VAL:O    | 49:DR:58:VAL:HG13 | 2.17        | 0.45     |
| 23:DB:1847:A:H4'  | 23:DB:1848:A:C8   | 2.52        | 0.45     |
| 23:BB:370:G:O2'   | 23:BB:423:A:H3'   | 2.15        | 0.45     |
| 1:CA:900:A:H2'    | 1:CA:901:A:C8     | 2.50        | 0.45     |
| 23:DB:841:G:O2'   | 23:DB:842:U:H5'   | 2.17        | 0.45     |
| 23:DB:1952:A:N3   | 27:DK:22:ILE:HD12 | 2.32        | 0.45     |
| 23:BB:2597:G:OP1  | 25:BC:240:GLY:HA3 | 2.16        | 0.45     |
| 23:DB:1064:C:H5'  | 24:DI:88:GLY:HA3  | 1.99        | 0.45     |
| 23:DB:553:G:H2'   | 23:DB:554:U:O4'   | 2.17        | 0.45     |
| 23:BB:797:G:H2'   | 23:BB:798:G:H8    | 1.82        | 0.45     |
| 23:DB:2508:G:O2'  | 23:DB:2509:G:H5'  | 2.16        | 0.45     |
| 23:DB:2509:G:O2'  | 23:DB:2510:C:H5'  | 2.17        | 0.45     |
| 1:CA:421:U:H5'    | 1:CA:422:C:C5     | 2.51        | 0.45     |
| 16:CQ:25:GLU:HA   | 16:CQ:39:ARG:O    | 2.17        | 0.45     |
| 23:BB:2643:G:H2'  | 23:BB:2644:G:O4'  | 2.15        | 0.45     |
| 48:BG:125:PRO:HB2 | 48:BG:129:GLU:OE2 | 2.16        | 0.45     |
| 8:AI:126:PHE:O    | 8:AI:128:LYS:N    | 2.49        | 0.45     |
| 23:BB:2588:G:H2'  | 23:BB:2589:A:O4'  | 2.17        | 0.45     |
| 23:BB:2523:G:O2'  | 23:BB:2524:G:H5'  | 2.17        | 0.45     |
| 19:AT:77:ASN:O    | 19:AT:81:GLN:HG3  | 2.16        | 0.45     |
| 10:AK:82:GLU:HG2  | 10:AK:108:ASN:HB2 | 1.99        | 0.45     |
| 23:DB:2208:C:H2'  | 23:DB:2209:G:C8   | 2.51        | 0.45     |
| 44:DQ:42:GLY:HA3  | 49:DR:75:VAL:HG21 | 1.99        | 0.45     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 41:BJ:9:GLU:H      | 41:BJ:9:GLU:CD     | 2.19        | 0.45     |
| 6:AG:10:LYS:HA     | 6:AG:10:LYS:HZ1    | 1.81        | 0.45     |
| 2:AC:91:ALA:O      | 2:AC:95:GLY:N      | 2.49        | 0.45     |
| 1:AA:421:U:H5'     | 1:AA:422:C:C5      | 2.51        | 0.45     |
| 23:BB:2534:A:C2    | 23:BB:2535:G:H1'   | 2.51        | 0.45     |
| 52:BW:28:GLU:HG3   | 52:BW:29:SER:H     | 1.82        | 0.45     |
| 23:DB:533:G:H5'    | 44:DQ:23:TYR:CD2   | 2.52        | 0.45     |
| 26:BD:48:ILE:HG23  | 26:BD:82:PHE:HB2   | 1.98        | 0.45     |
| 8:CI:56:MET:CG     | 8:CI:57:VAL:N      | 2.79        | 0.45     |
| 26:DD:109:VAL:HG11 | 26:DD:193:VAL:CG1  | 2.46        | 0.45     |
| 23:DB:2311:A:O4'   | 47:DF:76:PHE:HE2   | 1.99        | 0.45     |
| 41:BJ:3:THR:HB     | 41:BJ:44:TYR:OH    | 2.17        | 0.45     |
| 3:CD:25:ARG:O      | 3:CD:26:ALA:HB3    | 2.16        | 0.45     |
| 13:AN:70:HIS:O     | 13:AN:71:GLY:C     | 2.53        | 0.45     |
| 1:AA:430:A:P       | 3:AD:6:PRO:HA      | 2.56        | 0.45     |
| 47:BF:106:ALA:N    | 47:BF:108:PRO:HD2  | 2.32        | 0.45     |
| 42:DN:81:ASN:O     | 42:DN:85:PRO:HD2   | 2.17        | 0.45     |
| 1:AA:922:G:N3      | 1:AA:1398:A:H2     | 2.13        | 0.45     |
| 47:DF:169:LEU:HB3  | 47:DF:174:PHE:CD1  | 2.52        | 0.45     |
| 4:CE:37:VAL:HG11   | 4:CE:113:VAL:CG1   | 2.38        | 0.45     |
| 18:AS:39:ILE:HG13  | 18:AS:68:HIS:O     | 2.16        | 0.45     |
| 25:DC:18:VAL:CG1   | 25:DC:202:ARG:HD2  | 2.47        | 0.45     |
| 3:AD:173:ASP:OD1   | 3:AD:176:LYS:HD3   | 2.16        | 0.45     |
| 16:AQ:45:VAL:HA    | 16:AQ:72:TRP:O     | 2.17        | 0.45     |
| 23:DB:1025:G:OP1   | 23:DB:1025:G:H8    | 2.00        | 0.45     |
| 23:DB:26:G:H2'     | 23:DB:27:G:C1'     | 2.47        | 0.45     |
| 23:DB:978:G:O2'    | 23:DB:979:A:H5'    | 2.16        | 0.45     |
| 35:DV:77:VAL:HG12  | 38:DM:136:MET:CE   | 2.47        | 0.45     |
| 45:BS:74:ILE:O     | 45:BS:75:PHE:HB3   | 2.16        | 0.45     |
| 53:D6:1:MET:HB3    | 53:D6:143:LEU:CD2  | 2.42        | 0.45     |
| 38:BM:66:ARG:HE    | 38:BM:101:VAL:HG21 | 1.82        | 0.45     |
| 44:BQ:107:ALA:HB1  | 49:BR:48:LYS:CE    | 2.46        | 0.45     |
| 49:BR:1:MET:HG3    | 49:BR:101:ILE:HG21 | 1.98        | 0.45     |
| 49:DR:39:LEU:CA    | 49:DR:49:ILE:HG12  | 2.46        | 0.45     |
| 1:AA:244:U:O4      | 1:AA:906:A:H1'     | 2.16        | 0.45     |
| 30:BY:25:GLY:HA3   | 30:BY:46:MET:HE3   | 1.99        | 0.45     |
| 23:DB:1445:G:O2'   | 23:DB:1446:C:H5'   | 2.16        | 0.45     |
| 40:DH:68:ARG:NH2   | 40:DH:71:LYS:HD3   | 2.32        | 0.45     |
| 20:CB:86:CYS:HB3   | 20:CB:88:GLN:CD    | 2.37        | 0.45     |
| 25:DC:159:THR:O    | 25:DC:160:TYR:HB3  | 2.17        | 0.45     |
| 25:BC:43:ASN:CG    | 25:BC:44:ASN:H     | 2.20        | 0.45     |
| 21:AU:10:PRO:HB2   | 2:CC:71:ARG:NE     | 2.31        | 0.45     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 5:AF:96:VAL:HG12   | 5:AF:97:THR:H     | 1.81        | 0.45     |
| 23:BB:2755:C:O5'   | 23:BB:2755:C:H6   | 1.99        | 0.45     |
| 16:AQ:16:MET:HB3   | 16:AQ:19:SER:HB2  | 1.95        | 0.45     |
| 50:BT:31:VAL:HA    | 50:BT:84:TYR:H    | 1.81        | 0.45     |
| 23:BB:1484:U:H2'   | 23:BB:1485:U:H6   | 1.80        | 0.45     |
| 41:BJ:110:PRO:HB2  | 41:BJ:111:LYS:CE  | 2.47        | 0.45     |
| 1:AA:9:G:H5'       | 4:AE:107:GLY:CA   | 2.43        | 0.45     |
| 23:DB:1222:U:P     | 49:DR:90:ARG:HH12 | 2.40        | 0.45     |
| 23:DB:2590:A:O2'   | 23:DB:2591:C:H5'  | 2.17        | 0.45     |
| 23:DB:719:C:O2'    | 23:DB:720:U:H5'   | 2.16        | 0.45     |
| 1:AA:236:A:H2'     | 1:AA:237:G:C8     | 2.52        | 0.45     |
| 1:AA:191:G:H2'     | 1:AA:192:A:H8     | 1.80        | 0.45     |
| 24:BI:138:VAL:HG12 | 24:BI:139:VAL:N   | 2.31        | 0.45     |
| 1:CA:708:C:O2'     | 1:CA:709:U:H5'    | 2.16        | 0.45     |
| 23:DB:523:C:O2'    | 23:DB:524:G:H5'   | 2.17        | 0.45     |
| 23:DB:526:A:N6     | 23:DB:2626:C:C4'  | 2.80        | 0.45     |
| 48:DG:38:ASP:CG    | 48:DG:39:ALA:N    | 2.70        | 0.45     |
| 1:AA:373:A:H1'     | 1:AA:481:G:H1'    | 1.98        | 0.45     |
| 23:BB:2737:G:H2'   | 23:BB:2738:A:H8   | 1.82        | 0.45     |
| 23:BB:2368:C:H2'   | 23:BB:2369:A:H8   | 1.81        | 0.45     |
| 23:DB:1561:C:H2'   | 23:DB:1562:U:H6   | 1.82        | 0.45     |
| 23:DB:1562:U:H2'   | 23:DB:1563:U:H6   | 1.81        | 0.45     |
| 42:DN:61:ALA:C     | 42:DN:63:ARG:N    | 2.70        | 0.45     |
| 14:AO:43:PHE:CD1   | 14:AO:56:LEU:HD22 | 2.51        | 0.45     |
| 1:AA:1042:A:H2'    | 1:AA:1043:G:O4'   | 2.16        | 0.45     |
| 19:AT:49:ALA:HA    | 19:AT:52:GLU:OE2  | 2.17        | 0.45     |
| 23:BB:1930:G:H22   | 23:BB:1969:A:P    | 2.39        | 0.45     |
| 43:BO:100:HIS:CA   | 43:BO:104:GLN:HB2 | 2.47        | 0.45     |
| 23:DB:1465:G:H2'   | 23:DB:1466:U:O4'  | 2.16        | 0.45     |
| 1:CA:224:U:H2'     | 1:CA:225:C:C6     | 2.51        | 0.45     |
| 11:CL:30:ARG:O     | 11:CL:57:THR:HG23 | 2.16        | 0.45     |
| 23:DB:639:U:H2'    | 23:DB:640:C:C6    | 2.52        | 0.45     |
| 23:BB:2150:C:H2'   | 23:BB:2151:U:C6   | 2.52        | 0.45     |
| 46:DU:41:VAL:HG22  | 46:DU:60:LYS:O    | 2.17        | 0.45     |
| 48:DG:77:GLY:HA3   | 48:DG:135:ALA:O   | 2.16        | 0.45     |
| 25:BC:20:ASN:HB3   | 25:BC:23:LEU:HD22 | 1.98        | 0.45     |
| 8:AI:10:ARG:HA     | 8:AI:77:ALA:HB1   | 1.99        | 0.45     |
| 14:CO:68:ASP:O     | 14:CO:72:ARG:HG3  | 2.17        | 0.45     |
| 1:CA:355:C:O2'     | 1:CA:356:A:H5'    | 2.16        | 0.45     |
| 23:BB:1544:A:H2'   | 23:BB:1545:A:C8   | 2.51        | 0.45     |
| 23:BB:2397:G:H2'   | 23:BB:2398:U:H6   | 1.82        | 0.45     |
| 1:CA:276:G:O2'     | 1:CA:277:C:H5'    | 2.17        | 0.45     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2643:G:H2'   | 23:DB:2644:G:O4'   | 2.15        | 0.45     |
| 49:BR:79:ARG:C     | 49:BR:81:LYS:H     | 2.19        | 0.45     |
| 23:BB:490:C:H3'    | 23:BB:491:G:H5''   | 1.99        | 0.45     |
| 10:CK:36:ARG:HG3   | 10:CK:36:ARG:HH11  | 1.82        | 0.45     |
| 23:DB:397:U:H2'    | 23:DB:398:C:C6     | 2.52        | 0.45     |
| 15:AP:8:ARG:CZ     | 15:AP:15:PRO:HB3   | 2.47        | 0.45     |
| 23:BB:1973:G:O2'   | 23:BB:1974:C:H5'   | 2.17        | 0.45     |
| 10:CK:126:ARG:HE   | 10:CK:126:ARG:HA   | 1.82        | 0.45     |
| 23:BB:2331:G:N2    | 23:BB:2336:A:H8    | 2.07        | 0.45     |
| 25:DC:90:ILE:HD11  | 25:DC:102:TYR:HB3  | 1.99        | 0.45     |
| 25:DC:188:ARG:HG2  | 25:DC:188:ARG:NH2  | 2.31        | 0.45     |
| 22:BA:42:C:C6      | 47:BF:65:LEU:HD13  | 2.51        | 0.45     |
| 26:BD:90:PHE:O     | 26:BD:91:THR:C     | 2.54        | 0.45     |
| 23:DB:2352:A:N1    | 52:DW:30:VAL:HG11  | 2.32        | 0.45     |
| 41:BJ:54:ILE:HD12  | 41:BJ:55:ILE:H     | 1.81        | 0.45     |
| 26:DD:25:THR:O     | 26:DD:189:VAL:HG22 | 2.17        | 0.45     |
| 37:DL:79:LEU:HB2   | 37:DL:113:ALA:N    | 2.23        | 0.45     |
| 47:DF:78:ILE:HA    | 47:DF:79:ARG:HH11  | 1.82        | 0.45     |
| 29:DE:58:LYS:HD3   | 29:DE:58:LYS:N     | 2.32        | 0.45     |
| 7:CH:124:ILE:HG22  | 7:CH:125:ILE:N     | 2.31        | 0.45     |
| 48:BG:26:LYS:HB2   | 48:BG:32:LEU:HG    | 1.98        | 0.45     |
| 13:AN:78:LEU:HD23  | 13:AN:82:LYS:CB    | 2.46        | 0.45     |
| 53:B6:10:THR:HG22  | 53:B6:14:MET:HE2   | 1.98        | 0.45     |
| 24:DI:128:ILE:HA   | 24:DI:131:THR:CG2  | 2.45        | 0.45     |
| 47:BF:106:ALA:HA   | 47:BF:135:ILE:HD11 | 1.99        | 0.45     |
| 47:BF:107:VAL:HB   | 47:BF:108:PRO:HD3  | 1.99        | 0.45     |
| 37:BL:77:ILE:HB    | 37:BL:109:LYS:O    | 2.16        | 0.45     |
| 40:DH:126:GLY:O    | 40:DH:146:VAL:HG23 | 2.17        | 0.45     |
| 40:DH:5:LEU:C      | 40:DH:6:LEU:HD12   | 2.36        | 0.45     |
| 29:DE:59:PRO:CB    | 29:DE:67:ARG:HH22  | 2.19        | 0.45     |
| 47:DF:131:VAL:O    | 47:DF:133:GLU:N    | 2.47        | 0.45     |
| 47:DF:103:ILE:HD11 | 47:DF:174:PHE:CD1  | 2.52        | 0.45     |
| 42:DN:101:GLY:CA   | 42:DN:109:PRO:HA   | 2.47        | 0.45     |
| 43:DO:26:LEU:HA    | 43:DO:39:VAL:HA    | 1.98        | 0.45     |
| 29:DE:29:HIS:CE1   | 37:DL:8:PRO:HG3    | 2.52        | 0.45     |
| 16:AQ:60:ILE:HG12  | 16:AQ:72:TRP:HE3   | 1.81        | 0.45     |
| 38:DM:66:ARG:HE    | 38:DM:101:VAL:HG21 | 1.81        | 0.45     |
| 1:AA:719:C:H2'     | 17:AR:38:ILE:HD11  | 1.99        | 0.45     |
| 31:B0:48:TYR:O     | 31:B0:50:GLY:N     | 2.50        | 0.45     |
| 2:AC:148:ILE:HA    | 2:AC:200:TRP:O     | 2.17        | 0.45     |
| 13:CN:50:LEU:N     | 13:CN:51:PRO:HD2   | 2.31        | 0.45     |
| 23:BB:1080:A:H2'   | 23:BB:1081:U:C6    | 2.50        | 0.45     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 24:BI:129:GLU:CB   | 24:BI:133:ARG:HH12 | 2.21        | 0.45     |
| 44:DQ:111:LYS:HZ2  | 49:DR:48:LYS:HD2   | 1.82        | 0.45     |
| 3:AD:122:ILE:HG22  | 3:AD:123:MET:H     | 1.82        | 0.45     |
| 23:BB:1445:G:H2'   | 23:BB:1446:C:H6    | 1.80        | 0.45     |
| 9:CJ:15:HIS:O      | 9:CJ:18:ILE:HG22   | 2.17        | 0.45     |
| 7:AH:65:PHE:CE2    | 7:AH:66:GLN:HG3    | 2.51        | 0.45     |
| 29:DE:126:VAL:HG22 | 29:DE:133:LEU:HD12 | 1.99        | 0.45     |
| 23:BB:62:U:H2'     | 23:BB:63:A:H5'     | 1.96        | 0.45     |
| 3:AD:169:TRP:CD2   | 3:AD:185:PRO:HB3   | 2.50        | 0.45     |
| 14:AO:25:THR:CG2   | 14:AO:70:LEU:HD23  | 2.47        | 0.45     |
| 23:BB:1794:A:O2'   | 23:BB:1795:C:H5'   | 2.17        | 0.45     |
| 41:BJ:99:ARG:HA    | 41:BJ:102:GLU:HB2  | 1.99        | 0.45     |
| 12:AM:2:ARG:O      | 12:AM:4:ALA:N      | 2.50        | 0.45     |
| 12:AM:5:GLY:O      | 12:AM:7:ASN:N      | 2.48        | 0.45     |
| 23:BB:2842:G:O2'   | 23:BB:2843:G:H5'   | 2.17        | 0.45     |
| 16:CQ:18:LYS:HG2   | 16:CQ:48:GLU:HA    | 1.99        | 0.45     |
| 23:DB:1212:G:H1'   | 23:DB:1236:G:N2    | 2.31        | 0.45     |
| 23:BB:154:U:H2'    | 23:BB:155:A:H8     | 1.81        | 0.45     |
| 39:DX:8:GLU:O      | 39:DX:12:GLU:HB2   | 2.17        | 0.45     |
| 1:CA:805:C:O2'     | 1:CA:806:C:H5'     | 2.16        | 0.45     |
| 27:DK:24:VAL:CG1   | 27:DK:33:ALA:HB2   | 2.46        | 0.45     |
| 1:CA:677:U:H3      | 1:CA:713:G:H22     | 1.64        | 0.45     |
| 12:AM:103:THR:HG22 | 12:AM:104:ASN:OD1  | 2.17        | 0.45     |
| 11:CL:98:ARG:HB2   | 11:CL:116:TYR:HA   | 1.98        | 0.45     |
| 1:CA:1054:C:O2'    | 1:CA:1055:A:H5''   | 2.16        | 0.45     |
| 1:CA:1432:G:H8     | 1:CA:1432:G:H5''   | 1.82        | 0.45     |
| 23:DB:2578:G:O2'   | 23:DB:2579:C:H5'   | 2.17        | 0.45     |
| 20:AB:71:THR:HG23  | 20:AB:94:ARG:N     | 2.32        | 0.45     |
| 1:AA:833:G:H2'     | 1:AA:834:U:H6      | 1.80        | 0.45     |
| 23:BB:1958:C:H2'   | 23:BB:1959:G:H8    | 1.80        | 0.45     |
| 23:DB:2276:G:O2'   | 23:DB:2277:G:H5'   | 2.17        | 0.45     |
| 22:DA:94:A:H2'     | 22:DA:95:U:O4'     | 2.17        | 0.45     |
| 1:AA:591:U:OP2     | 7:AH:30:LYS:HD2    | 2.16        | 0.45     |
| 23:BB:2197:U:H1'   | 23:BB:2198:A:C8    | 2.52        | 0.45     |
| 1:AA:729:A:H2'     | 1:AA:730:G:H8      | 1.81        | 0.45     |
| 1:AA:900:A:H2'     | 1:AA:901:A:C8      | 2.51        | 0.45     |
| 6:CG:70:PRO:HA     | 6:CG:141:HIS:CE1   | 2.52        | 0.45     |
| 7:AH:34:ALA:HB1    | 7:AH:109:VAL:HB    | 1.99        | 0.45     |
| 22:DA:54:G:H21     | 47:DF:25:MET:CE    | 2.30        | 0.45     |
| 23:BB:2150:C:H2'   | 23:BB:2151:U:O4'   | 2.17        | 0.45     |
| 1:CA:652:U:H1'     | 1:CA:653:U:C5      | 2.52        | 0.45     |
| 23:DB:2047:C:H2'   | 23:DB:2048:G:C8    | 2.52        | 0.45     |

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| Atom-1              | Atom-2             | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 23:BB:728:G:O2'     | 23:BB:730:A:H8     | 2.00        | 0.45     |
| 1:CA:1241:G:O2'     | 1:CA:1242:G:H5'    | 2.17        | 0.45     |
| 1:AA:984:C:O2'      | 1:AA:985:C:H5'     | 2.17        | 0.45     |
| 23:DB:88:G:C2'      | 23:DB:89:A:H5'     | 2.46        | 0.45     |
| 23:DB:2714:G:O2'    | 23:DB:2715:C:H5'   | 2.16        | 0.45     |
| 26:DD:27:ILE:HG23   | 26:DD:201:LEU:HD12 | 1.98        | 0.45     |
| 1:CA:1253:G:N1      | 1:CA:1285:A:N6     | 2.65        | 0.45     |
| 23:BB:1830:C:H2'    | 23:BB:1831:G:H8    | 1.81        | 0.45     |
| 23:BB:380:G:O2'     | 23:BB:381:G:H5'    | 2.16        | 0.45     |
| 1:CA:755:G:H2'      | 1:CA:756:C:H6      | 1.82        | 0.45     |
| 1:CA:755:G:H2'      | 1:CA:756:C:C6      | 2.52        | 0.45     |
| 1:CA:594:U:H2'      | 1:CA:595:A:C8      | 2.52        | 0.45     |
| 29:BE:73:ILE:HG12   | 29:BE:73:ILE:O     | 2.17        | 0.45     |
| 55:BB:3111:PAR:H322 | 55:BB:3111:PAR:H51 | 1.81        | 0.45     |
| 37:DL:10:GLU:HA     | 37:DL:10:GLU:OE2   | 2.15        | 0.45     |
| 25:BC:151:GLY:C     | 25:BC:152:GLN:HG3  | 2.37        | 0.45     |
| 52:DW:23:LYS:HD2    | 52:DW:24:ARG:H     | 1.82        | 0.45     |
| 53:B6:48:ALA:C      | 53:B6:50:VAL:H     | 2.20        | 0.45     |
| 53:B6:50:VAL:O      | 53:B6:55:ILE:HG21  | 2.16        | 0.45     |
| 8:CI:74:GLN:O       | 8:CI:78:ILE:HG13   | 2.16        | 0.45     |
| 47:DF:177:ARG:HA    | 47:DF:177:ARG:CZ   | 2.47        | 0.45     |
| 41:BJ:58:ASN:O      | 41:BJ:59:ALA:HB3   | 2.17        | 0.45     |
| 23:DB:996:A:H4'     | 44:DQ:91:ARG:HG2   | 1.98        | 0.45     |
| 25:BC:70:LYS:HD3    | 25:BC:101:ARG:NH2  | 2.31        | 0.45     |
| 26:DD:105:LYS:N     | 26:DD:106:LYS:HZ3  | 2.11        | 0.45     |
| 35:BV:4:ILE:N       | 35:BV:62:THR:O     | 2.50        | 0.45     |
| 12:AM:30:LYS:HG3    | 12:AM:40:GLU:OE1   | 2.17        | 0.45     |
| 7:AH:103:VAL:HG22   | 7:AH:124:ILE:HA    | 1.99        | 0.45     |
| 25:BC:188:ARG:HG2   | 25:BC:188:ARG:NH2  | 2.32        | 0.45     |
| 47:BF:3:LEU:HB2     | 47:BF:100:GLU:OE1  | 2.16        | 0.45     |
| 47:BF:110:ILE:HB    | 47:BF:113:PHE:HB3  | 1.98        | 0.45     |
| 47:BF:137:PHE:CD2   | 47:BF:137:PHE:N    | 2.84        | 0.45     |
| 47:BF:1:ALA:O       | 47:BF:2:LYS:C      | 2.55        | 0.45     |
| 4:AE:28:ARG:NH2     | 4:AE:30:PHE:HB3    | 2.32        | 0.45     |
| 21:AU:16:ARG:HG3    | 21:AU:19:LYS:HD2   | 1.99        | 0.45     |
| 18:CS:20:LYS:HD2    | 18:CS:20:LYS:O     | 2.16        | 0.45     |
| 1:AA:1270:G:H2'     | 1:AA:1271:A:H8     | 1.82        | 0.45     |
| 25:DC:210:ALA:O     | 25:DC:213:ARG:HB3  | 2.17        | 0.45     |
| 23:DB:973:A:OP1     | 23:DB:973:A:H8     | 1.99        | 0.45     |
| 23:BB:1179:G:O2'    | 23:BB:1180:U:H5'   | 2.17        | 0.45     |
| 13:AN:50:LEU:N      | 13:AN:51:PRO:HD2   | 2.32        | 0.45     |
| 23:BB:2038:G:H2'    | 23:BB:2039:U:H6    | 1.81        | 0.45     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:2884:U:O4   | 31:B0:39:ARG:HD3   | 2.17        | 0.45     |
| 23:DB:849:A:H2'   | 23:DB:850:U:C6     | 2.51        | 0.45     |
| 32:D4:5:ALA:HA    | 32:D4:37:GLN:NE2   | 2.32        | 0.45     |
| 35:DV:30:ILE:HA   | 35:DV:91:PHE:O     | 2.17        | 0.45     |
| 35:DV:80:HIS:CD2  | 35:DV:82:TYR:H     | 2.15        | 0.45     |
| 22:DA:102:G:O2'   | 22:DA:103:U:H5'    | 2.17        | 0.45     |
| 48:BG:148:ARG:HD2 | 48:BG:149:ALA:N    | 2.32        | 0.45     |
| 23:DB:2772:C:H2'  | 23:DB:2773:C:H6    | 1.82        | 0.45     |
| 26:DD:113:SER:OG  | 26:DD:114:LYS:N    | 2.48        | 0.45     |
| 27:DK:121:GLU:O   | 27:DK:122:VAL:C    | 2.55        | 0.45     |
| 20:AB:212:TYR:O   | 20:AB:216:VAL:HG22 | 2.17        | 0.45     |
| 49:DR:4:VAL:H     | 49:DR:38:VAL:HG23  | 1.82        | 0.45     |
| 24:BI:19:PRO:HB2  | 24:BI:22:PRO:HD2   | 1.99        | 0.45     |
| 27:BK:99:ILE:H    | 27:BK:118:LEU:HD23 | 1.82        | 0.45     |
| 37:DL:93:ASN:HD22 | 37:DL:94:THR:H     | 1.64        | 0.45     |
| 23:BB:459:U:C2'   | 23:BB:460:A:H5'    | 2.47        | 0.45     |
| 23:BB:849:A:H2'   | 23:BB:850:U:C6     | 2.51        | 0.45     |
| 1:AA:82:G:OP2     | 1:AA:83:C:H6       | 1.99        | 0.45     |
| 20:CB:64:GLY:HA2  | 20:CB:158:ASP:OD1  | 2.16        | 0.45     |
| 34:D3:14:LYS:O    | 34:D3:21:PHE:O     | 2.35        | 0.45     |
| 37:BL:93:ASN:ND2  | 37:BL:94:THR:H     | 2.14        | 0.45     |
| 23:BB:1680:U:H2'  | 23:BB:1681:G:O4'   | 2.17        | 0.45     |
| 23:DB:2846:G:OP1  | 28:DP:51:ASN:HB2   | 2.17        | 0.45     |
| 3:AD:104:MET:SD   | 3:AD:179:GLY:HA3   | 2.57        | 0.45     |
| 1:CA:441:A:N6     | 1:CA:493:A:N6      | 2.65        | 0.45     |
| 23:DB:2602:A:C2'  | 23:DB:2602:A:N3    | 2.78        | 0.45     |
| 48:BG:137:LYS:O   | 48:BG:140:ILE:HG13 | 2.17        | 0.45     |
| 1:CA:553:A:H2'    | 1:CA:554:A:C8      | 2.51        | 0.45     |
| 23:DB:1210:G:H1'  | 23:DB:1212:G:C2    | 2.52        | 0.45     |
| 36:D2:10:LEU:HD11 | 36:D2:14:ARG:NH1   | 2.32        | 0.45     |
| 23:BB:1998:A:O2'  | 23:BB:1999:C:H5'   | 2.17        | 0.45     |
| 7:CH:74:ILE:HG13  | 7:CH:128:VAL:HG22  | 1.98        | 0.45     |
| 45:BS:31:GLN:C    | 45:BS:33:LEU:N     | 2.69        | 0.45     |
| 1:AA:676:A:H1'    | 10:AK:116:PRO:HB3  | 1.99        | 0.45     |
| 23:BB:523:C:O2'   | 23:BB:524:G:H5'    | 2.17        | 0.45     |
| 23:BB:1064:C:H2'  | 23:BB:1065:U:O4'   | 2.17        | 0.45     |
| 23:DB:123:G:H2'   | 23:DB:124:G:C8     | 2.52        | 0.45     |
| 50:DT:13:ALA:O    | 50:DT:32:LEU:HB2   | 2.17        | 0.45     |
| 51:DZ:65:ASP:O    | 51:DZ:69:ALA:N     | 2.48        | 0.45     |
| 41:BJ:13:ARG:HB3  | 41:BJ:53:TYR:HD2   | 1.82        | 0.45     |
| 1:AA:1384:C:O2'   | 1:AA:1385:G:H5'    | 2.16        | 0.45     |
| 1:AA:584:G:O2'    | 1:AA:585:G:H5'     | 2.17        | 0.45     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1429:G:H2'  | 23:BB:1430:G:C8    | 2.51        | 0.45     |
| 43:DO:28:VAL:HG21 | 43:DO:106:LEU:HD21 | 1.99        | 0.45     |
| 1:AA:204:G:H1'    | 1:AA:466:A:H62     | 1.82        | 0.45     |
| 23:BB:2804:U:H2'  | 23:BB:2805:C:H6    | 1.81        | 0.45     |
| 23:DB:459:U:O2'   | 23:DB:460:A:H5'    | 2.17        | 0.45     |
| 23:BB:2729:G:H2'  | 23:BB:2730:C:H6    | 1.82        | 0.45     |
| 1:CA:761:G:H2'    | 1:CA:762:U:H6      | 1.81        | 0.45     |
| 1:AA:975:A:H5''   | 1:AA:976:G:O5'     | 2.17        | 0.45     |
| 2:CC:172:VAL:O    | 2:CC:174:LEU:HD12  | 2.17        | 0.45     |
| 23:DB:2560:A:H2'  | 23:DB:2561:U:C6    | 2.52        | 0.45     |
| 23:DB:2561:U:O3'  | 27:DK:40:LYS:HE2   | 2.17        | 0.45     |
| 1:AA:358:U:H2'    | 1:AA:359:G:H8      | 1.80        | 0.45     |
| 46:DU:31:GLY:O    | 46:DU:66:VAL:HG12  | 2.16        | 0.45     |
| 48:BG:172:GLU:O   | 48:BG:173:ALA:HB2  | 2.17        | 0.45     |
| 49:BR:84:ARG:NH2  | 49:BR:84:ARG:HG3   | 2.32        | 0.45     |
| 49:BR:64:VAL:O    | 49:BR:65:ALA:HB3   | 2.17        | 0.45     |
| 1:CA:93:U:C2'     | 1:CA:94:G:H5'      | 2.47        | 0.45     |
| 23:DB:622:G:H2'   | 23:DB:623:C:H6     | 1.81        | 0.45     |
| 4:AE:17:VAL:HA    | 4:AE:33:THR:O      | 2.17        | 0.45     |
| 23:BB:688:U:O2'   | 23:BB:689:A:H5'    | 2.17        | 0.45     |
| 1:AA:970:C:N4     | 8:AI:128:LYS:HG2   | 2.32        | 0.45     |
| 16:AQ:3:LYS:HG2   | 16:AQ:4:ILE:H      | 1.81        | 0.45     |
| 23:BB:1159:U:H2'  | 23:BB:1160:G:H8    | 1.81        | 0.45     |
| 23:BB:911:A:H2'   | 38:BM:9:PHE:CZ     | 2.52        | 0.45     |
| 12:CM:72:ILE:O    | 12:CM:76:ILE:HG13  | 2.16        | 0.45     |
| 2:AC:182:ASP:HB2  | 2:AC:203:LYS:HE2   | 1.98        | 0.45     |
| 1:CA:454:G:H2'    | 1:CA:455:G:H8      | 1.81        | 0.45     |
| 27:BK:64:ARG:O    | 27:BK:82:ASN:HA    | 2.17        | 0.45     |
| 5:CF:49:TYR:CE1   | 17:CR:65:SER:HA    | 2.52        | 0.45     |
| 1:CA:200:G:O2'    | 1:CA:381:C:N4      | 2.50        | 0.45     |
| 50:DT:76:ARG:HB3  | 50:DT:76:ARG:NH1   | 2.32        | 0.45     |
| 23:DB:1099:G:H4'  | 24:DI:4:VAL:HG12   | 1.99        | 0.45     |
| 44:BQ:23:TYR:HB2  | 44:BQ:27:ARG:HB3   | 1.99        | 0.45     |
| 48:BG:108:PHE:H   | 48:BG:108:PHE:HD1  | 1.65        | 0.45     |
| 48:DG:6:ALA:HB3   | 48:DG:68:ARG:CD    | 2.47        | 0.45     |
| 16:CQ:45:VAL:HA   | 16:CQ:72:TRP:O     | 2.17        | 0.45     |
| 53:B6:64:ARG:HA   | 53:B6:103:ILE:O    | 2.17        | 0.45     |
| 8:CI:6:TYR:C      | 8:CI:85:ALA:HB2    | 2.37        | 0.45     |
| 51:DZ:40:VAL:O    | 51:DZ:42:SER:N     | 2.49        | 0.45     |
| 23:DB:2305:U:H1'  | 47:DF:132:ARG:HA   | 1.99        | 0.45     |
| 48:DG:15:ASP:HA   | 48:DG:26:LYS:NZ    | 2.32        | 0.45     |
| 46:DU:84:PHE:HB3  | 46:DU:91:LYS:HG3   | 1.97        | 0.45     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:BB:2305:U:H2'   | 23:BB:2306:C:O4'  | 2.17        | 0.45     |
| 23:BB:2393:U:H2'   | 23:BB:2394:C:O4'  | 2.17        | 0.45     |
| 1:CA:1207:G:O2'    | 1:CA:1208:C:H5'   | 2.17        | 0.45     |
| 47:BF:168:LEU:HD13 | 47:BF:172:PHE:HE2 | 1.82        | 0.45     |
| 1:AA:1077:G:N2     | 1:AA:1080:A:OP2   | 2.44        | 0.45     |
| 1:CA:1078:U:H4'    | 4:CE:137:ARG:NH1  | 2.32        | 0.45     |
| 1:CA:922:G:N3      | 1:CA:1398:A:H2    | 2.15        | 0.45     |
| 1:CA:921:U:O2      | 4:CE:23:THR:HG23  | 2.17        | 0.45     |
| 1:CA:764:C:H2'     | 1:CA:765:G:C5'    | 2.45        | 0.45     |
| 18:CS:44:ILE:O     | 18:CS:44:ILE:HG23 | 2.16        | 0.45     |
| 18:AS:20:LYS:O     | 18:AS:23:GLU:HG3  | 2.17        | 0.45     |
| 32:B4:3:VAL:HG23   | 32:B4:4:ARG:N     | 2.31        | 0.45     |
| 23:DB:2788:C:H1'   | 23:DB:2809:A:C2   | 2.52        | 0.45     |
| 23:DB:818:G:N1     | 23:DB:1187:G:H2'  | 2.32        | 0.45     |
| 1:CA:1269:A:H2     | 1:CA:1312:G:N3    | 2.15        | 0.45     |
| 48:DG:147:LEU:O    | 48:DG:150:TYR:HB2 | 2.17        | 0.45     |
| 35:DV:9:ARG:HA     | 35:DV:41:GLU:OE2  | 2.17        | 0.45     |
| 15:CP:66:THR:HG22  | 15:CP:67:ILE:H    | 1.82        | 0.45     |
| 27:DK:104:THR:HB   | 27:DK:106:GLU:OE1 | 2.16        | 0.45     |
| 23:DB:845:A:C2'    | 23:DB:846:U:H5''  | 2.42        | 0.45     |
| 11:CL:29:LYS:HB3   | 11:CL:56:LEU:HD22 | 1.98        | 0.45     |
| 24:BI:19:PRO:HG2   | 24:BI:22:PRO:HB2  | 1.99        | 0.45     |
| 35:BV:89:ILE:HD12  | 35:BV:89:ILE:O    | 2.17        | 0.45     |
| 23:DB:1198:U:H2'   | 23:DB:1199:U:H6   | 1.82        | 0.45     |
| 48:BG:30:GLY:O     | 48:BG:78:VAL:HG12 | 2.16        | 0.45     |
| 2:CC:11:LEU:HD11   | 13:CN:87:ALA:O    | 2.16        | 0.45     |
| 45:DS:81:SER:CA    | 45:DS:99:ARG:HA   | 2.43        | 0.45     |
| 20:CB:116:LEU:HA   | 20:CB:119:GLN:HG2 | 1.99        | 0.45     |
| 23:DB:362:A:C2'    | 23:DB:362:A:N3    | 2.80        | 0.45     |
| 5:AF:62:MET:O      | 5:AF:63:ASN:HB2   | 2.17        | 0.45     |
| 31:D0:33:SER:OG    | 31:D0:35:GLU:HG2  | 2.17        | 0.45     |
| 23:BB:191:A:H2'    | 23:BB:192:C:H6    | 1.76        | 0.45     |
| 23:BB:2015:A:C2    | 31:B0:2:VAL:HG22  | 2.52        | 0.45     |
| 2:CC:23:ALA:HB1    | 2:CC:27:GLU:OE2   | 2.17        | 0.45     |
| 23:BB:2746:U:O4    | 23:BB:2755:C:H5'  | 2.17        | 0.45     |
| 23:BB:2602:A:H3'   | 23:BB:2602:A:OP1  | 2.17        | 0.45     |
| 40:BH:44:ILE:C     | 40:BH:46:PHE:N    | 2.70        | 0.45     |
| 23:BB:647:G:H2'    | 23:BB:648:G:C8    | 2.52        | 0.45     |
| 22:BA:114:C:H1'    | 43:BO:47:VAL:HG21 | 1.98        | 0.45     |
| 43:BO:52:SER:OG    | 43:BO:54:VAL:HG12 | 2.17        | 0.45     |
| 35:BV:29:ILE:HD13  | 35:BV:31:TYR:HE2  | 1.81        | 0.45     |
| 37:BL:47:ARG:HB3   | 37:BL:47:ARG:HH21 | 1.82        | 0.45     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 43:DO:24:THR:HG1  | 43:DO:90:VAL:HG12  | 1.81        | 0.45     |
| 12:CM:2:ARG:O     | 12:CM:4:ALA:N      | 2.50        | 0.45     |
| 23:BB:2720:U:H2'  | 23:BB:2721:A:C8    | 2.52        | 0.45     |
| 22:DA:115:A:O2'   | 22:DA:116:G:H5'    | 2.17        | 0.45     |
| 23:DB:2415:G:O2'  | 23:DB:2416:C:H5'   | 2.17        | 0.45     |
| 19:AT:53:MET:HA   | 19:AT:56:ILE:HD12  | 1.98        | 0.45     |
| 1:AA:376:G:H5''   | 15:AP:5:ARG:HB2    | 1.98        | 0.45     |
| 25:BC:245:THR:C   | 25:BC:247:TRP:N    | 2.70        | 0.45     |
| 28:DP:107:ALA:O   | 28:DP:108:ARG:C    | 2.56        | 0.45     |
| 37:BL:65:GLY:O    | 37:BL:66:PHE:HB3   | 2.17        | 0.45     |
| 41:DJ:12:LYS:O    | 41:DJ:13:ARG:HB2   | 2.17        | 0.45     |
| 23:DB:1454:C:H5'  | 42:DN:63:ARG:NE    | 2.32        | 0.45     |
| 50:BT:45:ALA:HA   | 50:BT:48:GLN:CG    | 2.46        | 0.45     |
| 5:CF:47:LEU:HD21  | 5:CF:57:ALA:CB     | 2.46        | 0.45     |
| 41:DJ:96:ARG:O    | 41:DJ:99:ARG:HG3   | 2.16        | 0.45     |
| 23:BB:39:G:H2'    | 23:BB:40:U:H6      | 1.81        | 0.45     |
| 23:DB:1885:A:H2'  | 23:DB:1886:U:O4'   | 2.16        | 0.45     |
| 23:DB:1252:G:H5'' | 57:DB:3463:HOH:O   | 2.15        | 0.45     |
| 17:CR:57:ALA:HA   | 17:CR:60:ARG:HD2   | 1.99        | 0.45     |
| 23:DB:1848:A:H2'  | 23:DB:1849:G:C8    | 2.52        | 0.45     |
| 47:DF:120:SER:O   | 47:DF:127:TYR:HA   | 2.16        | 0.45     |
| 23:DB:2213:U:O2   | 23:DB:2213:U:H2'   | 2.15        | 0.45     |
| 4:AE:87:VAL:HG23  | 4:AE:92:ARG:HA     | 1.98        | 0.45     |
| 1:CA:435:A:H2'    | 1:CA:435:A:N3      | 2.32        | 0.45     |
| 7:CH:79:ARG:NH1   | 7:CH:82:LEU:HB3    | 2.32        | 0.45     |
| 49:DR:84:ARG:HG3  | 49:DR:84:ARG:NH2   | 2.32        | 0.45     |
| 23:BB:2081:U:H2'  | 23:BB:2082:A:H8    | 1.82        | 0.45     |
| 1:AA:106:C:O2'    | 1:AA:107:G:H5'     | 2.17        | 0.45     |
| 23:DB:2508:G:O3'  | 23:DB:2555:U:H5'   | 2.17        | 0.45     |
| 45:BS:4:ILE:HG22  | 45:BS:106:VAL:HG13 | 1.98        | 0.45     |
| 1:CA:241:G:O2'    | 1:CA:242:G:H5'     | 2.17        | 0.45     |
| 1:CA:175:C:O2'    | 1:CA:176:C:H5'     | 2.17        | 0.45     |
| 47:BF:94:ARG:O    | 47:BF:98:PHE:N     | 2.49        | 0.45     |
| 22:DA:19:C:O2'    | 22:DA:20:G:H5'     | 2.17        | 0.45     |
| 16:CQ:3:LYS:HG2   | 16:CQ:4:ILE:H      | 1.81        | 0.45     |
| 23:BB:1376:C:H5'' | 57:BB:3502:HOH:O   | 2.16        | 0.45     |
| 1:AA:1310:G:O2'   | 1:AA:1311:A:H5'    | 2.16        | 0.45     |
| 36:D2:12:ARG:HG3  | 36:D2:12:ARG:NH2   | 2.32        | 0.45     |
| 39:BX:45:GLN:O    | 39:BX:46:VAL:HB    | 2.16        | 0.45     |
| 23:DB:1753:G:N2   | 23:DB:1755:A:H3'   | 2.32        | 0.45     |
| 52:BW:35:ILE:O    | 52:BW:37:VAL:N     | 2.50        | 0.45     |
| 52:DW:35:ILE:O    | 52:DW:35:ILE:CG1   | 2.65        | 0.45     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:1819:A:H1'  | 23:DB:1821:A:C6    | 2.52        | 0.45     |
| 23:DB:2033:A:H3'  | 57:DB:3319:HOH:O   | 2.15        | 0.45     |
| 23:DB:2352:A:H8   | 23:DB:2352:A:O5'   | 2.00        | 0.45     |
| 8:CI:21:LYS:HB3   | 8:CI:61:ASP:O      | 2.17        | 0.45     |
| 20:CB:162:VAL:CG1 | 20:CB:184:ALA:HB2  | 2.39        | 0.45     |
| 51:DZ:5:CYS:O     | 51:DZ:6:GLN:HB3    | 2.16        | 0.45     |
| 25:BC:137:GLY:H   | 25:BC:163:ILE:HB   | 1.82        | 0.45     |
| 1:AA:1015:G:H2'   | 1:AA:1016:A:C8     | 2.52        | 0.45     |
| 1:AA:981:U:H2'    | 1:AA:982:U:C5      | 2.52        | 0.45     |
| 23:DB:2305:U:H2'  | 23:DB:2306:C:O4'   | 2.17        | 0.45     |
| 25:DC:75:ALA:CB   | 25:DC:93:VAL:HG22  | 2.46        | 0.45     |
| 42:DN:79:LEU:HA   | 42:DN:83:LEU:HD12  | 1.98        | 0.45     |
| 38:BM:21:ALA:HB3  | 38:BM:99:GLY:O     | 2.16        | 0.45     |
| 24:BI:27:LEU:HB2  | 24:BI:32:VAL:HG21  | 1.98        | 0.45     |
| 1:CA:951:G:OP2    | 12:CM:100:ARG:NH2  | 2.50        | 0.45     |
| 12:AM:53:ASP:HA   | 12:AM:56:ARG:NH2   | 2.32        | 0.45     |
| 33:D1:8:ILE:HG21  | 33:D1:51:ALA:CB    | 2.47        | 0.45     |
| 50:DT:29:THR:HB   | 50:DT:86:THR:HG22  | 1.98        | 0.45     |
| 23:DB:1789:A:OP1  | 25:DC:220:ARG:HD3  | 2.17        | 0.45     |
| 31:B0:50:GLY:C    | 31:B0:51:ARG:HG2   | 2.37        | 0.45     |
| 23:BB:2883:A:OP1  | 31:B0:48:TYR:OH    | 2.31        | 0.45     |
| 1:CA:1326:U:H2'   | 1:CA:1327:C:H6     | 1.79        | 0.45     |
| 32:D4:7:VAL:HG13  | 32:D4:8:LYS:N      | 2.29        | 0.45     |
| 52:DW:9:THR:OG1   | 52:DW:10:ARG:N     | 2.44        | 0.45     |
| 23:DB:1458:U:O3'  | 23:DB:1459:G:O4'   | 2.34        | 0.45     |
| 23:BB:845:A:C2'   | 23:BB:846:U:H5''   | 2.42        | 0.45     |
| 1:CA:1333:A:H2'   | 1:CA:1334:G:O4'    | 2.17        | 0.45     |
| 23:DB:592:A:H2'   | 23:DB:593:U:H6     | 1.78        | 0.45     |
| 42:DN:48:VAL:O    | 42:DN:51:LEU:N     | 2.50        | 0.45     |
| 1:CA:279:A:H5''   | 1:CA:280:C:C3'     | 2.44        | 0.45     |
| 24:DI:129:GLU:CB  | 24:DI:133:ARG:HH12 | 2.29        | 0.45     |
| 26:DD:48:ILE:HG23 | 26:DD:82:PHE:HB2   | 1.98        | 0.45     |
| 20:CB:83:ALA:CB   | 20:CB:90:PHE:HB3   | 2.47        | 0.45     |
| 49:DR:27:ILE:HG22 | 49:DR:28:ALA:N     | 2.32        | 0.45     |
| 37:BL:95:LEU:HB3  | 37:BL:100:ILE:CG2  | 2.46        | 0.45     |
| 2:CC:184:ASN:HD22 | 2:CC:185:THR:H     | 1.64        | 0.45     |
| 2:AC:26:LYS:HE2   | 2:AC:27:GLU:CG     | 2.46        | 0.45     |
| 7:CH:48:PHE:HA    | 7:CH:59:GLU:O      | 2.17        | 0.45     |
| 40:DH:111:ALA:O   | 40:DH:132:PHE:CZ   | 2.70        | 0.45     |
| 5:AF:97:THR:O     | 5:AF:98:GLU:CD     | 2.55        | 0.45     |
| 1:CA:974:A:H8     | 1:CA:974:A:OP1     | 1.98        | 0.45     |
| 14:AO:70:LEU:HD12 | 14:AO:78:TYR:CB    | 2.42        | 0.45     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:299:A:H2'   | 23:DB:300:A:C8     | 2.52        | 0.45     |
| 10:CK:80:ASN:HA   | 10:CK:105:ARG:HB3  | 1.99        | 0.45     |
| 50:DT:81:LYS:HG3  | 50:DT:82:LYS:N     | 2.32        | 0.45     |
| 23:DB:1210:G:H5'  | 23:DB:1212:G:H5'   | 1.98        | 0.45     |
| 3:CD:117:VAL:O    | 3:CD:130:ASN:HA    | 2.17        | 0.45     |
| 23:DB:1429:G:H2'  | 23:DB:1430:G:C8    | 2.52        | 0.45     |
| 53:B6:147:LEU:N   | 53:B6:147:LEU:HD23 | 2.32        | 0.45     |
| 27:DK:2:ILE:HG23  | 27:DK:33:ALA:O     | 2.17        | 0.45     |
| 1:AA:805:C:O2'    | 1:AA:806:C:H5'     | 2.17        | 0.45     |
| 23:DB:1353:A:O2'  | 23:DB:1354:A:H5'   | 2.17        | 0.45     |
| 46:BU:48:VAL:O    | 46:BU:48:VAL:HG22  | 2.17        | 0.45     |
| 23:DB:1350:C:H5'  | 23:DB:1351:C:OP2   | 2.17        | 0.45     |
| 23:DB:307:G:N2    | 23:DB:309:A:H3'    | 2.32        | 0.45     |
| 22:DA:113:C:H2'   | 22:DA:114:C:C6     | 2.52        | 0.45     |
| 19:AT:38:ILE:HG13 | 19:AT:82:ILE:HG22  | 1.98        | 0.45     |
| 1:CA:212:G:H2'    | 1:CA:213:G:C8      | 2.52        | 0.45     |
| 20:CB:23:ASN:HB3  | 20:CB:188:THR:O    | 2.16        | 0.45     |
| 1:AA:1180:A:OP1   | 8:AI:104:THR:HG22  | 2.16        | 0.45     |
| 1:AA:1495:U:O2'   | 1:AA:1496:C:H5'    | 2.17        | 0.45     |
| 3:CD:7:LYS:O      | 3:CD:20:LEU:HD12   | 2.17        | 0.45     |
| 23:BB:2277:G:H5'' | 38:BM:86:LYS:CB    | 2.47        | 0.45     |
| 23:BB:480:A:H3'   | 23:BB:481:G:H5''   | 1.98        | 0.45     |
| 23:BB:681:G:H2'   | 23:BB:682:G:H8     | 1.81        | 0.45     |
| 1:CA:1480:A:H2'   | 1:CA:1481:U:H6     | 1.80        | 0.45     |
| 19:AT:49:ALA:HA   | 19:AT:52:GLU:CD    | 2.36        | 0.45     |
| 1:AA:90:C:H2'     | 1:AA:91:U:H5       | 1.82        | 0.45     |
| 23:BB:39:G:H2'    | 23:BB:40:U:C6      | 2.52        | 0.45     |
| 43:DO:27:VAL:HG12 | 43:DO:28:VAL:N     | 2.30        | 0.45     |
| 23:DB:131:A:H2'   | 23:DB:132:G:H8     | 1.82        | 0.45     |
| 6:CG:45:ALA:HB2   | 6:CG:116:ALA:O     | 2.17        | 0.45     |
| 1:CA:223:A:H2'    | 1:CA:224:U:H6      | 1.80        | 0.45     |
| 10:AK:60:PHE:O    | 10:AK:63:GLN:HB3   | 2.17        | 0.45     |
| 23:BB:1495:A:H2'  | 23:BB:1496:A:H8    | 1.80        | 0.45     |
| 46:DU:14:THR:HG21 | 46:DU:64:ILE:HD13  | 1.99        | 0.45     |
| 1:AA:912:C:H2'    | 1:AA:913:A:C8      | 2.52        | 0.45     |
| 23:DB:1664:A:H1'  | 23:DB:2726:A:C2    | 2.52        | 0.45     |
| 4:AE:33:THR:HB    | 4:AE:49:TYR:CE1    | 2.52        | 0.45     |
| 49:DR:62:GLU:O    | 49:DR:96:VAL:HA    | 2.16        | 0.45     |
| 43:DO:56:LYS:HA   | 43:DO:59:ALA:HB3   | 1.99        | 0.45     |
| 23:DB:158:U:H2'   | 23:DB:159:G:O4'    | 2.17        | 0.45     |
| 1:AA:200:G:O2'    | 1:AA:381:C:N4      | 2.49        | 0.45     |
| 1:AA:220:G:O2'    | 1:AA:221:C:H5'     | 2.16        | 0.45     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:138:G:C6     | 1:AA:226:G:C6      | 3.05        | 0.45     |
| 8:CI:126:PHE:O    | 8:CI:128:LYS:N     | 2.50        | 0.45     |
| 23:DB:2582:G:O2'  | 23:DB:2583:G:H5'   | 2.16        | 0.45     |
| 15:CP:36:VAL:O    | 15:CP:36:VAL:HG13  | 2.17        | 0.45     |
| 24:DI:59:THR:O    | 24:DI:59:THR:HG23  | 2.17        | 0.45     |
| 23:BB:686:U:H2'   | 23:BB:788:A:N1     | 2.32        | 0.45     |
| 1:CA:1047:G:H21   | 1:CA:1215:G:C4'    | 2.30        | 0.45     |
| 23:DB:1100:C:H41  | 24:DI:1:ALA:H2     | 1.65        | 0.44     |
| 23:BB:855:G:C2    | 52:BW:23:LYS:HG2   | 2.50        | 0.44     |
| 23:BB:2354:C:H4'  | 52:BW:31:LEU:HD22  | 1.99        | 0.44     |
| 25:DC:131:MET:HE1 | 25:DC:189:ALA:HB2  | 1.98        | 0.44     |
| 23:BB:2667:C:O2   | 48:BG:110:HIS:CE1  | 2.69        | 0.44     |
| 48:BG:93:TYR:O    | 48:BG:94:ARG:HG3   | 2.17        | 0.44     |
| 26:BD:107:VAL:H   | 26:BD:205:PRO:HA   | 1.82        | 0.44     |
| 26:BD:25:THR:O    | 26:BD:189:VAL:HG22 | 2.17        | 0.44     |
| 8:AI:24:ASN:HD22  | 8:AI:25:GLY:H      | 1.60        | 0.44     |
| 8:AI:39:GLY:HA2   | 8:AI:44:ARG:HD3    | 1.99        | 0.44     |
| 1:AA:1014:A:H4'   | 18:AS:13:HIS:CD2   | 2.52        | 0.44     |
| 48:DG:22:VAL:C    | 48:DG:23:ILE:HG13  | 2.38        | 0.44     |
| 7:CH:86:LYS:HB3   | 7:CH:90:GLU:HG2    | 1.99        | 0.44     |
| 13:CN:60:ARG:HH21 | 13:CN:69:PRO:HD3   | 1.82        | 0.44     |
| 39:BX:27:ASN:O    | 39:BX:28:LEU:C     | 2.55        | 0.44     |
| 34:D3:36:ALA:HB3  | 34:D3:39:ARG:HB2   | 1.98        | 0.44     |
| 25:BC:107:LYS:N   | 25:BC:193:GLU:O    | 2.49        | 0.44     |
| 47:BF:45:ASP:C    | 47:BF:47:LYS:H     | 2.20        | 0.44     |
| 47:BF:108:PRO:C   | 47:BF:110:ILE:H    | 2.21        | 0.44     |
| 23:BB:625:G:O2'   | 23:BB:626:A:H5'    | 2.16        | 0.44     |
| 37:BL:115:GLU:OE1 | 37:BL:115:GLU:N    | 2.50        | 0.44     |
| 29:BE:184:ASP:O   | 29:BE:185:LYS:HG3  | 2.17        | 0.44     |
| 40:DH:89:LYS:HD2  | 40:DH:89:LYS:N     | 2.33        | 0.44     |
| 1:CA:1320:C:OP2   | 18:CS:2:ARG:HG3    | 2.17        | 0.44     |
| 23:BB:518:G:H4'   | 45:BS:18:ARG:CZ    | 2.47        | 0.44     |
| 33:D1:49:LYS:CG   | 33:D1:50:GLU:H     | 2.17        | 0.44     |
| 33:D1:8:ILE:CG2   | 33:D1:51:ALA:HA    | 2.47        | 0.44     |
| 6:CG:110:ARG:HE   | 6:CG:122:GLU:HB2   | 1.81        | 0.44     |
| 46:BU:81:ARG:HB2  | 46:BU:96:LYS:HG2   | 1.98        | 0.44     |
| 15:AP:72:ALA:HA   | 15:AP:75:ILE:CD1   | 2.47        | 0.44     |
| 1:AA:1352:C:H2'   | 1:AA:1353:G:C8     | 2.52        | 0.44     |
| 45:BS:69:LEU:HG   | 45:BS:107:VAL:HG22 | 1.98        | 0.44     |
| 32:D4:2:LYS:HG2   | 32:D4:4:ARG:HG3    | 1.98        | 0.44     |
| 29:DE:151:GLY:HA2 | 29:DE:195:GLN:HE22 | 1.82        | 0.44     |
| 44:BQ:7:VAL:O     | 44:BQ:11:ALA:HB2   | 2.16        | 0.44     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:333:U:H2'    | 1:CA:334:C:H6      | 1.82        | 0.44     |
| 20:CB:30:ILE:HD13 | 20:CB:38:HIS:CD2   | 2.52        | 0.44     |
| 3:CD:152:SER:O    | 3:CD:155:LYS:HG2   | 2.17        | 0.44     |
| 49:BR:39:LEU:CA   | 49:BR:53:PHE:HA    | 2.46        | 0.44     |
| 49:DR:38:VAL:HG22 | 49:DR:40:MET:H     | 1.83        | 0.44     |
| 23:DB:1794:A:O2'  | 23:DB:1795:C:H5'   | 2.17        | 0.44     |
| 23:BB:1416:G:O2'  | 23:BB:1417:C:H6    | 1.97        | 0.44     |
| 36:B2:34:ARG:O    | 36:B2:38:GLY:N     | 2.50        | 0.44     |
| 44:DQ:9:ALA:C     | 44:DQ:11:ALA:N     | 2.69        | 0.44     |
| 23:DB:1700:A:C2'  | 23:DB:1701:A:H5'   | 2.43        | 0.44     |
| 1:CA:845:A:C5     | 1:CA:846:G:H1'     | 2.52        | 0.44     |
| 25:BC:157:ALA:HA  | 25:BC:194:VAL:CG2  | 2.47        | 0.44     |
| 11:AL:20:VAL:HB   | 11:AL:94:TYR:CE1   | 2.53        | 0.44     |
| 16:AQ:77:VAL:HG12 | 16:AQ:79:GLU:H     | 1.82        | 0.44     |
| 37:BL:96:LYS:HD3  | 37:BL:103:ILE:HA   | 1.98        | 0.44     |
| 37:BL:96:LYS:HE2  | 37:BL:102:GLY:O    | 2.17        | 0.44     |
| 1:AA:325:A:H2'    | 1:AA:326:G:O4'     | 2.17        | 0.44     |
| 23:BB:182:A:H2'   | 23:BB:183:C:C6     | 2.52        | 0.44     |
| 23:BB:1789:A:O2'  | 23:BB:1790:C:H5'   | 2.16        | 0.44     |
| 49:BR:25:LEU:H    | 49:BR:94:THR:HG21  | 1.82        | 0.44     |
| 26:BD:169:ARG:O   | 26:BD:170:VAL:O    | 2.36        | 0.44     |
| 1:CA:238:A:H3'    | 1:CA:239:U:H5''    | 1.99        | 0.44     |
| 16:CQ:18:LYS:HD3  | 16:CQ:48:GLU:HG2   | 1.98        | 0.44     |
| 10:CK:80:ASN:H    | 10:CK:80:ASN:ND2   | 2.14        | 0.44     |
| 3:CD:169:TRP:CD2  | 3:CD:185:PRO:HB3   | 2.51        | 0.44     |
| 38:DM:69:PRO:HA   | 38:DM:94:ALA:HA    | 1.99        | 0.44     |
| 6:CG:41:ILE:CG2   | 6:CG:115:MET:HG3   | 2.47        | 0.44     |
| 23:DB:1204:A:N1   | 23:DB:1241:A:N1    | 2.65        | 0.44     |
| 1:AA:618:C:N3     | 1:AA:622:A:N6      | 2.65        | 0.44     |
| 25:DC:245:THR:OG1 | 25:DC:249:VAL:HG23 | 2.17        | 0.44     |
| 8:AI:9:GLY:CA     | 8:AI:80:HIS:HB3    | 2.47        | 0.44     |
| 24:BI:12:VAL:HG23 | 24:BI:41:PHE:CE2   | 2.53        | 0.44     |
| 23:BB:704:G:H1'   | 23:BB:727:A:H61    | 1.82        | 0.44     |
| 23:DB:1432:G:H2'  | 23:DB:1433:A:H8    | 1.82        | 0.44     |
| 23:DB:1684:G:O2'  | 23:DB:1685:C:H5'   | 2.18        | 0.44     |
| 23:DB:936:A:H2'   | 23:DB:937:C:H6     | 1.80        | 0.44     |
| 19:AT:71:ALA:O    | 19:AT:74:HIS:HB2   | 2.17        | 0.44     |
| 23:BB:1042:G:H2'  | 23:BB:1043:C:H6    | 1.81        | 0.44     |
| 1:AA:376:G:H2'    | 1:AA:377:G:H8      | 1.80        | 0.44     |
| 1:AA:376:G:O3'    | 15:AP:5:ARG:HD3    | 2.17        | 0.44     |
| 23:BB:1183:U:H2'  | 23:BB:1184:U:C6    | 2.52        | 0.44     |
| 17:CR:51:GLN:HE22 | 17:CR:54:LEU:HD22  | 1.82        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 16:CQ:30:HIS:HB3  | 16:CQ:33:TYR:HB2  | 1.97        | 0.44     |
| 6:AG:91:ARG:HD2   | 6:AG:91:ARG:H     | 1.82        | 0.44     |
| 23:BB:6:A:O2'     | 23:BB:7:G:H5'     | 2.18        | 0.44     |
| 20:AB:23:ASN:HD22 | 20:AB:24:PRO:CD   | 2.28        | 0.44     |
| 1:CA:1277:C:H1'   | 1:CA:1282:C:O2    | 2.18        | 0.44     |
| 43:BO:7:ARG:HA    | 43:BO:10:ARG:CD   | 2.47        | 0.44     |
| 1:CA:796:C:H2'    | 1:CA:797:C:H6     | 1.81        | 0.44     |
| 23:DB:6:A:O2'     | 23:DB:7:G:H5'     | 2.17        | 0.44     |
| 1:CA:818:G:H3'    | 1:CA:819:A:C5'    | 2.47        | 0.44     |
| 3:AD:81:LEU:C     | 3:AD:83:GLY:H     | 2.20        | 0.44     |
| 2:AC:16:PRO:HG2   | 2:AC:53:ARG:HH22  | 1.82        | 0.44     |
| 1:AA:153:C:O2'    | 1:AA:154:U:H5'    | 2.17        | 0.44     |
| 7:AH:29:SER:OG    | 7:AH:32:LYS:HG3   | 2.17        | 0.44     |
| 23:BB:2358:A:H2'  | 23:BB:2359:C:C6   | 2.52        | 0.44     |
| 48:DG:91:VAL:HG23 | 48:DG:92:GLY:N    | 2.31        | 0.44     |
| 29:BE:40:ARG:NH2  | 29:BE:92:HIS:NE2  | 2.65        | 0.44     |
| 17:CR:63:TYR:HD2  | 17:CR:63:TYR:N    | 2.15        | 0.44     |
| 7:AH:79:ARG:NH1   | 7:AH:82:LEU:HB3   | 2.32        | 0.44     |
| 23:BB:2757:A:H2   | 48:BG:63:GLN:NE2  | 2.14        | 0.44     |
| 23:DB:2595:G:N1   | 23:DB:2599:G:C6   | 2.85        | 0.44     |
| 23:DB:2818:U:H4'  | 23:DB:2837:A:O4'  | 2.18        | 0.44     |
| 23:BB:553:G:H2'   | 23:BB:554:U:O4'   | 2.16        | 0.44     |
| 1:AA:1363:A:H2'   | 1:AA:1363:A:N3    | 2.32        | 0.44     |
| 23:DB:622:G:H2'   | 23:DB:623:C:C6    | 2.52        | 0.44     |
| 25:DC:57:HIS:ND1  | 25:DC:58:LYS:N    | 2.59        | 0.44     |
| 40:DH:11:ASN:O    | 40:DH:12:LEU:HB3  | 2.17        | 0.44     |
| 23:BB:332:A:O2'   | 23:BB:334:C:OP2   | 2.34        | 0.44     |
| 1:CA:1345:U:H2'   | 57:CA:1747:HOH:O  | 2.16        | 0.44     |
| 23:DB:1973:G:O2'  | 23:DB:1974:C:H5'  | 2.17        | 0.44     |
| 1:CA:1496:C:H2'   | 1:CA:1497:G:O4'   | 2.17        | 0.44     |
| 1:AA:594:U:H2'    | 1:AA:595:A:C8     | 2.52        | 0.44     |
| 23:DB:1449:G:O2'  | 23:DB:1450:G:H5'  | 2.17        | 0.44     |
| 23:BB:2516:A:O2'  | 23:BB:2517:C:H5'  | 2.17        | 0.44     |
| 36:D2:3:ARG:NE    | 36:D2:3:ARG:HA    | 2.31        | 0.44     |
| 49:BR:70:GLU:CD   | 49:BR:70:GLU:N    | 2.69        | 0.44     |
| 14:CO:28:GLN:O    | 14:CO:32:LEU:HD23 | 2.16        | 0.44     |
| 1:AA:814:A:O2'    | 1:AA:815:A:H3'    | 2.18        | 0.44     |
| 23:BB:918:A:C2'   | 23:BB:919:U:H5'   | 2.43        | 0.44     |
| 10:CK:41:LEU:HD22 | 10:CK:76:TYR:CE2  | 2.52        | 0.44     |
| 37:DL:141:LYS:HD3 | 37:DL:141:LYS:C   | 2.38        | 0.44     |
| 16:CQ:45:VAL:HG11 | 16:CQ:60:ILE:CG2  | 2.46        | 0.44     |
| 22:DA:44:G:N2     | 22:DA:48:U:C2     | 2.86        | 0.44     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:852:U:H2'    | 23:DB:853:C:H6     | 1.82        | 0.44     |
| 52:DW:49:ASN:HB2   | 52:DW:60:ALA:CA    | 2.46        | 0.44     |
| 8:AI:119:LYS:C     | 8:AI:121:ARG:H     | 2.21        | 0.44     |
| 25:BC:140:VAL:HG12 | 25:BC:141:HIS:N    | 2.32        | 0.44     |
| 37:DL:112:LEU:O    | 37:DL:112:LEU:HD23 | 2.17        | 0.44     |
| 47:DF:79:ARG:HE    | 47:DF:79:ARG:H     | 1.64        | 0.44     |
| 45:BS:1:MET:SD     | 45:BS:62:ASP:HB3   | 2.57        | 0.44     |
| 43:DO:31:THR:HG23  | 43:DO:34:HIS:O     | 2.17        | 0.44     |
| 7:AH:101:ALA:O     | 7:AH:103:VAL:HG23  | 2.17        | 0.44     |
| 33:B1:33:LEU:HB3   | 33:B1:51:ALA:HB3   | 1.98        | 0.44     |
| 37:BL:51:GLU:OE1   | 37:BL:57:LEU:HB2   | 2.17        | 0.44     |
| 42:DN:52:ILE:HD13  | 42:DN:87:PHE:CE2   | 2.52        | 0.44     |
| 42:DN:83:LEU:HA    | 42:DN:86:ARG:HG3   | 1.99        | 0.44     |
| 40:DH:89:LYS:O     | 40:DH:90:LEU:C     | 2.55        | 0.44     |
| 42:BN:101:GLY:CA   | 42:BN:109:PRO:HA   | 2.46        | 0.44     |
| 12:CM:106:ARG:NH1  | 12:CM:109:LYS:HD2  | 2.20        | 0.44     |
| 1:CA:922:G:H2'     | 1:CA:923:A:H8      | 1.81        | 0.44     |
| 50:DT:42:GLU:O     | 50:DT:46:ALA:HB2   | 2.17        | 0.44     |
| 25:DC:14:HIS:O     | 25:DC:16:VAL:HG23  | 2.16        | 0.44     |
| 53:D6:18:LEU:HD21  | 53:D6:171:LYS:HG3  | 1.99        | 0.44     |
| 45:DS:32:ALA:O     | 45:DS:36:LEU:HD23  | 2.17        | 0.44     |
| 23:BB:2789:C:H2'   | 23:BB:2893:A:N7    | 2.32        | 0.44     |
| 2:CC:106:ARG:HG2   | 2:CC:106:ARG:O     | 2.16        | 0.44     |
| 53:B6:113:ASP:O    | 53:B6:116:ARG:HG2  | 2.17        | 0.44     |
| 26:DD:113:SER:HB3  | 26:DD:167:ASN:H    | 1.79        | 0.44     |
| 23:BB:1197:G:H2'   | 23:BB:1198:U:H6    | 1.82        | 0.44     |
| 23:BB:1727:C:H2'   | 23:BB:1728:C:O4'   | 2.17        | 0.44     |
| 26:BD:149:ASN:C    | 26:BD:152:PRO:HD2  | 2.38        | 0.44     |
| 31:D0:2:VAL:HG12   | 31:D0:3:GLN:N      | 2.33        | 0.44     |
| 46:DU:10:VAL:HG21  | 46:DU:35:VAL:HG21  | 1.98        | 0.44     |
| 10:AK:80:ASN:HA    | 10:AK:105:ARG:HB3  | 1.98        | 0.44     |
| 23:BB:2821:A:OP2   | 23:BB:2822:G:OP2   | 2.34        | 0.44     |
| 26:BD:112:THR:O    | 26:BD:113:SER:HB2  | 2.16        | 0.44     |
| 26:BD:116:LYS:HB3  | 26:BD:118:PHE:CE2  | 2.53        | 0.44     |
| 23:DB:2794:C:H2'   | 23:DB:2795:C:C6    | 2.52        | 0.44     |
| 12:CM:90:HIS:CE1   | 12:CM:96:VAL:HG21  | 2.53        | 0.44     |
| 12:AM:1:ALA:CA     | 12:AM:8:ILE:HG22   | 2.48        | 0.44     |
| 1:AA:617:G:H4'     | 15:AP:46:LYS:CE    | 2.46        | 0.44     |
| 23:DB:1724:G:H2'   | 23:DB:1725:U:H6    | 1.80        | 0.44     |
| 40:DH:96:THR:HG23  | 40:DH:97:ARG:N     | 2.29        | 0.44     |
| 35:DV:55:GLU:H     | 35:DV:55:GLU:CD    | 2.20        | 0.44     |
| 2:AC:129:PHE:CE2   | 2:AC:156:LEU:HD13  | 2.52        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DC:245:THR:C   | 25:DC:247:TRP:N   | 2.70        | 0.44     |
| 1:CA:618:C:N3     | 1:CA:622:A:N6     | 2.65        | 0.44     |
| 2:AC:119:ILE:HD11 | 2:AC:133:MET:HA   | 1.98        | 0.44     |
| 23:BB:1470:A:H2'  | 23:BB:1471:G:O4'  | 2.17        | 0.44     |
| 1:CA:676:A:H1'    | 10:CK:116:PRO:HB3 | 1.99        | 0.44     |
| 1:CA:482:A:C2     | 1:CA:483:C:H1'    | 2.51        | 0.44     |
| 1:CA:1385:G:O2'   | 1:CA:1386:G:H5'   | 2.17        | 0.44     |
| 23:DB:2700:A:H2'  | 23:DB:2701:U:C6   | 2.50        | 0.44     |
| 23:BB:1317:G:H2'  | 23:BB:1318:U:H6   | 1.82        | 0.44     |
| 23:DB:871:U:H2'   | 23:DB:872:U:C6    | 2.52        | 0.44     |
| 14:CO:36:ILE:HD11 | 14:CO:59:MET:HB2  | 2.00        | 0.44     |
| 23:DB:1092:C:H2'  | 23:DB:1093:G:C5'  | 2.47        | 0.44     |
| 19:CT:49:ALA:HA   | 19:CT:52:GLU:OE2  | 2.17        | 0.44     |
| 29:DE:40:ARG:NH2  | 29:DE:92:HIS:NE2  | 2.65        | 0.44     |
| 20:CB:62:ARG:HG3  | 20:CB:62:ARG:HH11 | 1.81        | 0.44     |
| 23:DB:2649:C:H2'  | 23:DB:2650:U:C6   | 2.52        | 0.44     |
| 1:CA:939:G:H2'    | 1:CA:940:C:C6     | 2.52        | 0.44     |
| 1:CA:729:A:H2'    | 1:CA:730:G:H8     | 1.82        | 0.44     |
| 1:CA:69:G:N2      | 1:CA:71:A:H62     | 2.15        | 0.44     |
| 46:BU:18:LYS:O    | 46:BU:20:LYS:N    | 2.50        | 0.44     |
| 24:BI:48:ILE:HG22 | 24:BI:49:GLU:HG2  | 1.98        | 0.44     |
| 23:BB:599:A:O2'   | 23:BB:600:G:H5'   | 2.17        | 0.44     |
| 23:BB:1370:C:H2'  | 23:BB:1371:G:C8   | 2.52        | 0.44     |
| 23:DB:1368:G:O2'  | 23:DB:1369:G:H5'  | 2.17        | 0.44     |
| 23:DB:2828:G:O2'  | 23:DB:2829:A:H5'  | 2.16        | 0.44     |
| 23:BB:2598:A:H5'' | 25:BC:233:GLY:CA  | 2.48        | 0.44     |
| 23:BB:2836:U:H2'  | 23:BB:2837:A:C8   | 2.53        | 0.44     |
| 7:CH:34:ALA:HB1   | 7:CH:109:VAL:HB   | 1.98        | 0.44     |
| 23:DB:2187:U:H2'  | 23:DB:2188:U:C6   | 2.52        | 0.44     |
| 1:AA:224:U:O2'    | 1:AA:225:C:H5'    | 2.17        | 0.44     |
| 23:BB:245:G:H2'   | 23:BB:246:C:H6    | 1.82        | 0.44     |
| 38:DM:54:THR:C    | 38:DM:56:ALA:H    | 2.21        | 0.44     |
| 12:CM:71:GLU:HA   | 12:CM:74:MET:SD   | 2.57        | 0.44     |
| 48:BG:60:GLY:O    | 48:BG:62:ALA:N    | 2.49        | 0.44     |
| 2:AC:38:VAL:HG23  | 2:AC:39:ARG:N     | 2.31        | 0.44     |
| 1:AA:1019:A:H2'   | 1:AA:1020:G:C8    | 2.53        | 0.44     |
| 1:AA:1023:U:O2'   | 1:AA:1024:G:H5'   | 2.18        | 0.44     |
| 23:BB:2693:G:H2'  | 23:BB:2694:G:H8   | 1.82        | 0.44     |
| 37:DL:14:LYS:O    | 37:DL:16:GLY:N    | 2.50        | 0.44     |
| 23:BB:1765:U:H2'  | 23:BB:1766:G:H8   | 1.82        | 0.44     |
| 23:DB:915:C:H3'   | 23:DB:916:G:H8    | 1.82        | 0.44     |
| 23:DB:288:U:O2    | 23:DB:288:U:H2'   | 2.16        | 0.44     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:CD:57:LYS:HD3    | 3:CD:57:LYS:C      | 2.38        | 0.44     |
| 23:BB:1130:U:C2    | 23:BB:2025:C:H5''  | 2.52        | 0.44     |
| 1:CA:140:U:H2'     | 1:CA:141:G:H8      | 1.81        | 0.44     |
| 23:DB:1098:A:H2'   | 24:DI:4:VAL:C      | 2.38        | 0.44     |
| 23:DB:2355:G:H4'   | 52:DW:20:LEU:HD12  | 1.99        | 0.44     |
| 48:BG:3:VAL:O      | 48:BG:68:ARG:HG3   | 2.18        | 0.44     |
| 25:DC:131:MET:C    | 25:DC:133:ASN:N    | 2.70        | 0.44     |
| 25:DC:52:HIS:NE2   | 25:DC:218:THR:HG23 | 2.33        | 0.44     |
| 48:BG:89:VAL:HG12  | 48:BG:90:GLY:H     | 1.83        | 0.44     |
| 40:BH:116:ARG:CB   | 40:BH:131:SER:HB2  | 2.37        | 0.44     |
| 40:BH:65:ALA:HB1   | 40:BH:68:ARG:NH1   | 2.32        | 0.44     |
| 53:B6:61:PRO:HB2   | 53:B6:62:ASP:OD1   | 2.18        | 0.44     |
| 53:B6:83:ILE:HG22  | 53:B6:90:LEU:H     | 1.81        | 0.44     |
| 1:CA:1251:A:H1'    | 1:CA:1370:G:O4'    | 2.17        | 0.44     |
| 41:BJ:25:LEU:HB2   | 41:BJ:62:VAL:CG2   | 2.47        | 0.44     |
| 41:DJ:44:TYR:CZ    | 44:DQ:59:LEU:HD11  | 2.52        | 0.44     |
| 41:DJ:59:ALA:O     | 41:DJ:62:VAL:HG12  | 2.17        | 0.44     |
| 30:DY:16:LEU:N     | 30:DY:16:LEU:HD22  | 2.16        | 0.44     |
| 50:BT:38:ALA:HB1   | 50:BT:43:ILE:CD1   | 2.47        | 0.44     |
| 3:CD:160:LEU:HD23  | 3:CD:164:ARG:NH2   | 2.32        | 0.44     |
| 3:CD:164:ARG:HG2   | 3:CD:164:ARG:NH1   | 2.32        | 0.44     |
| 46:DU:85:ARG:HA    | 46:DU:85:ARG:CZ    | 2.48        | 0.44     |
| 25:BC:90:ILE:HD13  | 25:BC:103:ILE:C    | 2.38        | 0.44     |
| 33:B1:8:ILE:HG21   | 33:B1:51:ALA:CB    | 2.47        | 0.44     |
| 42:BN:83:LEU:HA    | 42:BN:86:ARG:HG3   | 1.98        | 0.44     |
| 47:BF:134:GLN:HE21 | 47:BF:134:GLN:HB3  | 1.53        | 0.44     |
| 12:CM:10:ASP:HA    | 12:CM:44:ILE:CD1   | 2.46        | 0.44     |
| 12:CM:47:LEU:HD22  | 12:CM:51:GLN:HB3   | 1.98        | 0.44     |
| 23:BB:340:A:H2'    | 23:BB:341:C:O4'    | 2.18        | 0.44     |
| 4:AE:89:THR:HG21   | 4:AE:134:ASN:HD21  | 1.78        | 0.44     |
| 35:BV:44:HIS:NE2   | 35:BV:85:LYS:HB2   | 2.33        | 0.44     |
| 1:CA:923:A:OP1     | 4:CE:25:LYS:HB3    | 2.17        | 0.44     |
| 45:BS:15:GLN:HA    | 45:BS:18:ARG:HG2   | 1.99        | 0.44     |
| 23:BB:2109:U:C2'   | 23:BB:2110:G:H5'   | 2.47        | 0.44     |
| 23:DB:971:G:H2'    | 23:DB:972:A:O4'    | 2.17        | 0.44     |
| 3:CD:173:ASP:OD1   | 3:CD:176:LYS:HD3   | 2.17        | 0.44     |
| 13:AN:88:MET:C     | 13:AN:90:GLY:H     | 2.20        | 0.44     |
| 39:DX:28:LEU:HD13  | 39:DX:37:LEU:CD1   | 2.38        | 0.44     |
| 22:DA:105:G:O2'    | 22:DA:106:G:H5'    | 2.17        | 0.44     |
| 48:BG:144:ALA:HB1  | 48:BG:163:TYR:HE1  | 1.81        | 0.44     |
| 27:DK:20:MET:O     | 27:DK:41:ILE:HD12  | 2.18        | 0.44     |
| 44:BQ:8:ILE:O      | 44:BQ:11:ALA:HB3   | 2.17        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 10:CK:25:SER:HG   | 10:CK:28:ASN:H    | 1.65        | 0.44     |
| 23:DB:1199:U:H5'' | 57:DB:3621:HOH:O  | 2.16        | 0.44     |
| 1:AA:81:A:N3      | 1:AA:82:G:N7      | 2.65        | 0.44     |
| 5:CF:97:THR:O     | 5:CF:98:GLU:CD    | 2.56        | 0.44     |
| 16:CQ:18:LYS:H    | 16:CQ:50:ASN:HD21 | 1.65        | 0.44     |
| 39:DX:44:LYS:NZ   | 39:DX:48:ARG:CZ   | 2.81        | 0.44     |
| 1:AA:620:C:O2     | 3:AD:131:ILE:HG21 | 2.17        | 0.44     |
| 23:DB:2135:A:C2'  | 23:DB:2136:G:H5'  | 2.47        | 0.44     |
| 1:AA:1227:A:H4'   | 12:AM:113:LYS:HD3 | 1.99        | 0.44     |
| 1:AA:58:C:O2'     | 1:AA:59:A:H5'     | 2.17        | 0.44     |
| 20:CB:22:TRP:CG   | 20:CB:23:ASN:N    | 2.82        | 0.44     |
| 1:CA:376:G:H5''   | 15:CP:5:ARG:HB2   | 1.99        | 0.44     |
| 23:DB:1316:U:H2'  | 23:DB:1317:G:C8   | 2.53        | 0.44     |
| 23:DB:1317:G:H2'  | 23:DB:1318:U:H6   | 1.81        | 0.44     |
| 1:AA:499:A:H1'    | 1:AA:500:G:C8     | 2.53        | 0.44     |
| 41:DJ:13:ARG:HB3  | 41:DJ:53:TYR:HD2  | 1.83        | 0.44     |
| 23:BB:2369:A:H2'  | 23:BB:2370:G:C8   | 2.51        | 0.44     |
| 16:AQ:30:HIS:HB3  | 16:AQ:33:TYR:HB2  | 1.98        | 0.44     |
| 22:BA:94:A:O2'    | 22:BA:95:U:H5'    | 2.18        | 0.44     |
| 31:B0:12:ARG:HD2  | 31:B0:16:ARG:NH1  | 2.32        | 0.44     |
| 23:BB:936:A:H2'   | 23:BB:937:C:H6    | 1.78        | 0.44     |
| 1:CA:167:A:H2'    | 1:CA:168:G:H8     | 1.82        | 0.44     |
| 46:BU:18:LYS:HD2  | 46:BU:19:GLY:N    | 2.32        | 0.44     |
| 23:BB:1749:A:H2'  | 23:BB:1750:G:C8   | 2.53        | 0.44     |
| 1:CA:26:A:N6      | 1:CA:558:G:H1'    | 2.32        | 0.44     |
| 23:BB:1843:C:H2'  | 23:BB:1844:C:H6   | 1.82        | 0.44     |
| 23:BB:840:C:H2'   | 23:BB:841:G:C8    | 2.52        | 0.44     |
| 3:AD:43:ARG:HB3   | 3:AD:43:ARG:NH1   | 2.32        | 0.44     |
| 29:DE:3:LEU:O     | 29:DE:12:LEU:HD23 | 2.17        | 0.44     |
| 5:AF:46:GLN:HE21  | 5:AF:46:GLN:HA    | 1.81        | 0.44     |
| 23:BB:285:G:O2'   | 23:BB:286:U:H5'   | 2.16        | 0.44     |
| 2:AC:180:ASP:OD1  | 2:AC:203:LYS:HB2  | 2.18        | 0.44     |
| 2:AC:32:LEU:O     | 2:AC:35:ASP:HB2   | 2.17        | 0.44     |
| 1:CA:814:A:O2'    | 1:CA:815:A:H3'    | 2.17        | 0.44     |
| 23:DB:1845:G:C6   | 23:DB:1896:G:C6   | 3.06        | 0.44     |
| 38:BM:29:GLY:HA2  | 38:BM:106:ASP:HB2 | 1.99        | 0.44     |
| 42:BN:11:ASN:HD22 | 42:BN:11:ASN:HA   | 1.53        | 0.44     |
| 23:DB:1098:A:O2'  | 24:DI:4:VAL:C     | 2.56        | 0.44     |
| 2:CC:122:GLN:O    | 2:CC:127:VAL:HG22 | 2.17        | 0.44     |
| 44:BQ:24:TYR:CG   | 44:BQ:25:GLY:N    | 2.86        | 0.44     |
| 44:BQ:33:VAL:O    | 44:BQ:37:ALA:N    | 2.51        | 0.44     |
| 48:DG:104:LEU:O   | 48:DG:111:PRO:HA  | 2.17        | 0.44     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 16:CQ:74:LEU:HD22  | 16:CQ:75:VAL:H     | 1.83        | 0.44     |
| 1:CA:1148:U:H2'    | 1:CA:1149:C:O4'    | 2.17        | 0.44     |
| 44:DQ:79:ILE:C     | 44:DQ:79:ILE:HD13  | 2.38        | 0.44     |
| 8:AI:90:ASP:O      | 8:AI:93:LEU:HG     | 2.16        | 0.44     |
| 25:BC:114:GLN:HB3  | 25:BC:114:GLN:HE21 | 1.62        | 0.44     |
| 13:AN:5:MET:HE2    | 13:AN:60:ARG:NH1   | 2.33        | 0.44     |
| 13:CN:70:HIS:O     | 13:CN:72:PHE:N     | 2.49        | 0.44     |
| 48:DG:17:LYS:HZ2   | 48:DG:18:ILE:H     | 1.65        | 0.44     |
| 23:DB:675:A:N3     | 23:DB:2443:C:O2'   | 2.50        | 0.44     |
| 1:CA:600:A:H2'     | 1:CA:601:G:H8      | 1.82        | 0.44     |
| 50:BT:10:VAL:O     | 50:BT:11:LEU:C     | 2.55        | 0.44     |
| 12:CM:13:HIS:HB2   | 12:CM:16:ILE:HG22  | 1.98        | 0.44     |
| 34:B3:36:ALA:HB3   | 34:B3:39:ARG:HB2   | 1.99        | 0.44     |
| 12:CM:53:ASP:HA    | 12:CM:56:ARG:NH2   | 2.32        | 0.44     |
| 12:CM:3:ILE:CA     | 12:CM:56:ARG:HG2   | 2.44        | 0.44     |
| 47:BF:3:LEU:HD11   | 47:BF:172:PHE:CD1  | 2.52        | 0.44     |
| 47:DF:138:PRO:HA   | 47:DF:142:TYR:CZ   | 2.53        | 0.44     |
| 12:CM:109:LYS:HG3  | 12:CM:110:GLY:H    | 1.83        | 0.44     |
| 1:CA:1227:A:O3'    | 12:CM:113:LYS:HB2  | 2.18        | 0.44     |
| 1:CA:1076:U:H2'    | 1:CA:1077:G:C8     | 2.52        | 0.44     |
| 1:AA:1270:G:H2'    | 1:AA:1271:A:C8     | 2.51        | 0.44     |
| 1:AA:1361:G:C2'    | 1:AA:1362:A:H5''   | 2.44        | 0.44     |
| 33:D1:33:LEU:HB3   | 33:D1:51:ALA:HB3   | 1.99        | 0.44     |
| 11:AL:89:LEU:HD22  | 11:AL:89:LEU:N     | 2.33        | 0.44     |
| 23:BB:673:C:H4'    | 29:BE:77:ILE:HD11  | 1.99        | 0.44     |
| 23:BB:2472:G:O6    | 23:BB:2476:A:H4'   | 2.18        | 0.44     |
| 25:DC:202:ARG:HH21 | 25:DC:202:ARG:HB2  | 1.83        | 0.44     |
| 39:DX:27:ASN:O     | 39:DX:28:LEU:C     | 2.56        | 0.44     |
| 38:BM:53:MET:SD    | 38:BM:63:ILE:HG21  | 2.57        | 0.44     |
| 27:DK:110:GLU:HA   | 27:DK:113:MET:HG2  | 2.00        | 0.44     |
| 44:DQ:108:LEU:O    | 44:DQ:111:LYS:HB3  | 2.18        | 0.44     |
| 37:DL:85:VAL:HG22  | 37:DL:94:THR:HG21  | 1.99        | 0.44     |
| 3:AD:152:SER:O     | 3:AD:155:LYS:HG2   | 2.18        | 0.44     |
| 1:AA:845:A:C5      | 1:AA:846:G:H1'     | 2.53        | 0.44     |
| 48:BG:75:VAL:O     | 48:BG:78:VAL:HG22  | 2.17        | 0.44     |
| 29:DE:154:ASP:C    | 29:DE:156:ASN:H    | 2.21        | 0.44     |
| 23:DB:1418:G:C2'   | 23:DB:1580:A:H61   | 2.30        | 0.44     |
| 5:AF:61:LEU:HD12   | 5:AF:63:ASN:OD1    | 2.18        | 0.44     |
| 26:BD:69:ALA:N     | 26:BD:73:VAL:HB    | 2.32        | 0.44     |
| 14:AO:81:LEU:O     | 14:AO:85:LEU:HD13  | 2.18        | 0.44     |
| 12:AM:90:HIS:CE1   | 12:AM:96:VAL:HG21  | 2.51        | 0.44     |
| 31:B0:2:VAL:HG12   | 31:B0:3:GLN:N      | 2.32        | 0.44     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 28:DP:31:VAL:HG13  | 28:DP:32:VAL:N    | 2.33        | 0.44     |
| 4:CE:81:GLN:CD     | 4:CE:148:SER:HA   | 2.37        | 0.44     |
| 4:CE:158:LYS:HZ1   | 7:CH:65:PHE:HA    | 1.80        | 0.44     |
| 11:AL:33:CYS:HB2   | 11:AL:77:SER:O    | 2.18        | 0.44     |
| 29:BE:48:THR:C     | 29:BE:50:ALA:N    | 2.71        | 0.44     |
| 1:AA:15:G:H2'      | 1:AA:16:A:H8      | 1.82        | 0.44     |
| 29:BE:148:ILE:HD13 | 29:BE:187:VAL:CG2 | 2.43        | 0.44     |
| 6:AG:57:GLU:O      | 6:AG:61:PHE:N     | 2.48        | 0.44     |
| 1:AA:191:G:H8      | 1:AA:191:G:OP2    | 1.99        | 0.44     |
| 23:DB:51:G:O2'     | 23:DB:119:A:N1    | 2.44        | 0.44     |
| 46:DU:48:VAL:O     | 46:DU:48:VAL:HG22 | 2.18        | 0.44     |
| 23:DB:2339:C:H2'   | 23:DB:2340:A:H8   | 1.81        | 0.44     |
| 25:BC:30:ALA:C     | 25:BC:32:LEU:H    | 2.21        | 0.44     |
| 23:BB:2217:G:H2'   | 23:BB:2218:G:H8   | 1.83        | 0.44     |
| 4:CE:106:ALA:HB1   | 4:CE:110:MET:CB   | 2.45        | 0.44     |
| 11:CL:33:CYS:H     | 11:CL:54:VAL:HG13 | 1.82        | 0.44     |
| 44:DQ:65:ASN:CB    | 44:DQ:75:TYR:HB2  | 2.47        | 0.44     |
| 23:DB:866:A:H61    | 23:DB:913:U:C1'   | 2.30        | 0.44     |
| 14:CO:56:LEU:O     | 14:CO:59:MET:HG3  | 2.18        | 0.44     |
| 31:D0:16:ARG:O     | 31:D0:19:ASP:HB2  | 2.18        | 0.44     |
| 1:AA:1517:G:H1'    | 23:BB:1919:A:O3'  | 2.18        | 0.44     |
| 23:DB:755:U:H2'    | 23:DB:756:A:H8    | 1.82        | 0.44     |
| 41:DJ:106:LYS:HD2  | 41:DJ:106:LYS:HA  | 1.84        | 0.44     |
| 23:DB:1201:U:H2'   | 23:DB:1202:G:C8   | 2.51        | 0.44     |
| 1:CA:1097:C:H2'    | 1:CA:1098:C:C6    | 2.53        | 0.44     |
| 49:BR:91:GLN:HG3   | 49:BR:92:TRP:N    | 2.32        | 0.44     |
| 17:AR:22:TYR:CZ    | 17:AR:23:LYS:HE3  | 2.53        | 0.44     |
| 40:BH:25:TYR:CZ    | 40:BH:30:LEU:HD21 | 2.52        | 0.44     |
| 3:CD:22:SER:N      | 3:CD:109:THR:HG22 | 2.32        | 0.44     |
| 23:DB:248:G:N7     | 23:DB:250:G:N3    | 2.66        | 0.44     |
| 23:DB:1517:G:O2'   | 23:DB:1518:C:H5'  | 2.17        | 0.44     |
| 23:BB:2181:U:H2'   | 23:BB:2182:U:C6   | 2.51        | 0.44     |
| 23:BB:1712:U:H2'   | 23:BB:1713:A:C8   | 2.53        | 0.44     |
| 23:BB:1893:C:H2'   | 23:BB:1894:C:O4'  | 2.18        | 0.44     |
| 23:DB:1144:A:O2'   | 23:DB:1145:C:H5'  | 2.18        | 0.44     |
| 46:BU:94:PHE:HB3   | 46:BU:101:THR:HA  | 1.99        | 0.44     |
| 1:AA:1198:G:H2'    | 1:AA:1199:U:C6    | 2.52        | 0.44     |
| 11:AL:23:LEU:O     | 11:AL:25:ALA:N    | 2.51        | 0.44     |
| 34:D3:9:ALA:C      | 34:D3:11:LYS:H    | 2.21        | 0.44     |
| 23:DB:1996:C:OP1   | 27:DK:31:ARG:CZ   | 2.66        | 0.44     |
| 5:AF:55:HIS:O      | 5:AF:56:LYS:HG3   | 2.17        | 0.44     |
| 23:DB:1462:C:O2'   | 23:DB:1463:C:H5'  | 2.17        | 0.44     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1228:G:H2'  | 23:BB:1229:C:H6    | 1.83        | 0.44     |
| 23:BB:2714:G:O2'  | 23:BB:2715:C:H5'   | 2.17        | 0.44     |
| 1:AA:711:G:O2'    | 1:AA:712:A:H5'     | 2.17        | 0.44     |
| 1:AA:1439:G:H2'   | 1:AA:1440:U:O4'    | 2.17        | 0.44     |
| 37:BL:81:ASP:O    | 37:BL:83:ALA:N     | 2.44        | 0.44     |
| 1:AA:1265:C:O2'   | 1:AA:1266:G:H5'    | 2.17        | 0.44     |
| 26:BD:56:LYS:C    | 26:BD:58:ASN:N     | 2.71        | 0.44     |
| 52:BW:23:LYS:H    | 52:BW:68:PHE:HE2   | 1.66        | 0.44     |
| 52:DW:35:ILE:O    | 52:DW:37:VAL:N     | 2.51        | 0.44     |
| 23:DB:1824:G:O2'  | 23:DB:1825:U:H5'   | 2.17        | 0.44     |
| 23:BB:17:G:H2'    | 23:BB:18:U:H6      | 1.81        | 0.44     |
| 23:BB:2667:C:H2'  | 23:BB:2668:G:O4'   | 2.17        | 0.44     |
| 44:DQ:20:ALA:HA   | 44:DQ:23:TYR:CE1   | 2.52        | 0.44     |
| 40:BH:133:GLN:HG2 | 40:BH:139:PHE:CD2  | 2.51        | 0.44     |
| 53:D6:81:LYS:HA   | 53:D6:84:ARG:HH22  | 1.80        | 0.44     |
| 53:D6:90:LEU:HB3  | 53:D6:101:ILE:CG2  | 2.47        | 0.44     |
| 23:DB:2365:G:H4'  | 52:DW:59:PHE:CD1   | 2.53        | 0.44     |
| 53:B6:83:ILE:CG2  | 53:B6:90:LEU:HD12  | 2.46        | 0.44     |
| 53:B6:80:GLU:OE1  | 53:B6:91:ASN:ND2   | 2.50        | 0.44     |
| 40:BH:84:ALA:HA   | 40:BH:91:PHE:N     | 2.31        | 0.44     |
| 8:CI:114:LYS:H    | 8:CI:120:ALA:HA    | 1.83        | 0.44     |
| 41:BJ:28:LEU:HG   | 41:BJ:32:LEU:HD12  | 1.99        | 0.44     |
| 8:AI:15:ALA:O     | 8:AI:66:VAL:HG23   | 2.17        | 0.44     |
| 8:AI:120:ALA:O    | 8:AI:121:ARG:HG2   | 2.18        | 0.44     |
| 23:DB:2312:U:H5'  | 47:DF:84:ILE:HD12  | 1.99        | 0.44     |
| 2:AC:87:ARG:HG2   | 2:AC:98:ALA:O      | 2.17        | 0.44     |
| 7:AH:124:ILE:HG22 | 7:AH:125:ILE:N     | 2.32        | 0.44     |
| 23:BB:397:U:OP1   | 51:BZ:31:PRO:HA    | 2.18        | 0.44     |
| 37:BL:78:ARG:HB3  | 37:BL:113:ALA:HB2  | 1.98        | 0.44     |
| 40:DH:87:GLU:HB2  | 40:DH:89:LYS:HZ2   | 1.81        | 0.44     |
| 47:DF:102:LEU:C   | 47:DF:102:LEU:HD13 | 2.38        | 0.44     |
| 47:DF:106:ALA:HA  | 47:DF:135:ILE:HD11 | 2.00        | 0.44     |
| 13:AN:40:ARG:O    | 13:AN:41:TRP:HE3   | 2.01        | 0.44     |
| 18:AS:47:THR:HA   | 18:AS:60:PHE:CD1   | 2.53        | 0.44     |
| 23:BB:1091:G:O2'  | 23:BB:1092:C:H5'   | 2.17        | 0.44     |
| 23:DB:2893:A:H4'  | 23:DB:2894:G:C5'   | 2.48        | 0.44     |
| 23:DB:2787:C:H5'  | 26:DD:66:GLY:HA3   | 1.99        | 0.44     |
| 23:DB:1023:U:H2'  | 23:DB:1024:G:C5'   | 2.47        | 0.44     |
| 34:D3:31:ILE:HG12 | 34:D3:31:ILE:O     | 2.17        | 0.44     |
| 9:CJ:56:HIS:O     | 9:CJ:57:VAL:HG12   | 2.16        | 0.44     |
| 27:BK:5:GLN:HA    | 27:BK:20:MET:SD    | 2.58        | 0.44     |
| 8:CI:87:MET:HB2   | 8:CI:94:ARG:CD     | 2.47        | 0.44     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 49:DR:16:GLU:HG2   | 49:DR:101:ILE:CG1 | 2.48        | 0.44     |
| 10:CK:28:ASN:HD22  | 10:CK:29:THR:H    | 1.64        | 0.44     |
| 23:DB:783:A:H4'    | 23:DB:1779:U:O2   | 2.17        | 0.44     |
| 44:DQ:8:ILE:O      | 44:DQ:11:ALA:HB3  | 2.18        | 0.44     |
| 1:AA:1057:G:H2'    | 1:AA:1058:G:O4'   | 2.16        | 0.44     |
| 3:AD:171:GLU:O     | 3:AD:180:THR:N    | 2.51        | 0.44     |
| 3:AD:89:LEU:CD2    | 3:AD:199:ILE:HD11 | 2.48        | 0.44     |
| 1:CA:1048:G:OP1    | 13:CN:3:GLN:HB2   | 2.17        | 0.44     |
| 23:BB:557:C:H2'    | 23:BB:558:U:H6    | 1.80        | 0.44     |
| 3:CD:104:MET:CE    | 3:CD:170:LEU:HD13 | 2.48        | 0.44     |
| 1:AA:441:A:N6      | 1:AA:493:A:N6     | 2.65        | 0.44     |
| 1:AA:472:U:H2'     | 1:AA:473:U:C6     | 2.51        | 0.44     |
| 23:BB:419:U:H2'    | 23:BB:420:C:H6    | 1.80        | 0.44     |
| 1:CA:1085:U:H3'    | 1:CA:1086:U:C5    | 2.52        | 0.44     |
| 23:BB:2462:C:H2'   | 23:BB:2463:C:H6   | 1.83        | 0.44     |
| 23:DB:1572:A:O2'   | 23:DB:1573:G:H5'  | 2.18        | 0.44     |
| 23:DB:1260:A:H2'   | 23:DB:1261:C:H6   | 1.83        | 0.44     |
| 37:BL:127:VAL:HG22 | 37:BL:128:THR:N   | 2.32        | 0.44     |
| 11:AL:14:LYS:CG    | 11:AL:15:VAL:N    | 2.80        | 0.44     |
| 28:DP:24:THR:C     | 28:DP:25:VAL:HG13 | 2.37        | 0.44     |
| 23:DB:692:C:H2'    | 23:DB:693:A:H8    | 1.83        | 0.44     |
| 1:CA:375:U:O2'     | 1:CA:376:G:H5'    | 2.17        | 0.44     |
| 1:CA:389:A:H3'     | 1:CA:390:U:H6     | 1.82        | 0.44     |
| 23:BB:1316:U:H2'   | 23:BB:1317:G:H8   | 1.81        | 0.44     |
| 23:BB:1573:G:C2'   | 23:BB:1574:C:H5'  | 2.47        | 0.44     |
| 23:DB:2368:C:H2'   | 23:DB:2369:A:C8   | 2.53        | 0.44     |
| 1:AA:1333:A:H2'    | 1:AA:1334:G:O4'   | 2.17        | 0.44     |
| 23:BB:958:U:H3     | 38:BM:16:ARG:HB3  | 1.82        | 0.44     |
| 1:AA:1458:G:O3'    | 19:AT:22:SER:HA   | 2.17        | 0.44     |
| 23:DB:1883:U:H2'   | 23:DB:1884:G:O4'  | 2.18        | 0.44     |
| 22:DA:8:C:H4'      | 43:DO:27:VAL:HG21 | 2.00        | 0.44     |
| 1:CA:584:G:O2'     | 1:CA:585:G:H5'    | 2.18        | 0.44     |
| 23:DB:234:U:O2'    | 23:DB:235:U:H5'   | 2.17        | 0.44     |
| 19:CT:27:MET:CE    | 19:CT:28:ARG:HG2  | 2.48        | 0.44     |
| 23:DB:955:U:OP1    | 38:DM:86:LYS:HE3  | 2.18        | 0.44     |
| 15:CP:34:GLU:CD    | 15:CP:60:TRP:HE1  | 2.21        | 0.44     |
| 49:BR:58:VAL:O     | 49:BR:58:VAL:HG13 | 2.16        | 0.44     |
| 6:CG:72:VAL:HA     | 6:CG:89:GLU:HA    | 2.00        | 0.44     |
| 23:DB:1849:G:H2'   | 23:DB:1850:G:C8   | 2.51        | 0.44     |
| 1:CA:96:U:H2'      | 1:CA:97:G:H8      | 1.82        | 0.44     |
| 1:AA:766:A:H2'     | 1:AA:767:A:C8     | 2.53        | 0.44     |
| 23:BB:1107:G:O2'   | 23:BB:1108:U:H5'  | 2.18        | 0.44     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 34:B3:9:ALA:C      | 34:B3:11:LYS:H     | 2.20        | 0.44     |
| 22:DA:80:U:H2'     | 22:DA:81:G:C8      | 2.52        | 0.44     |
| 1:CA:248:C:O2'     | 1:CA:249:U:H5'     | 2.18        | 0.44     |
| 3:CD:81:LEU:C      | 3:CD:83:GLY:H      | 2.19        | 0.44     |
| 15:CP:10:GLY:HA3   | 15:CP:15:PRO:HA    | 1.99        | 0.44     |
| 23:BB:2485:G:O2'   | 23:BB:2486:C:H5'   | 2.17        | 0.44     |
| 1:AA:1202:U:H2'    | 1:AA:1203:C:O4'    | 2.17        | 0.44     |
| 23:DB:531:C:O2'    | 23:DB:563:A:H5''   | 2.17        | 0.44     |
| 1:CA:1292:G:H2'    | 1:CA:1293:C:C6     | 2.51        | 0.44     |
| 23:DB:1366:A:H2'   | 23:DB:1367:A:O4'   | 2.17        | 0.44     |
| 49:DR:74:ILE:HB    | 49:DR:87:GLN:O     | 2.17        | 0.44     |
| 6:AG:11:ILE:HD12   | 6:AG:11:ILE:H      | 1.82        | 0.44     |
| 1:AA:1429:A:O2'    | 1:AA:1430:A:H5'    | 2.17        | 0.44     |
| 1:AA:1241:G:O2'    | 1:AA:1242:G:H5'    | 2.17        | 0.44     |
| 25:BC:131:MET:CE   | 25:BC:189:ALA:HB2  | 2.47        | 0.44     |
| 25:DC:107:LYS:N    | 25:DC:193:GLU:O    | 2.50        | 0.44     |
| 47:BF:91:ARG:HD3   | 47:BF:91:ARG:N     | 2.32        | 0.44     |
| 48:DG:3:VAL:O      | 48:DG:68:ARG:HG3   | 2.17        | 0.44     |
| 16:CQ:66:LEU:HD12  | 16:CQ:70:LYS:HG2   | 1.98        | 0.44     |
| 53:D6:84:ARG:NH1   | 53:D6:92:PRO:HG2   | 2.32        | 0.44     |
| 52:DW:61:LYS:HB3   | 52:DW:62:ALA:H     | 1.43        | 0.44     |
| 8:CI:5:TYR:HB3     | 8:CI:88:GLU:OE2    | 2.18        | 0.44     |
| 1:CA:1287:A:H1'    | 1:CA:1353:G:O2'    | 2.17        | 0.44     |
| 1:AA:1128:C:H4'    | 1:AA:1148:U:O2     | 2.17        | 0.44     |
| 8:AI:56:MET:CG     | 8:AI:57:VAL:N      | 2.81        | 0.44     |
| 8:AI:21:LYS:HB3    | 8:AI:61:ASP:O      | 2.17        | 0.44     |
| 1:AA:1348:U:H4'    | 8:AI:121:ARG:HE    | 1.82        | 0.44     |
| 37:DL:111:ILE:HD13 | 37:DL:128:THR:HG23 | 1.98        | 0.44     |
| 45:DS:61:ASN:HB3   | 45:DS:62:ASP:H     | 1.45        | 0.44     |
| 7:CH:77:VAL:HG12   | 7:CH:78:SER:N      | 2.32        | 0.44     |
| 23:DB:2734:A:H2'   | 23:DB:2735:G:C5'   | 2.45        | 0.44     |
| 30:BY:12:ALA:HB2   | 30:BY:53:MET:HE1   | 1.99        | 0.44     |
| 47:BF:78:ILE:CA    | 47:BF:79:ARG:HH11  | 2.31        | 0.44     |
| 23:BB:1076:C:H2'   | 23:BB:1077:A:C8    | 2.52        | 0.44     |
| 23:DB:2882:A:OP1   | 42:DN:96:ARG:HD2   | 2.17        | 0.44     |
| 45:DS:12:SER:O     | 45:DS:13:SER:HB3   | 2.17        | 0.44     |
| 25:DC:180:MET:HB2  | 25:DC:268:ARG:H    | 1.82        | 0.44     |
| 23:BB:1025:G:H8    | 23:BB:1025:G:OP1   | 2.00        | 0.44     |
| 23:BB:673:C:H5''   | 29:BE:76:PRO:HD2   | 2.00        | 0.44     |
| 23:BB:1072:C:N3    | 23:BB:1092:C:N4    | 2.64        | 0.44     |
| 45:DS:69:LEU:HG    | 45:DS:107:VAL:HG22 | 1.98        | 0.44     |
| 6:CG:2:ARG:HH11    | 6:CG:2:ARG:CB      | 2.20        | 0.44     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 53:B6:107:THR:HG22 | 53:B6:108:GLU:N   | 2.32        | 0.44     |
| 10:CK:89:GLY:O     | 10:CK:92:ARG:HB2  | 2.18        | 0.44     |
| 32:D4:15:LYS:O     | 32:D4:16:ILE:HB   | 2.17        | 0.44     |
| 13:CN:26:LEU:CD1   | 13:CN:44:VAL:HG22 | 2.47        | 0.44     |
| 48:BG:147:LEU:HA   | 48:BG:150:TYR:HD1 | 1.82        | 0.44     |
| 48:BG:86:LEU:HD23  | 48:BG:162:ARG:O   | 2.18        | 0.44     |
| 1:AA:1269:A:N3     | 1:AA:1326:U:H1'   | 2.32        | 0.44     |
| 8:CI:87:MET:HB2    | 8:CI:94:ARG:HD3   | 1.99        | 0.44     |
| 3:CD:123:MET:HG3   | 3:CD:127:ARG:C    | 2.37        | 0.44     |
| 27:BK:121:GLU:O    | 27:BK:122:VAL:C   | 2.55        | 0.44     |
| 3:AD:126:GLY:O     | 3:AD:127:ARG:HD2  | 2.18        | 0.44     |
| 4:CE:52:ALA:N      | 4:CE:58:ALA:HB2   | 2.32        | 0.44     |
| 9:AJ:12:ALA:HB3    | 9:AJ:18:ILE:HB    | 2.00        | 0.44     |
| 48:BG:30:GLY:HA3   | 48:BG:78:VAL:CA   | 2.41        | 0.44     |
| 23:BB:2772:C:H2'   | 23:BB:2773:C:H6   | 1.82        | 0.44     |
| 23:DB:357:C:H2'    | 23:DB:358:U:H6    | 1.80        | 0.44     |
| 23:DB:684:G:C6     | 23:DB:774:G:C4    | 3.05        | 0.44     |
| 15:CP:46:LYS:C     | 15:CP:48:GLU:H    | 2.21        | 0.44     |
| 23:BB:265:A:O2'    | 23:BB:266:G:H4'   | 2.17        | 0.44     |
| 23:DB:1138:G:H21   | 41:DJ:108:MET:CE  | 2.30        | 0.44     |
| 39:BX:44:LYS:NZ    | 39:BX:48:ARG:CZ   | 2.80        | 0.44     |
| 52:DW:44:PHE:HB3   | 52:DW:78:PHE:CE1  | 2.53        | 0.44     |
| 1:CA:1514:G:H2'    | 1:CA:1515:G:C8    | 2.52        | 0.44     |
| 23:BB:1372:U:H1'   | 23:BB:2214:C:C4   | 2.53        | 0.44     |
| 53:D6:62:ASP:HB2   | 53:D6:64:ARG:NH1  | 2.32        | 0.44     |
| 25:BC:245:THR:HG23 | 25:BC:249:VAL:HB  | 2.00        | 0.44     |
| 23:BB:506:G:H1'    | 23:BB:507:A:C8    | 2.52        | 0.44     |
| 41:DJ:35:ARG:HG3   | 41:DJ:52:ASP:OD1  | 2.18        | 0.44     |
| 23:DB:1292:G:H2'   | 23:DB:1293:C:H6   | 1.81        | 0.44     |
| 14:AO:59:MET:HG2   | 14:AO:59:MET:H    | 1.49        | 0.44     |
| 27:BK:76:VAL:HG12  | 27:BK:77:ILE:N    | 2.32        | 0.44     |
| 23:DB:2511:U:H2'   | 23:DB:2512:C:C6   | 2.53        | 0.44     |
| 23:BB:690:G:N3     | 25:BC:42:ARG:NH2  | 2.66        | 0.44     |
| 1:AA:518:C:H2'     | 1:AA:530:G:H8     | 1.80        | 0.44     |
| 17:AR:27:THR:HG22  | 17:AR:31:TYR:HE1  | 1.83        | 0.44     |
| 1:AA:900:A:O2'     | 1:AA:901:A:H5'    | 2.17        | 0.44     |
| 23:DB:2758:A:C2'   | 23:DB:2759:G:H5'  | 2.47        | 0.44     |
| 1:CA:900:A:O2'     | 1:CA:901:A:H5'    | 2.17        | 0.44     |
| 23:DB:1052:C:H2'   | 23:DB:1053:C:H6   | 1.82        | 0.44     |
| 23:BB:2818:U:O2'   | 23:BB:2819:G:H5'  | 2.18        | 0.44     |
| 32:B4:27:CYS:CB    | 32:B4:33:HIS:HB2  | 2.48        | 0.44     |
| 1:CA:159:G:H5'     | 1:CA:160:A:OP2    | 2.17        | 0.44     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1387:G:H2'    | 1:AA:1388:C:C6     | 2.52        | 0.44     |
| 23:DB:1870:C:H5''  | 23:DB:1871:A:C6    | 2.52        | 0.44     |
| 38:DM:110:GLU:HG2  | 38:DM:111:GLU:N    | 2.33        | 0.44     |
| 23:BB:820:A:H2'    | 23:BB:821:A:O4'    | 2.18        | 0.44     |
| 1:AA:1415:G:O2'    | 1:AA:1416:G:H5'    | 2.18        | 0.44     |
| 23:BB:1136:G:H2'   | 23:BB:1137:G:H8    | 1.81        | 0.44     |
| 1:CA:1229:A:H2'    | 1:CA:1230:C:C6     | 2.52        | 0.44     |
| 23:BB:2327:A:N7    | 23:BB:2388:A:N6    | 2.65        | 0.44     |
| 23:BB:2353:G:H1'   | 52:BW:30:VAL:CG1   | 2.48        | 0.44     |
| 44:BQ:24:TYR:CD1   | 44:BQ:25:GLY:N     | 2.86        | 0.44     |
| 44:DQ:24:TYR:CG    | 44:DQ:25:GLY:N     | 2.86        | 0.44     |
| 44:DQ:29:ARG:HG2   | 44:DQ:29:ARG:NH1   | 2.33        | 0.44     |
| 37:DL:125:LEU:HB2  | 37:DL:143:GLU:OE2  | 2.17        | 0.44     |
| 53:B6:44:GLU:CA    | 53:B6:49:HIS:HA    | 2.36        | 0.44     |
| 40:BH:117:LEU:HD13 | 40:BH:121:VAL:HG23 | 1.99        | 0.44     |
| 1:CA:1346:A:H5''   | 8:CI:121:ARG:HH21  | 1.83        | 0.44     |
| 20:CB:204:ASP:O    | 20:CB:205:ALA:HB3  | 2.17        | 0.44     |
| 23:DB:625:G:O2'    | 23:DB:626:A:H5'    | 2.18        | 0.44     |
| 41:DJ:25:LEU:HB2   | 41:DJ:62:VAL:HG22  | 2.00        | 0.44     |
| 7:AH:86:LYS:CG     | 7:AH:124:ILE:HD11  | 2.47        | 0.44     |
| 50:BT:11:LEU:N     | 50:BT:11:LEU:HD22  | 2.27        | 0.44     |
| 40:DH:143:ILE:HG22 | 40:DH:144:VAL:N    | 2.33        | 0.44     |
| 46:BU:87:GLU:OE2   | 46:BU:88:ASP:HB3   | 2.17        | 0.44     |
| 37:BL:3:LEU:O      | 37:BL:5:THR:N      | 2.50        | 0.44     |
| 47:BF:138:PRO:HA   | 47:BF:142:TYR:CZ   | 2.52        | 0.44     |
| 23:BB:1076:C:H2'   | 23:BB:1077:A:H8    | 1.82        | 0.44     |
| 40:DH:85:GLY:N     | 40:DH:89:LYS:H     | 2.15        | 0.44     |
| 38:BM:21:ALA:HB1   | 38:BM:100:LYS:HE2  | 1.99        | 0.44     |
| 20:AB:41:ASN:HD22  | 20:AB:44:LYS:CB    | 2.31        | 0.44     |
| 20:CB:41:ASN:HD22  | 20:CB:44:LYS:HB3   | 1.83        | 0.44     |
| 12:AM:47:LEU:HD22  | 12:AM:51:GLN:HB3   | 1.99        | 0.44     |
| 10:AK:86:LYS:HB2   | 10:AK:113:THR:HA   | 2.00        | 0.44     |
| 46:DU:47:PRO:HB3   | 46:DU:55:GLY:CA    | 2.47        | 0.44     |
| 45:DS:26:GLY:HA2   | 45:DS:71:VAL:O     | 2.18        | 0.44     |
| 45:DS:29:VAL:HG11  | 45:DS:55:ILE:CD1   | 2.47        | 0.44     |
| 23:BB:2787:C:H2'   | 23:BB:2788:C:C6    | 2.52        | 0.44     |
| 23:BB:1169:A:H2'   | 23:BB:1170:C:C6    | 2.52        | 0.44     |
| 23:DB:2266:A:H1'   | 23:DB:2267:A:N6    | 2.32        | 0.44     |
| 21:CU:19:LYS:CD    | 21:CU:20:ARG:HH21  | 2.29        | 0.44     |
| 23:DB:1057:A:H62   | 23:DB:1086:A:H2'   | 1.82        | 0.44     |
| 45:BS:28:LYS:HB3   | 45:BS:29:VAL:H     | 1.42        | 0.44     |
| 37:DL:85:VAL:HG22  | 37:DL:94:THR:CG2   | 2.47        | 0.44     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:968:C:O2'   | 23:DB:969:G:H5'    | 2.18        | 0.44     |
| 24:DI:45:THR:O    | 24:DI:48:ILE:HG22  | 2.17        | 0.44     |
| 46:BU:58:VAL:HG12 | 46:BU:59:GLU:N     | 2.24        | 0.44     |
| 11:AL:66:ILE:HG21 | 11:AL:71:HIS:CB    | 2.48        | 0.44     |
| 26:BD:8:LYS:O     | 26:BD:9:VAL:HB     | 2.17        | 0.44     |
| 20:CB:119:GLN:HA  | 20:CB:124:THR:HG23 | 2.00        | 0.44     |
| 46:DU:58:VAL:HG12 | 46:DU:59:GLU:N     | 2.27        | 0.44     |
| 25:DC:30:ALA:C    | 25:DC:32:LEU:H     | 2.21        | 0.44     |
| 23:BB:2840:C:O2'  | 23:BB:2841:C:H5'   | 2.17        | 0.44     |
| 23:BB:559:G:P     | 41:BJ:111:LYS:HD3  | 2.57        | 0.44     |
| 35:BV:29:ILE:HD12 | 35:BV:90:ASP:HA    | 1.99        | 0.44     |
| 23:BB:2689:U:H4'  | 23:BB:2690:U:OP2   | 2.18        | 0.44     |
| 23:DB:1583:A:H2   | 23:DB:1583:A:OP2   | 2.01        | 0.44     |
| 1:AA:856:C:O2'    | 1:AA:857:C:H5'     | 2.18        | 0.44     |
| 23:DB:1591:A:H2'  | 23:DB:1592:C:C6    | 2.52        | 0.44     |
| 39:BX:56:LEU:O    | 39:BX:58:ASN:N     | 2.50        | 0.44     |
| 12:AM:113:LYS:N   | 12:AM:114:PRO:CD   | 2.81        | 0.44     |
| 38:BM:68:PHE:CD1  | 38:BM:69:PRO:HD2   | 2.53        | 0.44     |
| 1:CA:213:G:H2'    | 1:CA:213:G:N3      | 2.33        | 0.44     |
| 23:DB:2219:U:O2'  | 23:DB:2220:U:H5'   | 2.18        | 0.44     |
| 6:AG:91:ARG:N     | 6:AG:91:ARG:HD2    | 2.33        | 0.44     |
| 1:CA:1472:U:H2'   | 1:CA:1473:G:H8     | 1.83        | 0.44     |
| 44:BQ:65:ASN:CB   | 44:BQ:75:TYR:HB2   | 2.48        | 0.44     |
| 23:DB:1930:G:H2'  | 23:DB:1968:G:N1    | 2.33        | 0.44     |
| 6:AG:68:VAL:CG1   | 6:AG:133:ALA:HB1   | 2.46        | 0.44     |
| 41:DJ:28:LEU:HG   | 41:DJ:32:LEU:HD12  | 1.99        | 0.44     |
| 53:B6:16:LYS:HA   | 53:B6:19:GLU:OE2   | 2.18        | 0.44     |
| 12:AM:22:TYR:HB2  | 12:AM:65:GLU:HA    | 1.99        | 0.44     |
| 23:BB:1637:A:H2'  | 23:BB:1638:C:H6    | 1.83        | 0.44     |
| 24:BI:109:ALA:HB1 | 24:BI:124:MET:CG   | 2.47        | 0.44     |
| 1:CA:128:G:H2'    | 1:CA:129:A:H8      | 1.81        | 0.44     |
| 23:BB:1013:C:H2'  | 23:BB:1014:A:H8    | 1.83        | 0.44     |
| 47:BF:119:LYS:N   | 47:BF:119:LYS:HD2  | 2.33        | 0.44     |
| 23:DB:2730:C:O2'  | 23:DB:2731:G:H5'   | 2.17        | 0.44     |
| 23:BB:1273:U:H4'  | 23:BB:1275:A:OP2   | 2.18        | 0.44     |
| 23:DB:189:G:H2'   | 23:DB:205:G:N2     | 2.33        | 0.44     |
| 23:BB:1465:G:H2'  | 23:BB:1466:U:O4'   | 2.17        | 0.44     |
| 23:DB:77:G:O2'    | 23:DB:78:U:H5'     | 2.17        | 0.44     |
| 1:CA:912:C:H2'    | 1:CA:913:A:C8      | 2.52        | 0.44     |
| 4:AE:92:ARG:HB3   | 4:AE:92:ARG:HH11   | 1.83        | 0.44     |
| 23:DB:1749:A:H2'  | 23:DB:1750:G:C8    | 2.52        | 0.44     |
| 23:DB:1749:A:H2'  | 23:DB:1750:G:H8    | 1.83        | 0.44     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 6:AG:30:MET:HA    | 6:AG:38:ALA:HB2    | 2.00        | 0.44     |
| 23:DB:2655:G:H1'  | 23:DB:2656:U:H5    | 1.83        | 0.44     |
| 23:DB:607:U:O4    | 23:DB:620:G:H5''   | 2.17        | 0.44     |
| 23:BB:622:G:H2'   | 23:BB:623:C:H6     | 1.83        | 0.44     |
| 23:BB:2829:A:O2'  | 23:BB:2830:C:H5'   | 2.18        | 0.44     |
| 23:BB:1266:G:N2   | 23:BB:2012:G:H2'   | 2.32        | 0.44     |
| 40:BH:9:VAL:HB    | 40:BH:12:LEU:O     | 2.18        | 0.44     |
| 5:AF:10:VAL:HA    | 5:AF:84:VAL:HA     | 2.00        | 0.44     |
| 23:BB:910:A:H2'   | 23:BB:911:A:C8     | 2.53        | 0.44     |
| 1:CA:454:G:O2'    | 1:CA:455:G:H5'     | 2.17        | 0.44     |
| 52:DW:54:ARG:C    | 52:DW:56:HIS:H     | 2.21        | 0.44     |
| 23:DB:2361:G:O2'  | 23:DB:2362:C:H5'   | 2.18        | 0.44     |
| 16:CQ:47:ASP:OD2  | 16:CQ:51:GLU:HG2   | 2.17        | 0.44     |
| 20:AB:118:THR:HA  | 20:AB:121:GLN:HB3  | 1.99        | 0.44     |
| 23:BB:2408:U:H2'  | 23:BB:2409:G:C8    | 2.53        | 0.44     |
| 40:DH:110:VAL:O   | 40:DH:110:VAL:HG22 | 2.18        | 0.44     |
| 23:DB:2749:A:H3'  | 23:DB:2750:A:H2'   | 2.00        | 0.44     |
| 14:AO:28:GLN:O    | 14:AO:32:LEU:HD23  | 2.18        | 0.44     |
| 23:BB:2057:G:H2'  | 23:BB:2058:A:O4'   | 2.17        | 0.44     |
| 9:CJ:31:ARG:HB2   | 9:CJ:31:ARG:HE     | 1.64        | 0.44     |
| 25:BC:34:GLU:O    | 25:BC:34:GLU:HG3   | 2.17        | 0.44     |
| 23:DB:1936:A:H2   | 23:DB:1943:U:O4    | 2.01        | 0.44     |
| 23:BB:146:A:H2'   | 23:BB:147:C:C6     | 2.53        | 0.44     |
| 21:CU:33:ARG:NH1  | 21:CU:34:ARG:HH11  | 2.15        | 0.44     |
| 52:BW:59:PHE:CD2  | 52:BW:61:LYS:HD2   | 2.53        | 0.44     |
| 23:BB:1799:G:N2   | 23:BB:1818:U:O2'   | 2.51        | 0.44     |
| 25:BC:121:ALA:HB3 | 25:BC:129:LEU:CD1  | 2.48        | 0.44     |
| 25:BC:184:GLU:O   | 25:BC:186:ASP:N    | 2.43        | 0.44     |
| 25:DC:64:VAL:O    | 25:DC:102:TYR:O    | 2.36        | 0.44     |
| 21:CU:40:PRO:C    | 21:CU:42:THR:N     | 2.71        | 0.44     |
| 48:BG:108:PHE:C   | 48:BG:110:HIS:H    | 2.21        | 0.44     |
| 6:AG:144:ALA:O    | 6:AG:146:ALA:N     | 2.46        | 0.44     |
| 6:AG:145:GLU:C    | 6:AG:147:ASN:N     | 2.69        | 0.44     |
| 48:DG:10:VAL:CG2  | 48:DG:49:LEU:HD13  | 2.48        | 0.44     |
| 53:B6:48:ALA:O    | 53:B6:50:VAL:HG22  | 2.17        | 0.44     |
| 40:BH:128:HIS:CG  | 40:BH:130:VAL:HG22 | 2.53        | 0.44     |
| 40:BH:99:ILE:O    | 40:BH:103:VAL:HG13 | 2.18        | 0.44     |
| 8:AI:78:ILE:O     | 8:AI:82:ILE:HG13   | 2.18        | 0.44     |
| 26:DD:51:THR:HG22 | 26:DD:52:THR:H     | 1.83        | 0.44     |
| 23:DB:634:C:H6    | 23:DB:634:C:O5'    | 2.01        | 0.44     |
| 23:DB:2393:U:H2'  | 23:DB:2394:C:O4'   | 2.18        | 0.44     |
| 23:DB:675:A:C6    | 23:DB:676:A:C6     | 3.06        | 0.44     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:600:A:H2'    | 1:AA:601:G:H8      | 1.83        | 0.44     |
| 7:CH:124:ILE:HG22 | 7:CH:125:ILE:H     | 1.83        | 0.44     |
| 51:BZ:77:LYS:CG   | 51:BZ:78:TYR:H     | 2.29        | 0.44     |
| 42:BN:52:ILE:O    | 42:BN:55:ALA:HB3   | 2.18        | 0.44     |
| 29:BE:157:LEU:HG  | 29:BE:169:VAL:HG11 | 2.00        | 0.44     |
| 29:BE:166:LYS:O   | 29:BE:167:VAL:HB   | 2.18        | 0.44     |
| 47:DF:110:ILE:HB  | 47:DF:113:PHE:HB3  | 1.98        | 0.44     |
| 47:DF:174:PHE:HB3 | 47:DF:176:PHE:CE1  | 2.53        | 0.44     |
| 47:DF:4:HIS:O     | 47:DF:7:TYR:HB3    | 2.17        | 0.44     |
| 21:AU:16:ARG:NH2  | 21:AU:19:LYS:NZ    | 2.66        | 0.44     |
| 18:CS:62:THR:HG22 | 18:CS:63:ASP:N     | 2.30        | 0.44     |
| 13:AN:30:ILE:O    | 13:AN:32:ASP:N     | 2.45        | 0.44     |
| 23:BB:675:A:O2'   | 29:BE:62:GLN:NE2   | 2.50        | 0.44     |
| 23:DB:139:U:H3    | 50:DT:49:LYS:HZ1   | 1.65        | 0.44     |
| 23:BB:2893:A:H4'  | 23:BB:2894:G:O5'   | 2.17        | 0.44     |
| 23:BB:1170:C:H2'  | 23:BB:1171:G:O4'   | 2.17        | 0.44     |
| 38:DM:26:VAL:HG13 | 38:DM:133:LYS:HA   | 1.99        | 0.44     |
| 38:DM:26:VAL:HA   | 38:DM:66:ARG:HH21  | 1.82        | 0.44     |
| 23:BB:2037:A:H2'  | 23:BB:2038:G:C8    | 2.51        | 0.44     |
| 23:BB:2734:A:H2'  | 23:BB:2735:G:C5'   | 2.44        | 0.44     |
| 28:BP:107:ALA:O   | 28:BP:108:ARG:C    | 2.56        | 0.44     |
| 23:BB:593:U:H2'   | 23:BB:594:U:H6     | 1.82        | 0.44     |
| 49:BR:59:ILE:HG13 | 49:BR:59:ILE:H     | 1.60        | 0.44     |
| 24:BI:29:GLN:HA   | 24:BI:29:GLN:NE2   | 2.32        | 0.44     |
| 38:DM:18:ARG:HA   | 38:DM:18:ARG:HD2   | 1.59        | 0.44     |
| 38:DM:55:ARG:HH21 | 38:DM:55:ARG:CA    | 2.24        | 0.44     |
| 23:BB:173:A:H2'   | 23:BB:174:U:H6     | 1.81        | 0.44     |
| 20:AB:95:TRP:HZ3  | 20:AB:174:GLU:OE2  | 2.00        | 0.44     |
| 37:BL:82:LEU:O    | 37:BL:85:VAL:HG12  | 2.18        | 0.44     |
| 45:DS:42:LYS:O    | 45:DS:46:LEU:HG    | 2.18        | 0.44     |
| 45:DS:25:ARG:CZ   | 45:DS:74:ILE:HG23  | 2.48        | 0.44     |
| 1:CA:34:C:H2'     | 1:CA:35:G:C8       | 2.53        | 0.44     |
| 1:CA:716:A:N3     | 10:CK:118:ASN:O    | 2.50        | 0.44     |
| 46:DU:40:LEU:HB3  | 46:DU:59:GLU:HG2   | 1.99        | 0.44     |
| 23:DB:299:A:N6    | 23:DB:322:A:O2'    | 2.50        | 0.44     |
| 23:DB:719:C:H2'   | 23:DB:720:U:C6     | 2.53        | 0.44     |
| 23:BB:1824:G:H1'  | 25:BC:251:THR:CG2  | 2.48        | 0.44     |
| 39:BX:9:LYS:HZ2   | 39:BX:60:LYS:HE3   | 1.81        | 0.44     |
| 9:AJ:37:ARG:HA    | 9:AJ:37:ARG:CZ     | 2.48        | 0.44     |
| 23:BB:2460:U:O2'  | 23:BB:2461:A:H5'   | 2.17        | 0.44     |
| 1:AA:1514:G:H2'   | 1:AA:1515:G:C8     | 2.52        | 0.44     |
| 40:BH:54:LEU:O    | 40:BH:58:LEU:N     | 2.51        | 0.44     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 9:CJ:92:LEU:HB2    | 9:CJ:93:ALA:H     | 1.61        | 0.44     |
| 1:CA:829:G:H4'     | 20:CB:24:PRO:HG3  | 1.99        | 0.44     |
| 23:DB:1946:U:H2'   | 23:DB:1947:C:C6   | 2.52        | 0.44     |
| 9:AJ:92:LEU:HB2    | 9:AJ:93:ALA:H     | 1.61        | 0.44     |
| 1:CA:1036:A:H2'    | 1:CA:1037:C:H6    | 1.83        | 0.44     |
| 23:DB:2252:G:H2'   | 23:DB:2253:G:C8   | 2.52        | 0.44     |
| 23:BB:316:C:O2'    | 23:BB:317:G:H5'   | 2.18        | 0.44     |
| 23:DB:2785:C:H2'   | 23:DB:2786:U:H6   | 1.82        | 0.44     |
| 14:AO:43:PHE:CE1   | 14:AO:56:LEU:HD22 | 2.53        | 0.44     |
| 1:AA:1306:A:H1'    | 1:AA:1332:A:C2    | 2.53        | 0.44     |
| 29:DE:106:LYS:O    | 29:DE:110:SER:HB2 | 2.17        | 0.44     |
| 4:CE:98:ALA:HB3    | 4:CE:121:ASN:C    | 2.38        | 0.44     |
| 2:CC:19:SER:HB3    | 2:CC:21:TRP:HE1   | 1.83        | 0.44     |
| 26:DD:15:PHE:CD1   | 26:DD:15:PHE:N    | 2.82        | 0.44     |
| 1:AA:204:G:C2'     | 1:AA:466:A:H62    | 2.30        | 0.44     |
| 23:DB:235:U:H2'    | 23:DB:236:C:H6    | 1.83        | 0.44     |
| 1:CA:1096:C:O2'    | 1:CA:1097:C:H5'   | 2.17        | 0.44     |
| 23:BB:1847:A:H4'   | 23:BB:1848:A:C8   | 2.53        | 0.44     |
| 19:CT:19:HIS:CE1   | 19:CT:23:ARG:HG3  | 2.53        | 0.44     |
| 48:DG:172:GLU:O    | 48:DG:173:ALA:HB2 | 2.18        | 0.44     |
| 51:BZ:19:SER:OG    | 51:BZ:23:ASN:HB2  | 2.17        | 0.44     |
| 6:CG:30:MET:HA     | 6:CG:38:ALA:HB2   | 2.00        | 0.44     |
| 23:BB:438:G:H2'    | 23:BB:439:A:C8    | 2.53        | 0.44     |
| 23:DB:2298:A:N1    | 23:DB:2321:U:C5   | 2.85        | 0.44     |
| 23:BB:1689:A:H2'   | 23:BB:1690:A:H8   | 1.82        | 0.44     |
| 23:DB:1984:G:O2'   | 23:DB:1985:C:H5'  | 2.17        | 0.44     |
| 23:DB:1345:C:H5'   | 23:DB:1396:U:C5   | 2.53        | 0.44     |
| 23:BB:425:G:O2'    | 23:BB:426:C:H5'   | 2.17        | 0.44     |
| 23:BB:800:A:H4'    | 23:BB:801:G:O5'   | 2.18        | 0.44     |
| 23:BB:1541:C:H2'   | 23:BB:1542:U:C6   | 2.52        | 0.44     |
| 43:BO:14:ALA:C     | 43:BO:16:ARG:H    | 2.21        | 0.44     |
| 24:DI:53:PRO:CG    | 24:DI:77:VAL:HG11 | 2.47        | 0.44     |
| 23:DB:380:G:O2'    | 23:DB:381:G:H5'   | 2.18        | 0.44     |
| 3:CD:32:LYS:O      | 3:CD:35:GLN:HB2   | 2.17        | 0.44     |
| 1:CA:220:G:O2'     | 1:CA:221:C:H5'    | 2.17        | 0.44     |
| 25:DC:67:LYS:O     | 25:DC:188:ARG:HD3 | 2.18        | 0.44     |
| 25:DC:20:ASN:O     | 25:DC:23:LEU:HD13 | 2.18        | 0.44     |
| 48:BG:104:LEU:O    | 48:BG:111:PRO:HA  | 2.17        | 0.44     |
| 23:DB:573:U:N3     | 23:DB:2031:A:OP1  | 2.38        | 0.44     |
| 20:AB:162:VAL:HG21 | 20:AB:168:GLU:HB2 | 1.99        | 0.44     |
| 26:BD:111:GLY:N    | 26:BD:194:PRO:HG2 | 2.31        | 0.44     |
| 16:CQ:61:ARG:HD2   | 16:CQ:61:ARG:C    | 2.38        | 0.44     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 52:DW:30:VAL:O     | 52:DW:30:VAL:HG13  | 2.18        | 0.44     |
| 52:DW:49:ASN:HB3   | 52:DW:81:ILE:CD1   | 2.48        | 0.44     |
| 52:DW:59:PHE:O     | 52:DW:60:ALA:HB3   | 2.17        | 0.44     |
| 53:B6:36:ALA:O     | 53:B6:39:LEU:HG    | 2.17        | 0.44     |
| 53:B6:79:ILE:O     | 53:B6:83:ILE:HG12  | 2.18        | 0.44     |
| 40:BH:99:ILE:HD12  | 40:BH:144:VAL:HG21 | 1.98        | 0.44     |
| 44:DQ:80:ASN:O     | 44:DQ:84:LYS:HG3   | 2.17        | 0.44     |
| 20:CB:166:ASP:OD2  | 20:CB:190:SER:HA   | 2.17        | 0.44     |
| 26:DD:107:VAL:H    | 26:DD:205:PRO:HA   | 1.83        | 0.44     |
| 29:BE:108:ILE:HD11 | 29:BE:181:ILE:CB   | 2.33        | 0.44     |
| 42:DN:8:ARG:HB2    | 42:DN:43:GLU:OE1   | 2.17        | 0.44     |
| 50:BT:57:VAL:O     | 50:BT:85:VAL:O     | 2.36        | 0.44     |
| 12:CM:15:VAL:HG21  | 12:CM:40:GLU:HB3   | 2.00        | 0.44     |
| 25:BC:67:LYS:O     | 25:BC:188:ARG:HD3  | 2.18        | 0.44     |
| 3:AD:24:VAL:HG12   | 3:AD:160:LEU:HD12  | 2.00        | 0.44     |
| 24:DI:72:THR:OG1   | 24:DI:73:PRO:HD2   | 2.18        | 0.44     |
| 47:BF:140:ILE:H    | 47:BF:140:ILE:HG13 | 1.58        | 0.44     |
| 24:BI:91:LYS:O     | 24:BI:94:LYS:HB2   | 2.18        | 0.44     |
| 40:DH:88:GLY:C     | 40:DH:89:LYS:HD2   | 2.38        | 0.44     |
| 47:DF:113:PHE:HE1  | 47:DF:116:LEU:HB2  | 1.83        | 0.44     |
| 47:DF:142:TYR:HD1  | 47:DF:142:TYR:H    | 1.61        | 0.44     |
| 23:BB:2471:A:O2'   | 23:BB:2472:G:C8    | 2.58        | 0.44     |
| 29:DE:29:HIS:O     | 29:DE:33:VAL:HG23  | 2.16        | 0.44     |
| 16:AQ:74:LEU:HD13  | 16:AQ:74:LEU:C     | 2.38        | 0.44     |
| 1:AA:333:U:H2'     | 1:AA:334:C:H6      | 1.83        | 0.44     |
| 10:CK:92:ARG:HE    | 21:CU:20:ARG:NH2   | 2.15        | 0.44     |
| 35:DV:44:HIS:NE2   | 35:DV:85:LYS:HB2   | 2.33        | 0.44     |
| 27:BK:8:LEU:O      | 27:BK:19:VAL:HG22  | 2.17        | 0.44     |
| 27:BK:113:MET:HA   | 27:BK:116:ILE:HD11 | 1.99        | 0.44     |
| 3:AD:153:ARG:HG3   | 3:AD:154:VAL:N     | 2.33        | 0.44     |
| 23:BB:1737:G:H8    | 23:BB:1737:G:OP2   | 2.00        | 0.44     |
| 1:AA:1074:G:C4'    | 20:AB:102:ASN:HB2  | 2.48        | 0.44     |
| 46:DU:35:VAL:HB    | 46:DU:38:ILE:HB    | 2.00        | 0.44     |
| 41:DJ:112:GLY:N    | 41:DJ:113:PRO:HD2  | 2.32        | 0.44     |
| 3:AD:96:ARG:NH1    | 3:AD:133:SER:HA    | 2.33        | 0.44     |
| 1:AA:34:C:H2'      | 1:AA:35:G:H8       | 1.82        | 0.44     |
| 12:CM:89:ARG:HH22  | 12:CM:94:LEU:HD12  | 1.81        | 0.44     |
| 19:CT:68:LYS:CA    | 19:CT:68:LYS:HE2   | 2.48        | 0.44     |
| 40:BH:41:LYS:HA    | 40:BH:44:ILE:CG1   | 2.46        | 0.44     |
| 35:DV:78:GLN:O     | 35:DV:87:GLN:N     | 2.43        | 0.44     |
| 23:BB:276:U:O2'    | 23:BB:278:A:N7     | 2.51        | 0.44     |
| 23:BB:153:U:O2'    | 23:BB:154:U:H5'    | 2.18        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:150:U:H2'   | 23:DB:151:C:O4'   | 2.18        | 0.44     |
| 1:AA:190:A:H2'    | 1:AA:191:G:O4'    | 2.18        | 0.44     |
| 22:DA:69:G:H3'    | 22:DA:70:C:H6     | 1.83        | 0.44     |
| 1:CA:1314:C:H2'   | 1:CA:1315:U:H6    | 1.82        | 0.44     |
| 20:CB:71:THR:HG23 | 20:CB:94:ARG:N    | 2.33        | 0.44     |
| 1:CA:58:C:O2'     | 1:CA:59:A:H5'     | 2.18        | 0.44     |
| 23:DB:666:A:H2'   | 23:DB:667:U:C6    | 2.53        | 0.44     |
| 42:BN:58:ASP:OD2  | 42:BN:63:ARG:NH2  | 2.51        | 0.44     |
| 23:DB:2020:A:O2'  | 23:DB:2021:C:H5'  | 2.18        | 0.44     |
| 23:BB:866:A:H61   | 23:BB:913:U:C1'   | 2.31        | 0.44     |
| 1:CA:513:C:H2'    | 1:CA:514:C:C6     | 2.53        | 0.44     |
| 43:BO:83:LEU:HA   | 43:BO:83:LEU:HD12 | 1.84        | 0.44     |
| 4:CE:103:GLY:O    | 4:CE:121:ASN:HA   | 2.17        | 0.44     |
| 23:BB:2491:U:H5'' | 23:BB:2570:G:C5'  | 2.47        | 0.44     |
| 23:BB:834:G:O2'   | 23:BB:835:C:H5'   | 2.17        | 0.44     |
| 23:DB:459:U:H5''  | 36:D2:40:ALA:HB2  | 1.99        | 0.44     |
| 20:AB:13:VAL:CG1  | 20:AB:207:ARG:HG2 | 2.48        | 0.44     |
| 17:CR:22:TYR:HB2  | 17:CR:61:ALA:HB2  | 2.00        | 0.44     |
| 23:DB:1273:U:H4'  | 23:DB:1275:A:OP2  | 2.17        | 0.44     |
| 1:CA:821:G:H2'    | 1:CA:822:U:H6     | 1.82        | 0.44     |
| 1:AA:160:A:H1'    | 1:AA:344:A:C5     | 2.53        | 0.44     |
| 23:DB:1773:A:H2'  | 23:DB:1774:C:O4'  | 2.18        | 0.44     |
| 23:BB:1313:U:C2'  | 23:BB:1313:U:O2   | 2.66        | 0.44     |
| 1:AA:1234:C:H2'   | 1:AA:1235:U:C6    | 2.52        | 0.44     |
| 23:DB:218:A:H2'   | 23:DB:219:A:O4'   | 2.18        | 0.44     |
| 23:BB:737:C:O2'   | 23:BB:738:G:H5'   | 2.17        | 0.44     |
| 23:BB:2818:U:H4'  | 23:BB:2837:A:C4'  | 2.47        | 0.44     |
| 1:AA:1119:C:OP2   | 8:AI:10:ARG:NH2   | 2.51        | 0.44     |
| 25:DC:79:ARG:HD2  | 25:DC:81:GLU:HG3  | 2.00        | 0.44     |
| 1:CA:1439:G:H2'   | 1:CA:1440:U:O4'   | 2.17        | 0.44     |
| 23:BB:1607:C:N4   | 23:BB:1622:G:OP2  | 2.51        | 0.44     |
| 1:AA:1292:G:H2'   | 1:AA:1293:C:C6    | 2.53        | 0.44     |
| 1:AA:1486:G:H2'   | 1:AA:1487:G:O4'   | 2.17        | 0.44     |
| 3:AD:32:LYS:O     | 3:AD:35:GLN:HB2   | 2.18        | 0.44     |
| 23:BB:282:A:H2'   | 23:BB:283:G:C8    | 2.53        | 0.44     |
| 1:CA:575:G:H4'    | 1:CA:576:C:OP1    | 2.18        | 0.44     |
| 1:CA:1202:U:H2'   | 1:CA:1203:C:O4'   | 2.18        | 0.44     |
| 49:DR:86:GLN:HB2  | 49:DR:86:GLN:HE21 | 1.53        | 0.44     |
| 23:DB:114:U:O2    | 23:DB:114:U:H2'   | 2.16        | 0.44     |
| 49:BR:86:GLN:HE21 | 49:BR:86:GLN:HB2  | 1.53        | 0.44     |
| 8:CI:90:ASP:O     | 8:CI:93:LEU:HG    | 2.17        | 0.44     |
| 38:BM:74:THR:O    | 38:BM:75:GLU:HB2  | 2.18        | 0.44     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:175:C:O2'    | 1:AA:176:C:H5'     | 2.18        | 0.44     |
| 23:DB:1098:A:C3'  | 24:DI:3:LYS:C      | 2.86        | 0.43     |
| 52:BW:49:ASN:HB3  | 52:BW:81:ILE:CD1   | 2.47        | 0.43     |
| 48:DG:9:VAL:HG12  | 48:DG:11:PRO:CD    | 2.42        | 0.43     |
| 41:BJ:25:LEU:HB2  | 41:BJ:62:VAL:HG22  | 2.00        | 0.43     |
| 35:DV:1:MET:HE2   | 35:DV:2:PHE:H      | 1.82        | 0.43     |
| 35:BV:62:THR:CG2  | 35:BV:71:LYS:HG2   | 2.48        | 0.43     |
| 41:DJ:54:ILE:O    | 41:DJ:122:LEU:HA   | 2.17        | 0.43     |
| 48:BG:22:VAL:C    | 48:BG:23:ILE:HG13  | 2.39        | 0.43     |
| 33:B1:49:LYS:CG   | 33:B1:50:GLU:H     | 2.17        | 0.43     |
| 23:BB:2110:G:N2   | 23:BB:2180:U:H3    | 2.15        | 0.43     |
| 23:DB:2787:C:H2'  | 23:DB:2788:C:C6    | 2.53        | 0.43     |
| 37:BL:14:LYS:O    | 37:BL:16:GLY:N     | 2.51        | 0.43     |
| 23:BB:2893:A:H4'  | 23:BB:2894:G:C5'   | 2.48        | 0.43     |
| 23:BB:2893:A:H4'  | 23:BB:2894:G:H5'   | 2.00        | 0.43     |
| 34:D3:33:THR:HG23 | 34:D3:34:LYS:N     | 2.33        | 0.43     |
| 23:BB:2834:G:H1'  | 23:BB:2883:A:H61   | 1.81        | 0.43     |
| 48:DG:144:ALA:O   | 48:DG:147:LEU:HB2  | 2.17        | 0.43     |
| 29:BE:151:GLY:HA2 | 29:BE:195:GLN:HE22 | 1.83        | 0.43     |
| 27:DK:19:VAL:HG12 | 27:DK:43:ILE:HA    | 1.99        | 0.43     |
| 5:CF:60:VAL:HG12  | 5:CF:61:LEU:N      | 2.33        | 0.43     |
| 42:DN:32:GLU:HB3  | 42:DN:115:LEU:HG   | 2.00        | 0.43     |
| 15:CP:23:ASP:CG   | 15:CP:25:ARG:HE    | 2.22        | 0.43     |
| 37:DL:93:ASN:ND2  | 37:DL:94:THR:H     | 2.16        | 0.43     |
| 34:B3:16:THR:HG21 | 34:B3:48:MET:SD    | 2.57        | 0.43     |
| 11:AL:66:ILE:N    | 11:AL:66:ILE:HD12  | 2.33        | 0.43     |
| 9:AJ:7:ARG:CZ     | 9:AJ:101:SER:HB2   | 2.48        | 0.43     |
| 45:BS:81:SER:CA   | 45:BS:99:ARG:HA    | 2.44        | 0.43     |
| 45:DS:74:ILE:O    | 45:DS:75:PHE:HB3   | 2.18        | 0.43     |
| 2:AC:155:ARG:HD2  | 2:AC:155:ARG:HA    | 1.88        | 0.43     |
| 1:AA:92:U:H2'     | 1:AA:92:U:O2       | 2.18        | 0.43     |
| 1:CA:191:G:H8     | 1:CA:191:G:OP2     | 2.01        | 0.43     |
| 23:BB:2746:U:C4'  | 48:BG:138:GLN:HA   | 2.48        | 0.43     |
| 28:DP:33:GLU:OE1  | 28:DP:33:GLU:HA    | 2.18        | 0.43     |
| 1:AA:1048:G:H5''  | 13:AN:2:LYS:HD2    | 1.99        | 0.43     |
| 23:BB:642:U:O2'   | 23:BB:644:A:N7     | 2.44        | 0.43     |
| 38:DM:69:PRO:HA   | 38:DM:94:ALA:CA    | 2.47        | 0.43     |
| 3:AD:117:VAL:HG12 | 3:AD:130:ASN:HA    | 2.00        | 0.43     |
| 23:BB:1418:G:C2'  | 23:BB:1580:A:H61   | 2.31        | 0.43     |
| 3:CD:117:VAL:HG12 | 3:CD:130:ASN:HA    | 2.00        | 0.43     |
| 1:CA:620:C:C1'    | 3:CD:131:ILE:HD13  | 2.48        | 0.43     |
| 20:AB:19:THR:HG23 | 20:AB:20:ARG:N     | 2.33        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:1171:G:H2'  | 23:DB:1172:C:C6   | 2.53        | 0.43     |
| 20:AB:86:CYS:C    | 20:AB:88:GLN:H    | 2.21        | 0.43     |
| 1:AA:404:G:OP1    | 3:AD:114:ARG:HD3  | 2.18        | 0.43     |
| 41:BJ:74:TYR:CD1  | 41:BJ:92:MET:HG3  | 2.54        | 0.43     |
| 23:DB:2854:G:H2'  | 23:DB:2855:C:H6   | 1.82        | 0.43     |
| 23:BB:2461:A:H1'  | 23:BB:2492:U:C2   | 2.53        | 0.43     |
| 1:AA:214:C:H2'    | 1:AA:215:C:H6     | 1.82        | 0.43     |
| 1:AA:450:G:N7     | 1:AA:481:G:O6     | 2.50        | 0.43     |
| 26:BD:125:TRP:HE1 | 26:BD:161:MET:N   | 2.16        | 0.43     |
| 23:DB:2756:U:H4'  | 23:DB:2757:A:OP1  | 2.18        | 0.43     |
| 1:AA:499:A:O4'    | 1:AA:547:A:N6     | 2.51        | 0.43     |
| 26:DD:125:TRP:HE1 | 26:DD:161:MET:N   | 2.16        | 0.43     |
| 26:DD:125:TRP:NE1 | 26:DD:161:MET:N   | 2.65        | 0.43     |
| 23:DB:6:A:O3'     | 41:DJ:132:HIS:CE1 | 2.71        | 0.43     |
| 14:CO:43:PHE:CE1  | 14:CO:56:LEU:HD22 | 2.53        | 0.43     |
| 50:DT:48:GLN:CA   | 50:DT:48:GLN:HE21 | 2.28        | 0.43     |
| 1:AA:658:C:H2'    | 1:AA:659:U:H6     | 1.83        | 0.43     |
| 10:CK:52:ARG:HD2  | 10:CK:52:ARG:HA   | 1.62        | 0.43     |
| 23:BB:2552:U:C2   | 23:BB:2554:U:H5'  | 2.53        | 0.43     |
| 23:DB:484:C:H2'   | 23:DB:485:C:H6    | 1.83        | 0.43     |
| 24:BI:14:ALA:HA   | 24:BI:45:THR:HG21 | 1.98        | 0.43     |
| 23:DB:1341:G:N2   | 23:DB:1398:C:H4'  | 2.33        | 0.43     |
| 23:BB:1885:A:H2'  | 23:BB:1886:U:O4'  | 2.18        | 0.43     |
| 23:BB:2873:A:O4'  | 42:BN:6:SER:HB3   | 2.18        | 0.43     |
| 1:AA:327:A:O2'    | 1:AA:328:C:O4'    | 2.35        | 0.43     |
| 26:BD:40:LEU:HD12 | 26:BD:41:ALA:H    | 1.83        | 0.43     |
| 24:DI:90:GLY:C    | 24:DI:92:PRO:HD3  | 2.39        | 0.43     |
| 23:DB:1313:U:O2   | 23:DB:1313:U:H2'  | 2.17        | 0.43     |
| 23:BB:1339:G:H21  | 23:BB:1603:A:H1'  | 1.82        | 0.43     |
| 46:BU:41:VAL:HG22 | 46:BU:60:LYS:O    | 2.18        | 0.43     |
| 23:BB:2007:U:O2'  | 23:BB:2008:C:H5'  | 2.18        | 0.43     |
| 23:DB:2597:G:OP1  | 25:DC:240:GLY:HA3 | 2.18        | 0.43     |
| 28:BP:8:GLU:HG2   | 28:BP:54:LEU:CD2  | 2.48        | 0.43     |
| 23:BB:797:G:OP2   | 29:BE:57:LYS:HB2  | 2.18        | 0.43     |
| 1:AA:960:U:H5''   | 1:AA:960:U:O2     | 2.17        | 0.43     |
| 23:BB:2047:C:H2'  | 23:BB:2048:G:C8   | 2.53        | 0.43     |
| 23:BB:822:G:H2'   | 23:BB:823:C:C6    | 2.53        | 0.43     |
| 24:BI:63:ASP:O    | 24:BI:65:SER:N    | 2.50        | 0.43     |
| 1:CA:176:C:H2'    | 1:CA:177:G:N3     | 2.34        | 0.43     |
| 2:AC:34:SER:O     | 2:AC:38:VAL:HG22  | 2.18        | 0.43     |
| 23:BB:282:A:H2'   | 23:BB:283:G:H8    | 1.83        | 0.43     |
| 3:AD:73:ASN:O     | 3:AD:76:LYS:HB2   | 2.18        | 0.43     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:711:G:O2'     | 1:CA:712:A:H5'     | 2.18        | 0.43     |
| 23:DB:1310:G:H1'   | 23:DB:1611:C:H5'   | 1.99        | 0.43     |
| 1:AA:771:G:H2'     | 1:AA:772:U:C6      | 2.53        | 0.43     |
| 52:BW:12:GLY:O     | 52:BW:13:ARG:HB2   | 2.18        | 0.43     |
| 3:AD:102:TYR:HE1   | 3:AD:108:ALA:O     | 2.01        | 0.43     |
| 1:CA:664:G:H22     | 1:CA:741:G:H1      | 1.66        | 0.43     |
| 52:DW:25:PHE:HD1   | 52:DW:26:GLY:H     | 1.64        | 0.43     |
| 23:DB:1098:A:C2'   | 24:DI:4:VAL:C      | 2.87        | 0.43     |
| 50:BT:4:GLU:OE2    | 50:BT:5:GLU:HG2    | 2.18        | 0.43     |
| 40:DH:27:ARG:H     | 40:DH:31:VAL:HG23  | 1.80        | 0.43     |
| 52:BW:30:VAL:O     | 52:BW:30:VAL:HG13  | 2.18        | 0.43     |
| 23:BB:1818:U:C4    | 25:BC:152:GLN:HB3  | 2.53        | 0.43     |
| 23:DB:2329:U:H2'   | 23:DB:2330:G:H8    | 1.82        | 0.43     |
| 25:DC:170:TYR:HD2  | 25:DC:184:GLU:HA   | 1.82        | 0.43     |
| 44:BQ:33:VAL:CG2   | 44:BQ:34:ALA:N     | 2.81        | 0.43     |
| 23:DB:2315:G:H2'   | 23:DB:2316:G:H8    | 1.83        | 0.43     |
| 47:DF:57:ALA:HB2   | 47:DF:64:PRO:HG2   | 1.99        | 0.43     |
| 23:DB:918:A:C2'    | 23:DB:919:U:H5'    | 2.43        | 0.43     |
| 44:DQ:90:ASP:C     | 49:DR:11:GLN:HE22  | 2.22        | 0.43     |
| 20:CB:162:VAL:HG21 | 20:CB:168:GLU:HB2  | 2.00        | 0.43     |
| 35:BV:4:ILE:HD11   | 35:BV:61:LEU:HB3   | 2.00        | 0.43     |
| 41:DJ:54:ILE:HD12  | 41:DJ:55:ILE:H     | 1.82        | 0.43     |
| 41:DJ:55:ILE:HG22  | 41:DJ:123:LYS:HB2  | 1.99        | 0.43     |
| 47:DF:38:GLY:HA2   | 47:DF:85:GLY:HA3   | 2.00        | 0.43     |
| 23:DB:673:C:C4'    | 29:DE:77:ILE:HD11  | 2.48        | 0.43     |
| 44:BQ:80:ASN:O     | 44:BQ:84:LYS:HG3   | 2.18        | 0.43     |
| 44:BQ:87:VAL:HG12  | 44:BQ:89:ILE:HD13  | 1.99        | 0.43     |
| 23:BB:337:C:OP1    | 46:BU:3:LYS:HG3    | 2.18        | 0.43     |
| 34:D3:28:LEU:HD22  | 34:D3:43:LEU:HB2   | 2.00        | 0.43     |
| 47:BF:116:LEU:HB3  | 47:BF:176:PHE:HA   | 1.99        | 0.43     |
| 42:BN:101:GLY:HA2  | 42:BN:109:PRO:HA   | 2.00        | 0.43     |
| 12:AM:79:LEU:HD22  | 12:AM:86:ARG:HH21  | 1.84        | 0.43     |
| 23:DB:141:G:N3     | 23:DB:141:G:C3'    | 2.78        | 0.43     |
| 37:DL:51:GLU:OE1   | 37:DL:57:LEU:HB2   | 2.18        | 0.43     |
| 23:DB:512:G:P      | 23:DB:1215:G:N2    | 2.91        | 0.43     |
| 38:DM:66:ARG:NE    | 38:DM:101:VAL:HG11 | 2.33        | 0.43     |
| 13:CN:30:ILE:CG2   | 13:CN:44:VAL:HG11  | 2.49        | 0.43     |
| 35:DV:89:ILE:HD12  | 35:DV:89:ILE:O     | 2.18        | 0.43     |
| 20:AB:212:TYR:HA   | 20:AB:215:ALA:HB3  | 2.00        | 0.43     |
| 1:CA:908:A:O2'     | 1:CA:909:A:H5'     | 2.18        | 0.43     |
| 27:BK:110:GLU:HA   | 27:BK:113:MET:HG2  | 1.99        | 0.43     |
| 23:BB:362:A:C8     | 23:BB:363:G:N7     | 2.86        | 0.43     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 28:DP:6:GLN:HE21   | 28:DP:7:LEU:N      | 2.16        | 0.43     |
| 1:AA:87:C:H2'      | 1:AA:88:U:C4'      | 2.48        | 0.43     |
| 23:BB:1445:G:O2'   | 23:BB:1446:C:H5'   | 2.16        | 0.43     |
| 20:AB:148:GLY:O    | 20:AB:151:LYS:HG2  | 2.18        | 0.43     |
| 45:BS:99:ARG:HB3   | 45:BS:99:ARG:HE    | 1.63        | 0.43     |
| 20:CB:98:GLY:HA2   | 20:CB:101:THR:CG2  | 2.48        | 0.43     |
| 5:AF:99:ALA:O      | 5:AF:100:SER:CB    | 2.67        | 0.43     |
| 42:DN:24:MET:CE    | 42:DN:44:LEU:HD13  | 2.47        | 0.43     |
| 23:BB:2794:C:H2'   | 23:BB:2795:C:H6    | 1.83        | 0.43     |
| 35:BV:9:ARG:HA     | 35:BV:41:GLU:OE2   | 2.18        | 0.43     |
| 23:DB:720:U:O2'    | 23:DB:721:A:H5'    | 2.18        | 0.43     |
| 1:AA:238:A:H3'     | 1:AA:239:U:H5''    | 2.00        | 0.43     |
| 25:DC:245:THR:HG23 | 25:DC:249:VAL:HB   | 2.00        | 0.43     |
| 45:BS:43:ALA:O     | 45:BS:46:LEU:HB2   | 2.19        | 0.43     |
| 20:CB:19:THR:HG23  | 20:CB:20:ARG:H     | 1.82        | 0.43     |
| 23:BB:526:A:H62    | 23:BB:2626:C:H4'   | 1.83        | 0.43     |
| 2:AC:42:LEU:O      | 2:AC:46:LEU:HD23   | 2.18        | 0.43     |
| 20:CB:160:LEU:HD21 | 20:CB:182:VAL:HG22 | 2.00        | 0.43     |
| 5:CF:53:LYS:CE     | 5:CF:53:LYS:HA     | 2.48        | 0.43     |
| 19:CT:53:MET:HA    | 19:CT:56:ILE:HD12  | 1.99        | 0.43     |
| 20:CB:8:MET:HG3    | 20:CB:9:LEU:H      | 1.81        | 0.43     |
| 11:AL:13:ARG:HB2   | 11:AL:14:LYS:H     | 1.44        | 0.43     |
| 38:DM:82:MET:HE3   | 38:DM:83:GLY:N     | 2.31        | 0.43     |
| 23:DB:2496:C:H5'   | 38:DM:82:MET:HG3   | 2.00        | 0.43     |
| 23:BB:2340:A:H2'   | 23:BB:2341:G:C8    | 2.49        | 0.43     |
| 1:AA:659:U:H2'     | 1:AA:660:C:C6      | 2.53        | 0.43     |
| 23:DB:1856:U:C2'   | 23:DB:1857:G:H5'   | 2.47        | 0.43     |
| 43:DO:66:GLY:O     | 43:DO:102:ARG:HD3  | 2.18        | 0.43     |
| 28:BP:61:ARG:HH21  | 28:BP:61:ARG:HB3   | 1.83        | 0.43     |
| 23:BB:1883:U:H2'   | 23:BB:1884:G:O4'   | 2.17        | 0.43     |
| 23:BB:2300:C:H2'   | 23:BB:2301:C:H6    | 1.82        | 0.43     |
| 23:DB:1422:G:H1'   | 23:DB:1495:A:H61   | 1.83        | 0.43     |
| 23:DB:226:A:H5''   | 23:DB:257:C:O2'    | 2.18        | 0.43     |
| 2:AC:172:VAL:O     | 2:AC:174:LEU:HD12  | 2.18        | 0.43     |
| 4:AE:92:ARG:NH1    | 4:AE:92:ARG:HB3    | 2.32        | 0.43     |
| 48:DG:173:ALA:HB3  | 48:DG:175:LYS:HZ3  | 1.82        | 0.43     |
| 23:BB:2818:U:H4'   | 23:BB:2837:A:O4'   | 2.17        | 0.43     |
| 23:BB:2559:C:O2'   | 23:BB:2560:A:H5'   | 2.18        | 0.43     |
| 39:BX:15:ASN:H     | 39:BX:15:ASN:ND2   | 2.16        | 0.43     |
| 22:DA:64:G:H2'     | 22:DA:65:U:H6      | 1.83        | 0.43     |
| 23:BB:428:A:O2'    | 23:BB:429:A:H5'    | 2.18        | 0.43     |
| 8:CI:45:MET:SD     | 8:CI:45:MET:N      | 2.91        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 6:CG:16:LYS:HD3   | 6:CG:17:PHE:CE1    | 2.54        | 0.43     |
| 2:CC:34:SER:O     | 2:CC:38:VAL:HG22   | 2.18        | 0.43     |
| 23:DB:2047:C:O2'  | 23:DB:2048:G:H5'   | 2.17        | 0.43     |
| 23:DB:822:G:H2'   | 23:DB:823:C:H6     | 1.83        | 0.43     |
| 1:AA:771:G:O2'    | 1:AA:772:U:H5'     | 2.18        | 0.43     |
| 1:AA:454:G:H2'    | 1:AA:455:G:H8      | 1.82        | 0.43     |
| 1:CA:984:C:O2'    | 1:CA:985:C:H5'     | 2.18        | 0.43     |
| 6:AG:125:ASP:HA   | 6:AG:128:GLU:OE1   | 2.19        | 0.43     |
| 24:BI:38:CYS:O    | 24:BI:42:ASN:ND2   | 2.51        | 0.43     |
| 23:DB:1501:G:O2'  | 23:DB:1502:A:H5'   | 2.18        | 0.43     |
| 38:DM:74:THR:O    | 38:DM:75:GLU:HB2   | 2.18        | 0.43     |
| 24:BI:103:ALA:O   | 24:BI:107:GLU:HG3  | 2.18        | 0.43     |
| 23:DB:1336:A:H3'  | 23:DB:1337:G:H8    | 1.83        | 0.43     |
| 23:DB:1623:G:O2'  | 23:DB:1624:U:H5'   | 2.18        | 0.43     |
| 23:DB:1633:G:O2'  | 23:DB:1634:A:H5''  | 2.17        | 0.43     |
| 47:DF:94:ARG:O    | 47:DF:98:PHE:N     | 2.49        | 0.43     |
| 24:BI:4:VAL:HG13  | 24:BI:4:VAL:O      | 2.17        | 0.43     |
| 23:DB:2754:U:H6   | 23:DB:2754:U:O5'   | 2.01        | 0.43     |
| 1:CA:397:A:H3'    | 1:CA:397:A:N3      | 2.34        | 0.43     |
| 23:BB:1304:A:H2'  | 23:BB:1305:C:C6    | 2.54        | 0.43     |
| 1:AA:1165:U:H2'   | 1:AA:1166:G:O4'    | 2.18        | 0.43     |
| 23:BB:2657:A:H4'  | 48:BG:91:VAL:HG21  | 2.00        | 0.43     |
| 48:DG:102:ILE:CD1 | 48:DG:116:LEU:HD11 | 2.48        | 0.43     |
| 53:D6:80:GLU:HB2  | 53:D6:99:LEU:CD1   | 2.48        | 0.43     |
| 47:DF:57:ALA:HB2  | 47:DF:64:PRO:CG    | 2.48        | 0.43     |
| 52:DW:59:PHE:CD2  | 52:DW:60:ALA:N     | 2.86        | 0.43     |
| 53:B6:68:VAL:O    | 53:B6:70:SER:N     | 2.51        | 0.43     |
| 53:B6:56:ALA:CB   | 53:B6:79:ILE:HD11  | 2.48        | 0.43     |
| 8:CI:48:ARG:HA    | 8:CI:51:LEU:CD1    | 2.46        | 0.43     |
| 41:BJ:17:VAL:CG2  | 41:BJ:137:PRO:HB2  | 2.31        | 0.43     |
| 8:AI:74:GLN:O     | 8:AI:78:ILE:HG13   | 2.19        | 0.43     |
| 8:AI:114:LYS:H    | 8:AI:120:ALA:HA    | 1.84        | 0.43     |
| 35:DV:62:THR:CG2  | 35:DV:71:LYS:HG2   | 2.48        | 0.43     |
| 25:BC:140:VAL:O   | 25:BC:141:HIS:HB2  | 2.18        | 0.43     |
| 35:BV:32:GLY:C    | 35:BV:93:ARG:HG3   | 2.39        | 0.43     |
| 23:DB:2308:G:O6   | 23:DB:2311:A:N7    | 2.51        | 0.43     |
| 7:AH:124:ILE:HG22 | 7:AH:125:ILE:H     | 1.83        | 0.43     |
| 38:DM:21:ALA:CB   | 38:DM:100:LYS:HG2  | 2.46        | 0.43     |
| 50:BT:50:LEU:O    | 50:BT:52:GLU:N     | 2.45        | 0.43     |
| 41:BJ:33:ALA:O    | 41:BJ:34:ARG:C     | 2.56        | 0.43     |
| 47:BF:141:ASP:O   | 47:BF:144:LYS:N    | 2.52        | 0.43     |
| 2:CC:87:ARG:HG2   | 2:CC:98:ALA:O      | 2.18        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 47:DF:141:ASP:O   | 47:DF:144:LYS:N    | 2.51        | 0.43     |
| 12:CM:84:CYS:SG   | 12:CM:86:ARG:HB2   | 2.59        | 0.43     |
| 29:DE:33:VAL:HA   | 29:DE:36:ALA:HB3   | 2.01        | 0.43     |
| 50:DT:40:LYS:O    | 50:DT:43:ILE:HB    | 2.17        | 0.43     |
| 45:DS:28:LYS:O    | 45:DS:71:VAL:HG12  | 2.17        | 0.43     |
| 23:BB:2788:C:H1'  | 23:BB:2809:A:C2    | 2.52        | 0.43     |
| 38:DM:63:ILE:N    | 38:DM:63:ILE:HD12  | 2.34        | 0.43     |
| 8:CI:33:SER:HB3   | 8:CI:36:GLN:HE21   | 1.82        | 0.43     |
| 2:AC:149:LYS:HE3  | 2:AC:166:TRP:CH2   | 2.54        | 0.43     |
| 1:AA:1325:C:O2'   | 1:AA:1326:U:H5'    | 2.19        | 0.43     |
| 45:BS:66:ILE:HG12 | 45:BS:67:ASP:N     | 2.33        | 0.43     |
| 17:CR:38:ILE:HG22 | 17:CR:58:ILE:HD13  | 2.01        | 0.43     |
| 3:CD:153:ARG:HG3  | 3:CD:154:VAL:N     | 2.33        | 0.43     |
| 23:DB:2884:U:O4   | 31:D0:39:ARG:HD3   | 2.18        | 0.43     |
| 1:CA:21:G:H2'     | 1:CA:22:G:H8       | 1.74        | 0.43     |
| 1:CA:909:A:H1'    | 1:CA:1414:U:H5'    | 1.99        | 0.43     |
| 1:AA:81:A:C2      | 1:AA:82:G:N7       | 2.87        | 0.43     |
| 24:DI:126:ARG:NH1 | 24:DI:126:ARG:CB   | 2.81        | 0.43     |
| 23:BB:1309:G:H4'  | 36:B2:7:PRO:HB2    | 1.99        | 0.43     |
| 25:BC:159:THR:O   | 25:BC:160:TYR:HB3  | 2.17        | 0.43     |
| 28:BP:9:GLN:HA    | 28:BP:12:MET:CG    | 2.49        | 0.43     |
| 34:D3:23:HIS:ND1  | 34:D3:24:LYS:N     | 2.66        | 0.43     |
| 20:CB:112:ARG:O   | 20:CB:116:LEU:HG   | 2.18        | 0.43     |
| 29:DE:130:LYS:C   | 29:DE:132:LYS:N    | 2.70        | 0.43     |
| 34:B3:33:THR:HG23 | 34:B3:34:LYS:N     | 2.33        | 0.43     |
| 51:DZ:20:HIS:O    | 51:DZ:21:ALA:HB3   | 2.18        | 0.43     |
| 1:CA:1343:G:H4'   | 8:CI:123:ARG:HB2   | 2.01        | 0.43     |
| 12:CM:95:PRO:HB2  | 12:CM:99:GLN:CD    | 2.38        | 0.43     |
| 1:CA:264:C:H2'    | 1:CA:265:G:O4'     | 2.18        | 0.43     |
| 20:CB:95:TRP:HZ2  | 20:CB:100:LEU:HD13 | 1.84        | 0.43     |
| 23:BB:1582:C:H3'  | 23:BB:1583:A:N3    | 2.34        | 0.43     |
| 1:AA:15:G:H2'     | 1:AA:16:A:C8       | 2.53        | 0.43     |
| 5:AF:53:LYS:HD3   | 5:AF:54:LEU:H      | 1.83        | 0.43     |
| 23:DB:741:U:H2'   | 23:DB:742:A:H8     | 1.83        | 0.43     |
| 25:DC:244:VAL:HA  | 25:DC:249:VAL:O    | 2.19        | 0.43     |
| 45:BS:51:LEU:HD12 | 45:BS:105:VAL:HG11 | 1.98        | 0.43     |
| 20:AB:86:CYS:HB3  | 20:AB:88:GLN:CD    | 2.39        | 0.43     |
| 23:BB:1470:A:H3'  | 23:BB:1471:G:H8    | 1.83        | 0.43     |
| 3:AD:22:SER:N     | 3:AD:109:THR:HG22  | 2.33        | 0.43     |
| 40:BH:47:PHE:C    | 40:BH:50:ARG:HH21  | 2.21        | 0.43     |
| 23:DB:1686:C:H2'  | 23:DB:1687:G:O4'   | 2.17        | 0.43     |
| 23:BB:1356:G:O2'  | 23:BB:1357:C:H5'   | 2.18        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 11:CL:115:LYS:O   | 11:CL:116:TYR:HB2 | 2.18        | 0.43     |
| 23:BB:1383:A:H2   | 23:BB:1405:U:O2   | 2.00        | 0.43     |
| 23:BB:7:G:H4'     | 41:BJ:15:TRP:CH2  | 2.53        | 0.43     |
| 22:DA:39:A:H2     | 22:DA:46:A:N6     | 2.15        | 0.43     |
| 37:DL:23:ILE:H    | 37:DL:23:ILE:CD1  | 2.30        | 0.43     |
| 23:BB:2784:U:H2'  | 23:BB:2785:C:C6   | 2.53        | 0.43     |
| 23:BB:2259:U:H2'  | 23:BB:2260:C:H6   | 1.83        | 0.43     |
| 23:BB:1341:G:N2   | 23:BB:1398:C:H4'  | 2.33        | 0.43     |
| 10:AK:52:ARG:HA   | 10:AK:52:ARG:HD2  | 1.64        | 0.43     |
| 5:CF:81:ASN:O     | 5:CF:82:ASP:C     | 2.56        | 0.43     |
| 23:BB:1292:G:O2'  | 23:BB:1293:C:H5'  | 2.19        | 0.43     |
| 23:DB:443:A:C8    | 29:DE:40:ARG:HD3  | 2.53        | 0.43     |
| 1:AA:592:G:O2'    | 1:AA:593:U:H5'    | 2.18        | 0.43     |
| 43:BO:94:ARG:HD2  | 43:BO:97:PHE:O    | 2.19        | 0.43     |
| 42:BN:2:ARG:HG2   | 42:BN:2:ARG:HH11  | 1.84        | 0.43     |
| 41:BJ:88:THR:HG22 | 41:BJ:91:GLU:OE1  | 2.17        | 0.43     |
| 23:BB:2008:C:H2'  | 23:BB:2009:A:C8   | 2.52        | 0.43     |
| 10:CK:63:GLN:O    | 10:CK:67:GLU:HG2  | 2.18        | 0.43     |
| 23:DB:2008:C:H2'  | 23:DB:2009:A:C8   | 2.53        | 0.43     |
| 42:DN:9:GLN:C     | 42:DN:17:ARG:HD3  | 2.39        | 0.43     |
| 8:CI:71:ILE:H     | 8:CI:71:ILE:HD12  | 1.83        | 0.43     |
| 23:BB:639:U:H2'   | 23:BB:640:C:C6    | 2.54        | 0.43     |
| 34:B3:12:ARG:NE   | 37:BL:58:TYR:O    | 2.52        | 0.43     |
| 23:DB:2514:U:H2'  | 23:DB:2515:C:C6   | 2.54        | 0.43     |
| 36:D2:12:ARG:HH21 | 36:D2:12:ARG:HG3  | 1.83        | 0.43     |
| 1:AA:1020:G:N3    | 1:AA:1020:G:H2'   | 2.33        | 0.43     |
| 23:BB:1227:G:O2'  | 23:BB:1228:G:H5'  | 2.18        | 0.43     |
| 1:CA:991:U:H2'    | 1:CA:1212:U:O2    | 2.18        | 0.43     |
| 1:AA:668:G:O2'    | 1:AA:669:G:H5'    | 2.18        | 0.43     |
| 5:AF:17:GLN:O     | 5:AF:21:MET:HG3   | 2.17        | 0.43     |
| 1:CA:291:U:H2'    | 1:CA:292:G:H8     | 1.84        | 0.43     |
| 41:BJ:98:GLU:CD   | 41:BJ:98:GLU:H    | 2.22        | 0.43     |
| 53:B6:177:GLU:O   | 53:B6:177:GLU:HG2 | 2.16        | 0.43     |
| 23:BB:527:C:O4'   | 23:BB:527:C:O2    | 2.31        | 0.43     |
| 53:B6:73:GLN:HG3  | 53:B6:73:GLN:H    | 1.64        | 0.43     |
| 14:AO:68:ASP:O    | 14:AO:72:ARG:HG3  | 2.17        | 0.43     |
| 52:DW:19:ARG:O    | 52:DW:20:LEU:HD23 | 2.18        | 0.43     |
| 20:AB:205:ALA:HB3 | 20:AB:208:ALA:HB3 | 2.00        | 0.43     |
| 52:DW:49:ASN:C    | 52:DW:50:VAL:HG22 | 2.38        | 0.43     |
| 40:BH:89:LYS:HB3  | 40:BH:89:LYS:HZ3  | 1.83        | 0.43     |
| 8:CI:24:ASN:CG    | 8:CI:25:GLY:H     | 2.21        | 0.43     |
| 44:DQ:86:SER:OG   | 49:DR:51:VAL:HG12 | 2.19        | 0.43     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 20:CB:17:HIS:CG    | 20:CB:202:ASN:ND2 | 2.87        | 0.43     |
| 5:AF:25:TYR:O      | 5:AF:29:ILE:HG13  | 2.18        | 0.43     |
| 26:DD:104:VAL:HG13 | 26:DD:106:LYS:HE2 | 2.00        | 0.43     |
| 35:BV:50:MET:O     | 35:BV:56:PHE:HB2  | 2.18        | 0.43     |
| 1:AA:599:C:H2'     | 1:AA:600:A:H8     | 1.83        | 0.43     |
| 12:CM:30:LYS:HG3   | 12:CM:40:GLU:OE1  | 2.18        | 0.43     |
| 47:BF:131:VAL:O    | 47:BF:133:GLU:N   | 2.50        | 0.43     |
| 45:DS:17:VAL:C     | 45:DS:19:LEU:N    | 2.70        | 0.43     |
| 47:DF:108:PRO:C    | 47:DF:110:ILE:H   | 2.22        | 0.43     |
| 1:CA:1227:A:H4'    | 12:CM:113:LYS:HD2 | 2.00        | 0.43     |
| 1:CA:1081:A:O2'    | 1:CA:1082:A:H5'   | 2.18        | 0.43     |
| 18:AS:10:ILE:HD13  | 18:AS:40:PHE:CE1  | 2.53        | 0.43     |
| 37:BL:19:LEU:HD23  | 37:BL:31:GLY:O    | 2.18        | 0.43     |
| 23:BB:1181:U:H2'   | 23:BB:1182:G:H8   | 1.83        | 0.43     |
| 46:BU:47:PRO:HB3   | 46:BU:55:GLY:HA3  | 2.01        | 0.43     |
| 2:AC:149:LYS:HE2   | 2:AC:200:TRP:CZ3  | 2.53        | 0.43     |
| 27:DK:8:LEU:O      | 27:DK:19:VAL:HG22 | 2.19        | 0.43     |
| 53:B6:24:ASN:HA    | 53:B6:24:ASN:HD22 | 1.54        | 0.43     |
| 49:BR:39:LEU:CA    | 49:BR:49:ILE:HG12 | 2.48        | 0.43     |
| 44:DQ:105:PHE:HA   | 44:DQ:108:LEU:CD1 | 2.49        | 0.43     |
| 49:DR:59:ILE:H     | 49:DR:59:ILE:HG13 | 1.59        | 0.43     |
| 18:AS:52:ASN:O     | 18:AS:76:THR:HG23 | 2.19        | 0.43     |
| 23:DB:2847:U:H5''  | 28:DP:94:ALA:CB   | 2.49        | 0.43     |
| 3:AD:167:PRO:HG3   | 3:AD:170:LEU:HD11 | 1.99        | 0.43     |
| 1:AA:1096:C:O2'    | 1:AA:1097:C:H5'   | 2.19        | 0.43     |
| 23:BB:2753:A:O2'   | 23:BB:2754:U:H5'  | 2.18        | 0.43     |
| 1:AA:491:G:O2'     | 1:AA:492:C:H5'    | 2.19        | 0.43     |
| 23:DB:1470:A:H2'   | 23:DB:1471:G:O4'  | 2.18        | 0.43     |
| 35:DV:53:LYS:HZ2   | 35:DV:53:LYS:HA   | 1.82        | 0.43     |
| 3:AD:117:VAL:O     | 3:AD:130:ASN:HA   | 2.18        | 0.43     |
| 20:AB:19:THR:HG23  | 20:AB:20:ARG:H    | 1.82        | 0.43     |
| 45:BS:44:ALA:C     | 45:BS:46:LEU:N    | 2.72        | 0.43     |
| 23:DB:19:A:OP1     | 44:DQ:22:GLY:N    | 2.52        | 0.43     |
| 23:DB:1431:A:O2'   | 23:DB:1432:G:H5'  | 2.18        | 0.43     |
| 23:DB:704:G:H1'    | 23:DB:727:A:H61   | 1.83        | 0.43     |
| 1:AA:1532:U:N1     | 1:AA:1534:A:H5'   | 2.33        | 0.43     |
| 2:CC:70:ALA:HA     | 2:CC:105:VAL:HG22 | 2.01        | 0.43     |
| 1:AA:56:U:H2'      | 1:AA:57:G:H8      | 1.83        | 0.43     |
| 23:BB:1326:U:H2'   | 23:BB:1327:A:C8   | 2.50        | 0.43     |
| 42:BN:61:ALA:C     | 42:BN:63:ARG:N    | 2.71        | 0.43     |
| 22:BA:60:C:H2'     | 22:BA:61:G:C8     | 2.48        | 0.43     |
| 21:CU:11:PHE:CD1   | 21:CU:11:PHE:O    | 2.70        | 0.43     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 14:AO:43:PHE:C     | 14:AO:45:GLU:N     | 2.71        | 0.43     |
| 2:CC:16:PRO:CG     | 2:CC:53:ARG:HH22   | 2.30        | 0.43     |
| 23:DB:1117:C:O2'   | 23:DB:1118:C:H5'   | 2.17        | 0.43     |
| 23:DB:1424:G:H2'   | 23:DB:1425:G:C8    | 2.53        | 0.43     |
| 1:AA:652:U:H1'     | 1:AA:653:U:C5      | 2.52        | 0.43     |
| 23:BB:2560:A:H2'   | 23:BB:2561:U:C6    | 2.54        | 0.43     |
| 5:CF:46:GLN:HE21   | 5:CF:46:GLN:HA     | 1.83        | 0.43     |
| 28:DP:13:LYS:HG2   | 28:DP:76:HIS:ND1   | 2.32        | 0.43     |
| 23:DB:2408:U:H2'   | 23:DB:2409:G:H8    | 1.83        | 0.43     |
| 23:BB:730:A:O2'    | 23:BB:731:C:H5'    | 2.17        | 0.43     |
| 23:BB:302:C:O2'    | 23:BB:303:G:H5'    | 2.18        | 0.43     |
| 1:AA:1426:G:H2'    | 1:AA:1427:C:C6     | 2.53        | 0.43     |
| 23:BB:1751:U:H2'   | 23:BB:1752:C:C6    | 2.53        | 0.43     |
| 23:DB:1863:G:H2'   | 23:DB:1864:U:O4'   | 2.18        | 0.43     |
| 28:BP:44:GLY:HA3   | 28:BP:60:VAL:HG12  | 2.01        | 0.43     |
| 23:DB:2563:U:H2'   | 23:DB:2565:A:OP2   | 2.19        | 0.43     |
| 25:BC:9:SER:HB2    | 25:BC:10:PRO:HD2   | 2.00        | 0.43     |
| 8:CI:112:ARG:HH22  | 9:CJ:64:GLN:HE22   | 1.65        | 0.43     |
| 22:BA:80:U:H2'     | 22:BA:81:G:C8      | 2.53        | 0.43     |
| 8:AI:118:ARG:HG2   | 8:AI:118:ARG:O     | 2.18        | 0.43     |
| 1:CA:282:A:H2'     | 1:CA:282:A:N3      | 2.33        | 0.43     |
| 15:AP:45:GLU:C     | 15:AP:47:GLU:H     | 2.21        | 0.43     |
| 1:AA:12:U:H4'      | 1:AA:526:C:H4'     | 2.01        | 0.43     |
| 26:DD:35:THR:N     | 26:DD:49:GLN:O     | 2.50        | 0.43     |
| 23:BB:95:A:H4'     | 39:BX:38:GLN:O     | 2.19        | 0.43     |
| 43:DO:15:ARG:HH21  | 43:DO:95:SER:CB    | 2.32        | 0.43     |
| 20:CB:80:LYS:HG3   | 20:CB:81:ASP:N     | 2.33        | 0.43     |
| 25:BC:121:ALA:HB3  | 25:BC:129:LEU:HD11 | 2.01        | 0.43     |
| 48:BG:47:ASN:CG    | 48:BG:48:THR:H     | 2.21        | 0.43     |
| 25:DC:53:ILE:HG23  | 25:DC:53:ILE:O     | 2.18        | 0.43     |
| 48:BG:120:ILE:HD13 | 48:BG:121:THR:N    | 2.34        | 0.43     |
| 47:BF:87:LYS:HG3   | 47:BF:88:VAL:N     | 2.23        | 0.43     |
| 53:D6:90:LEU:HB3   | 53:D6:101:ILE:HG21 | 2.00        | 0.43     |
| 22:DA:40:U:H1'     | 22:DA:43:C:C5      | 2.53        | 0.43     |
| 53:B6:61:PRO:HD2   | 53:B6:65:THR:O     | 2.19        | 0.43     |
| 8:CI:17:ARG:O      | 8:CI:64:ILE:HA     | 2.18        | 0.43     |
| 8:CI:50:PRO:HD3    | 8:CI:79:ARG:CG     | 2.48        | 0.43     |
| 41:BJ:54:ILE:O     | 41:BJ:122:LEU:HA   | 2.18        | 0.43     |
| 44:DQ:89:ILE:HB    | 44:DQ:90:ASP:H     | 1.73        | 0.43     |
| 8:AI:17:ARG:O      | 8:AI:64:ILE:HA     | 2.19        | 0.43     |
| 25:BC:75:ALA:HB1   | 25:BC:94:LEU:O     | 2.19        | 0.43     |
| 23:BB:144:A:H2'    | 23:BB:145:C:H6     | 1.83        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 48:DG:32:LEU:HB3  | 48:DG:34:ARG:CZ    | 2.49        | 0.43     |
| 25:DC:75:ALA:HB1  | 25:DC:94:LEU:O     | 2.19        | 0.43     |
| 25:BC:90:ILE:HD13 | 25:BC:103:ILE:O    | 2.19        | 0.43     |
| 23:BB:107:G:H21   | 23:BB:346:A:H62    | 1.65        | 0.43     |
| 24:DI:49:GLU:HB3  | 24:DI:52:LEU:HD12  | 2.00        | 0.43     |
| 47:BF:140:ILE:O   | 47:BF:145:VAL:HG12 | 2.19        | 0.43     |
| 47:BF:169:LEU:HA  | 47:BF:172:PHE:HD2  | 1.83        | 0.43     |
| 45:DS:76:VAL:HA   | 45:DS:102:HIS:O    | 2.18        | 0.43     |
| 4:AE:131:ASN:ND2  | 4:AE:134:ASN:H     | 2.16        | 0.43     |
| 21:AU:24:LYS:HZ3  | 21:AU:25:ALA:N     | 2.15        | 0.43     |
| 24:BI:32:VAL:HG22 | 24:BI:60:VAL:CG2   | 2.49        | 0.43     |
| 1:CA:1082:A:O2'   | 1:CA:1083:U:H5'    | 2.19        | 0.43     |
| 12:CM:79:LEU:HD22 | 12:CM:86:ARG:HE    | 1.82        | 0.43     |
| 1:AA:1320:C:N4    | 18:AS:36:ARG:HE    | 2.15        | 0.43     |
| 18:AS:42:ASN:ND2  | 18:AS:43:MET:N     | 2.66        | 0.43     |
| 11:AL:88:ASP:C    | 11:AL:89:LEU:HD22  | 2.39        | 0.43     |
| 23:BB:1255:U:H5'' | 23:BB:1256:G:H5''  | 2.01        | 0.43     |
| 23:BB:2060:A:H62  | 29:BE:69:ARG:HH12  | 1.64        | 0.43     |
| 23:BB:672:C:H2'   | 23:BB:673:C:H6     | 1.83        | 0.43     |
| 23:DB:1790:C:H2'  | 23:DB:1791:A:N7    | 2.33        | 0.43     |
| 29:BE:29:HIS:CE1  | 37:BL:8:PRO:HG3    | 2.52        | 0.43     |
| 23:DB:28:A:N6     | 23:DB:512:G:O2'    | 2.52        | 0.43     |
| 1:AA:1324:A:H2'   | 1:AA:1325:C:C6     | 2.54        | 0.43     |
| 15:CP:6:LEU:HD11  | 15:CP:71:VAL:HB    | 2.01        | 0.43     |
| 1:AA:1432:G:H5''  | 1:AA:1432:G:H8     | 1.83        | 0.43     |
| 38:BM:64:TRP:HE3  | 38:BM:104:GLU:O    | 2.02        | 0.43     |
| 27:BK:79:PHE:CD2  | 28:BP:69:VAL:HG12  | 2.53        | 0.43     |
| 24:DI:41:PHE:CE2  | 24:DI:45:THR:HG21  | 2.53        | 0.43     |
| 38:DM:40:ARG:HB2  | 38:DM:93:VAL:HG21  | 1.99        | 0.43     |
| 40:DH:69:ALA:HB1  | 40:DH:140:ALA:HB2  | 2.00        | 0.43     |
| 10:AK:25:SER:HG   | 10:AK:28:ASN:H     | 1.65        | 0.43     |
| 21:AU:10:PRO:HB2  | 2:CC:71:ARG:HE     | 1.83        | 0.43     |
| 7:CH:47:ASP:CG    | 7:CH:48:PHE:N      | 2.71        | 0.43     |
| 23:BB:2773:C:O2'  | 23:BB:2774:C:H5'   | 2.19        | 0.43     |
| 38:BM:111:GLU:O   | 38:BM:114:ARG:HB3  | 2.19        | 0.43     |
| 4:CE:45:VAL:CG1   | 4:CE:116:VAL:HG23  | 2.48        | 0.43     |
| 23:DB:340:A:H2'   | 23:DB:341:C:O4'    | 2.18        | 0.43     |
| 22:BA:114:C:H2'   | 22:BA:115:A:H8     | 1.83        | 0.43     |
| 3:AD:84:ASN:C     | 3:AD:84:ASN:ND2    | 2.71        | 0.43     |
| 23:DB:1150:C:H2'  | 23:DB:1151:A:C8    | 2.47        | 0.43     |
| 6:CG:104:VAL:HG12 | 6:CG:108:ARG:HD2   | 2.01        | 0.43     |
| 39:DX:13:GLU:HA   | 39:DX:13:GLU:OE2   | 2.19        | 0.43     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 22:DA:14:U:H4'   | 22:DA:70:C:O2      | 2.19        | 0.43     |
| 1:AA:620:C:C1'   | 3:AD:131:ILE:HD13  | 2.48        | 0.43     |
| 45:BS:46:LEU:O   | 45:BS:50:VAL:HG23  | 2.18        | 0.43     |
| 23:BB:2231:U:H2' | 23:BB:2232:C:C6    | 2.53        | 0.43     |
| 25:BC:52:HIS:NE2 | 25:BC:218:THR:HG23 | 2.32        | 0.43     |
| 25:BC:52:HIS:O   | 25:BC:53:ILE:HB    | 2.18        | 0.43     |
| 23:DB:1983:G:H4' | 23:DB:2606:C:H4'   | 1.99        | 0.43     |
| 1:AA:1064:G:OP1  | 1:AA:1386:G:H4'    | 2.18        | 0.43     |
| 4:CE:55:VAL:N    | 4:CE:56:PRO:CD     | 2.81        | 0.43     |
| 23:DB:285:G:C2'  | 23:DB:286:U:H5'    | 2.49        | 0.43     |
| 14:AO:45:GLU:O   | 14:AO:47:LYS:N     | 2.50        | 0.43     |
| 1:CA:591:U:O2'   | 1:CA:592:G:H5'     | 2.19        | 0.43     |
| 23:BB:2623:G:H4' | 23:BB:2825:G:C8    | 2.52        | 0.43     |
| 37:DL:136:GLU:HA | 37:DL:140:GLY:CA   | 2.49        | 0.43     |
| 1:CA:642:A:H2'   | 1:CA:643:C:C6      | 2.51        | 0.43     |
| 23:DB:2054:A:H2' | 31:D0:4:GLN:OE1    | 2.19        | 0.43     |
| 23:BB:2303:G:C1' | 47:BF:122:ASP:OD1  | 2.67        | 0.43     |
| 6:AG:72:VAL:HG12 | 6:AG:89:GLU:HA     | 2.01        | 0.43     |
| 23:DB:39:G:H2'   | 23:DB:40:U:H6      | 1.83        | 0.43     |
| 36:B2:13:ASN:C   | 36:B2:15:SER:H     | 2.21        | 0.43     |
| 23:DB:1050:A:H2' | 23:DB:1051:G:H8    | 1.83        | 0.43     |
| 17:AR:57:ALA:HA  | 17:AR:60:ARG:HD2   | 2.00        | 0.43     |
| 22:DA:54:G:O2'   | 22:DA:55:U:H5'     | 2.18        | 0.43     |
| 23:DB:2203:U:H2' | 23:DB:2204:G:OP2   | 2.18        | 0.43     |
| 8:CI:39:GLY:HA2  | 8:CI:44:ARG:HD3    | 1.99        | 0.43     |
| 23:BB:67:U:H2'   | 23:BB:68:G:C8      | 2.54        | 0.43     |
| 23:BB:1050:A:H2' | 23:BB:1051:G:H8    | 1.83        | 0.43     |
| 5:CF:10:VAL:HA   | 5:CF:84:VAL:HA     | 2.01        | 0.43     |
| 20:AB:35:ASN:O   | 20:AB:37:VAL:N     | 2.52        | 0.43     |
| 24:BI:63:ASP:C   | 24:BI:65:SER:N     | 2.72        | 0.43     |
| 23:BB:697:G:H2'  | 23:BB:698:C:C6     | 2.53        | 0.43     |
| 23:BB:686:U:H1'  | 36:B2:6:GLN:O      | 2.17        | 0.43     |
| 1:CA:1495:U:O2'  | 1:CA:1496:C:H5'    | 2.19        | 0.43     |
| 23:BB:2515:C:O2' | 23:BB:2516:A:H5'   | 2.18        | 0.43     |
| 14:AO:69:TYR:HA  | 14:AO:72:ARG:NH1   | 2.34        | 0.43     |
| 23:DB:308:G:H1'  | 23:DB:501:A:OP1    | 2.19        | 0.43     |
| 23:DB:1410:G:H2' | 23:DB:1411:U:C6    | 2.54        | 0.43     |
| 23:BB:1360:G:H2' | 23:BB:1361:G:O4'   | 2.18        | 0.43     |
| 1:AA:755:G:H2'   | 1:AA:756:C:C6      | 2.53        | 0.43     |
| 23:DB:425:G:O2'  | 23:DB:426:C:H5'    | 2.18        | 0.43     |
| 1:CA:360:G:O2'   | 1:CA:361:G:H5'     | 2.19        | 0.43     |
| 2:AC:52:SER:HB3  | 2:AC:114:LEU:HG    | 2.00        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1587:G:H2'  | 23:BB:1588:G:H8    | 1.82        | 0.43     |
| 23:BB:677:A:O2'   | 23:BB:678:C:H5'    | 2.18        | 0.43     |
| 23:BB:2256:G:H2'  | 23:BB:2257:U:H6    | 1.83        | 0.43     |
| 1:CA:1363:A:H2'   | 1:CA:1363:A:N3     | 2.33        | 0.43     |
| 23:BB:2771:C:H1'  | 26:BD:208:LYS:HZ1  | 1.83        | 0.43     |
| 23:DB:765:C:H2'   | 23:DB:766:U:H6     | 1.83        | 0.43     |
| 23:BB:2454:G:H1'  | 57:BB:3366:HOH:O   | 2.18        | 0.43     |
| 21:CU:33:ARG:NE   | 21:CU:34:ARG:HG2   | 2.33        | 0.43     |
| 23:DB:1824:G:H1'  | 25:DC:251:THR:CG2  | 2.49        | 0.43     |
| 48:BG:96:ALA:O    | 48:BG:97:VAL:HB    | 2.19        | 0.43     |
| 44:DQ:29:ARG:O    | 44:DQ:30:VAL:HB    | 2.18        | 0.43     |
| 22:BA:42:C:O2'    | 47:BF:91:ARG:NH1   | 2.51        | 0.43     |
| 10:CK:70:ALA:HA   | 10:CK:73:VAL:CG2   | 2.49        | 0.43     |
| 53:D6:53:ASN:HD22 | 53:D6:53:ASN:N     | 2.10        | 0.43     |
| 53:D6:79:ILE:HG22 | 53:D6:80:GLU:N     | 2.33        | 0.43     |
| 23:DB:2314:A:H2'  | 23:DB:2315:G:H8    | 1.82        | 0.43     |
| 53:B6:28:LEU:O    | 53:B6:37:LEU:HD21  | 2.18        | 0.43     |
| 53:B6:55:ILE:CG2  | 53:B6:56:ALA:H     | 2.13        | 0.43     |
| 53:B6:66:LEU:O    | 53:B6:100:TYR:HA   | 2.18        | 0.43     |
| 8:CI:15:ALA:O     | 8:CI:66:VAL:HG23   | 2.19        | 0.43     |
| 1:CA:1349:A:P     | 8:CI:119:LYS:HD2   | 2.58        | 0.43     |
| 41:BJ:36:LEU:HD21 | 41:BJ:122:LEU:HD12 | 2.00        | 0.43     |
| 41:BJ:28:LEU:HG   | 41:BJ:32:LEU:CD1   | 2.48        | 0.43     |
| 8:AI:26:LYS:HB2   | 8:AI:61:ASP:CB     | 2.49        | 0.43     |
| 1:AA:1346:A:H5''  | 8:AI:121:ARG:HH21  | 1.83        | 0.43     |
| 23:DB:636:G:H4'   | 23:DB:638:G:O3'    | 2.17        | 0.43     |
| 41:DJ:36:LEU:HD21 | 41:DJ:122:LEU:HD12 | 2.00        | 0.43     |
| 22:DA:29:A:C4     | 22:DA:56:G:N2      | 2.86        | 0.43     |
| 25:DC:76:VAL:O    | 25:DC:93:VAL:O     | 2.36        | 0.43     |
| 43:BO:53:THR:HG23 | 43:BO:74:VAL:HG21  | 2.00        | 0.43     |
| 24:DI:54:ILE:HD11 | 24:DI:71:LYS:N     | 2.33        | 0.43     |
| 23:BB:2394:C:H2'  | 23:BB:2395:C:O4'   | 2.19        | 0.43     |
| 1:AA:1258:G:C2    | 1:AA:1278:G:N2     | 2.87        | 0.43     |
| 23:BB:340:A:O2'   | 29:BE:162:ARG:NH1  | 2.52        | 0.43     |
| 1:AA:921:U:O2     | 4:AE:23:THR:HG23   | 2.19        | 0.43     |
| 1:CA:411:A:O2'    | 1:CA:412:A:N3      | 2.42        | 0.43     |
| 18:CS:30:LEU:HB2  | 18:CS:48:ILE:CG2   | 2.41        | 0.43     |
| 37:DL:42:SER:O    | 37:DL:44:GLY:N     | 2.51        | 0.43     |
| 12:AM:84:CYS:SG   | 12:AM:86:ARG:HB2   | 2.58        | 0.43     |
| 18:AS:43:MET:O    | 18:AS:61:VAL:HB    | 2.18        | 0.43     |
| 18:AS:62:THR:HG22 | 18:AS:63:ASP:N     | 2.33        | 0.43     |
| 11:AL:86:VAL:CG1  | 11:AL:89:LEU:HD23  | 2.48        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 46:DU:47:PRO:HB3  | 46:DU:55:GLY:HA3   | 2.01        | 0.43     |
| 23:DB:2789:C:H2'  | 23:DB:2893:A:N7    | 2.32        | 0.43     |
| 1:CA:1269:A:N3    | 1:CA:1326:U:H1'    | 2.34        | 0.43     |
| 48:DG:147:LEU:HA  | 48:DG:150:TYR:HD1  | 1.82        | 0.43     |
| 48:DG:152:ARG:HA  | 48:DG:152:ARG:HD2  | 1.80        | 0.43     |
| 23:BB:1057:A:H62  | 23:BB:1086:A:H2'   | 1.83        | 0.43     |
| 1:AA:1287:A:H1'   | 1:AA:1353:G:O2'    | 2.18        | 0.43     |
| 23:BB:2733:A:C3'  | 23:BB:2733:A:C8    | 3.01        | 0.43     |
| 23:BB:1080:A:O2'  | 24:BI:126:ARG:CB   | 2.66        | 0.43     |
| 53:D6:2:THR:O     | 53:D6:3:LEU:C      | 2.55        | 0.43     |
| 27:DK:71:ARG:HD2  | 27:DK:106:GLU:OE2  | 2.18        | 0.43     |
| 42:BN:34:ILE:HG22 | 42:BN:35:LYS:N     | 2.32        | 0.43     |
| 23:BB:28:A:O2'    | 23:BB:29:U:H5'     | 2.17        | 0.43     |
| 44:BQ:9:ALA:O     | 44:BQ:11:ALA:N     | 2.52        | 0.43     |
| 20:AB:212:TYR:O   | 20:AB:216:VAL:HG13 | 2.19        | 0.43     |
| 38:BM:66:ARG:NE   | 38:BM:101:VAL:HG11 | 2.34        | 0.43     |
| 49:BR:49:ILE:HB   | 49:BR:53:PHE:O     | 2.19        | 0.43     |
| 7:AH:49:LYS:HG3   | 7:AH:50:VAL:N      | 2.33        | 0.43     |
| 26:DD:92:VAL:O    | 26:DD:94:GLN:N     | 2.51        | 0.43     |
| 9:AJ:15:HIS:HA    | 9:AJ:18:ILE:CG2    | 2.49        | 0.43     |
| 28:BP:3:ILE:HG23  | 28:BP:4:ILE:H      | 1.81        | 0.43     |
| 23:BB:2651:C:O2'  | 23:BB:2652:C:H5'   | 2.19        | 0.43     |
| 7:AH:68:LYS:HA    | 7:AH:68:LYS:HD2    | 1.90        | 0.43     |
| 45:DS:6:LYS:HA    | 45:DS:50:VAL:HG11  | 2.01        | 0.43     |
| 23:DB:170:U:O2'   | 23:DB:171:U:H5'    | 2.18        | 0.43     |
| 2:CC:129:PHE:CG   | 2:CC:130:ARG:N     | 2.86        | 0.43     |
| 23:DB:1428:C:H2'  | 23:DB:1569:A:OP2   | 2.18        | 0.43     |
| 46:BU:24:VAL:HA   | 46:BU:35:VAL:HA    | 2.01        | 0.43     |
| 9:AJ:24:GLU:CD    | 9:AJ:90:LEU:HD11   | 2.39        | 0.43     |
| 39:DX:52:ARG:O    | 39:DX:55:THR:HB    | 2.18        | 0.43     |
| 1:CA:663:A:H5'    | 1:CA:836:G:OP1     | 2.18        | 0.43     |
| 25:BC:6:LYS:HA    | 25:BC:7:PRO:HD3    | 1.91        | 0.43     |
| 39:BX:1:MET:CG    | 39:BX:4:LYS:HD3    | 2.48        | 0.43     |
| 1:AA:102:G:H2'    | 1:AA:103:U:H6      | 1.82        | 0.43     |
| 1:CA:549:C:H2'    | 1:CA:550:G:C8      | 2.53        | 0.43     |
| 23:BB:2219:U:O2'  | 23:BB:2220:U:H5'   | 2.18        | 0.43     |
| 1:CA:676:A:O2'    | 1:CA:677:U:H5'     | 2.19        | 0.43     |
| 1:AA:1053:G:H4'   | 1:AA:1054:C:H5'    | 1.99        | 0.43     |
| 23:BB:2758:A:C2'  | 23:BB:2759:G:H5'   | 2.48        | 0.43     |
| 1:AA:677:U:H3     | 1:AA:713:G:H22     | 1.66        | 0.43     |
| 3:CD:10:LEU:HD12  | 3:CD:20:LEU:HD11   | 2.01        | 0.43     |
| 20:AB:23:ASN:HB3  | 20:AB:188:THR:O    | 2.18        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 41:BJ:13:ARG:HB3  | 41:BJ:53:TYR:CD2  | 2.53        | 0.43     |
| 1:AA:1464:U:H2'   | 1:AA:1465:A:H8    | 1.83        | 0.43     |
| 22:BA:97:C:C2'    | 22:BA:98:G:H5'    | 2.49        | 0.43     |
| 14:AO:56:LEU:O    | 14:AO:59:MET:HG3  | 2.19        | 0.43     |
| 23:BB:958:U:N3    | 38:BM:16:ARG:HB3  | 2.33        | 0.43     |
| 1:CA:659:U:H2'    | 1:CA:660:C:C6     | 2.54        | 0.43     |
| 1:CA:327:A:H1'    | 1:CA:329:A:O4'    | 2.19        | 0.43     |
| 28:DP:80:VAL:CG1  | 28:DP:81:ASP:N    | 2.82        | 0.43     |
| 23:DB:600:G:H1'   | 29:DE:100:MET:CG  | 2.48        | 0.43     |
| 26:DD:40:LEU:HD12 | 26:DD:41:ALA:H    | 1.83        | 0.43     |
| 25:DC:270:ARG:CZ  | 25:DC:270:ARG:HB3 | 2.49        | 0.43     |
| 23:BB:2756:U:OP2  | 32:B4:17:VAL:HG11 | 2.19        | 0.43     |
| 23:DB:769:U:H2'   | 23:DB:770:G:H8    | 1.81        | 0.43     |
| 53:B6:134:ARG:CZ  | 53:B6:135:GLU:HG3 | 2.48        | 0.43     |
| 23:BB:483:A:H5'   | 46:BU:44:HIS:O    | 2.18        | 0.43     |
| 25:BC:57:HIS:ND1  | 25:BC:58:LYS:N    | 2.58        | 0.43     |
| 29:DE:6:LYS:HB3   | 29:DE:7:ASP:H     | 1.59        | 0.43     |
| 1:AA:770:C:O2'    | 1:AA:771:G:H5'    | 2.19        | 0.43     |
| 26:DD:56:LYS:C    | 26:DD:58:ASN:N    | 2.72        | 0.43     |
| 1:AA:291:U:H2'    | 1:AA:292:G:H8     | 1.84        | 0.43     |
| 1:AA:933:G:N7     | 6:AG:2:ARG:NH1    | 2.67        | 0.43     |
| 23:DB:1607:C:N4   | 23:DB:1622:G:OP2  | 2.51        | 0.43     |
| 51:DZ:2:SER:HB3   | 51:DZ:4:VAL:HG23  | 1.99        | 0.43     |
| 1:AA:1045:C:H2'   | 1:AA:1046:A:O4'   | 2.18        | 0.43     |
| 1:AA:537:G:H2'    | 1:AA:538:G:C8     | 2.53        | 0.43     |
| 2:AC:171:ARG:HB2  | 2:AC:171:ARG:HH11 | 1.82        | 0.43     |
| 37:BL:10:GLU:OE2  | 37:BL:10:GLU:HA   | 2.16        | 0.43     |
| 26:DD:182:ALA:O   | 26:DD:184:ARG:HG2 | 2.18        | 0.43     |
| 1:CA:323:U:H2'    | 1:CA:324:G:O4'    | 2.18        | 0.43     |
| 23:DB:1765:U:H2'  | 23:DB:1766:G:H8   | 1.83        | 0.43     |
| 10:AK:126:ARG:HA  | 10:AK:126:ARG:HE  | 1.83        | 0.43     |
| 23:DB:2331:G:H4'  | 52:DW:39:GLN:HA   | 2.01        | 0.43     |
| 48:BG:6:ALA:HB3   | 48:BG:68:ARG:CD   | 2.49        | 0.43     |
| 23:BB:21:A:H2'    | 23:BB:22:C:H6     | 1.81        | 0.43     |
| 20:AB:204:ASP:O   | 20:AB:205:ALA:HB3 | 2.17        | 0.43     |
| 26:BD:54:ALA:N    | 26:BD:76:GLY:HA2  | 2.34        | 0.43     |
| 52:DW:59:PHE:CD2  | 52:DW:61:LYS:HD2  | 2.54        | 0.43     |
| 53:B6:61:PRO:HD2  | 53:B6:65:THR:C    | 2.39        | 0.43     |
| 40:BH:90:LEU:O    | 40:BH:123:ARG:HD3 | 2.18        | 0.43     |
| 40:BH:84:ALA:CA   | 40:BH:90:LEU:HA   | 2.37        | 0.43     |
| 8:CI:49:GLN:N     | 8:CI:50:PRO:HD2   | 2.32        | 0.43     |
| 35:DV:72:VAL:CG1  | 35:DV:93:ARG:HA   | 2.49        | 0.43     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1217:C:H2'    | 1:AA:1218:C:C6     | 2.54        | 0.43     |
| 1:AA:1216:A:O2'    | 1:AA:1217:C:H5'    | 2.19        | 0.43     |
| 23:DB:2394:C:H2'   | 23:DB:2395:C:O4'   | 2.19        | 0.43     |
| 1:CA:598:U:H4'     | 7:CH:85:TYR:CD2    | 2.52        | 0.43     |
| 1:CA:1217:C:H2'    | 1:CA:1218:C:C6     | 2.54        | 0.43     |
| 23:BB:2199:A:H3'   | 23:BB:2200:C:C6    | 2.52        | 0.43     |
| 30:BY:8:GLN:HB3    | 30:BY:31:ILE:O     | 2.18        | 0.43     |
| 3:AD:24:VAL:HG23   | 3:AD:25:ARG:N      | 2.27        | 0.43     |
| 24:DI:54:ILE:O     | 24:DI:54:ILE:HG23  | 2.19        | 0.43     |
| 23:BB:1060:U:C1'   | 23:BB:1062:G:H5'   | 2.49        | 0.43     |
| 24:BI:11:GLN:NE2   | 24:BI:74:PRO:HG2   | 2.33        | 0.43     |
| 47:BF:168:LEU:O    | 47:BF:169:LEU:CB   | 2.65        | 0.43     |
| 29:BE:126:VAL:HG22 | 29:BE:133:LEU:HD12 | 1.99        | 0.43     |
| 29:BE:147:LEU:O    | 29:BE:168:ASP:O    | 2.37        | 0.43     |
| 47:DF:3:LEU:HD11   | 47:DF:172:PHE:CE1  | 2.54        | 0.43     |
| 33:D1:8:ILE:HG23   | 33:D1:51:ALA:HA    | 1.99        | 0.43     |
| 11:AL:41:PRO:CB    | 11:AL:88:ASP:HB3   | 2.49        | 0.43     |
| 50:DT:11:LEU:N     | 50:DT:11:LEU:HD22  | 2.29        | 0.43     |
| 23:BB:1244:A:H5''  | 37:BL:8:PRO:CD     | 2.38        | 0.43     |
| 22:DA:75:G:N1      | 22:DA:102:G:N2     | 2.67        | 0.43     |
| 23:BB:2734:A:H61   | 23:BB:2770:G:H1'   | 1.83        | 0.43     |
| 1:CA:120:A:C5      | 1:CA:122:G:C6      | 3.07        | 0.43     |
| 20:AB:16:GLY:HA2   | 20:AB:40:ILE:HG13  | 1.98        | 0.43     |
| 23:BB:26:G:H1'     | 23:BB:514:A:H61    | 1.82        | 0.43     |
| 20:AB:64:GLY:HA2   | 20:AB:158:ASP:OD1  | 2.18        | 0.43     |
| 1:CA:1306:A:H1'    | 1:CA:1332:A:C2     | 2.52        | 0.43     |
| 27:BK:119:ALA:O    | 27:BK:120:PRO:O    | 2.37        | 0.43     |
| 24:DI:12:VAL:HG13  | 24:DI:41:PHE:CE2   | 2.54        | 0.43     |
| 23:DB:1445:G:H2'   | 23:DB:1446:C:H6    | 1.82        | 0.43     |
| 36:B2:42:LEU:O     | 36:B2:43:THR:HG23  | 2.19        | 0.43     |
| 20:CB:212:TYR:O    | 20:CB:216:VAL:HG22 | 2.19        | 0.43     |
| 20:CB:86:CYS:C     | 20:CB:88:GLN:H     | 2.22        | 0.43     |
| 36:D2:31:LEU:HD22  | 36:D2:42:LEU:HD12  | 2.00        | 0.43     |
| 9:AJ:7:ARG:NH1     | 9:AJ:7:ARG:HB2     | 2.33        | 0.43     |
| 16:CQ:77:VAL:HG12  | 16:CQ:79:GLU:H     | 1.84        | 0.43     |
| 37:BL:85:VAL:HG22  | 37:BL:94:THR:HG21  | 2.00        | 0.43     |
| 23:DB:1434:A:H62   | 23:DB:1558:C:H42   | 1.66        | 0.43     |
| 1:CA:1503:A:C8     | 1:CA:1531:A:H1'    | 2.53        | 0.43     |
| 41:BJ:112:GLY:N    | 41:BJ:113:PRO:HD2  | 2.31        | 0.43     |
| 1:AA:1479:C:H2'    | 1:AA:1480:A:C8     | 2.46        | 0.43     |
| 49:BR:27:ILE:HG22  | 49:BR:28:ALA:N     | 2.33        | 0.43     |
| 49:BR:63:VAL:O     | 49:BR:63:VAL:HG23  | 2.19        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:1123:U:C2'   | 1:CA:1124:G:H5'   | 2.49        | 0.43     |
| 9:CJ:35:GLN:HG2   | 9:CJ:77:VAL:HB    | 2.01        | 0.43     |
| 3:CD:96:ARG:O     | 3:CD:99:ASN:HB3   | 2.19        | 0.43     |
| 22:BA:14:U:H4'    | 22:BA:70:C:O2     | 2.19        | 0.43     |
| 23:DB:1582:C:H3'  | 23:DB:1583:A:N3   | 2.33        | 0.43     |
| 15:CP:76:LYS:HZ3  | 15:CP:80:LYS:HD3  | 1.81        | 0.43     |
| 23:DB:1405:U:H2'  | 23:DB:1406:U:H6   | 1.83        | 0.43     |
| 23:DB:1383:A:H2   | 23:DB:1405:U:O2   | 2.01        | 0.43     |
| 23:BB:1353:A:O2'  | 23:BB:1354:A:H5'  | 2.19        | 0.43     |
| 2:CC:111:ASP:OD2  | 2:CC:114:LEU:HG   | 2.19        | 0.43     |
| 1:AA:1229:A:H2'   | 1:AA:1230:C:C6    | 2.53        | 0.43     |
| 1:AA:1229:A:OP2   | 12:AM:112:ARG:HD2 | 2.18        | 0.43     |
| 11:CL:107:LYS:C   | 11:CL:109:ARG:H   | 2.20        | 0.43     |
| 1:AA:213:G:H2'    | 1:AA:213:G:N3     | 2.33        | 0.43     |
| 27:BK:2:ILE:HA    | 27:BK:33:ALA:H    | 1.83        | 0.43     |
| 23:BB:2449:U:H4'  | 23:BB:2450:A:OP1  | 2.19        | 0.43     |
| 23:DB:2217:G:H2'  | 23:DB:2218:G:H8   | 1.83        | 0.43     |
| 17:CR:27:THR:HG22 | 17:CR:31:TYR:HE1  | 1.83        | 0.43     |
| 23:BB:1561:C:H2'  | 23:BB:1562:U:H6   | 1.82        | 0.43     |
| 23:BB:1562:U:O2'  | 23:BB:1563:U:H5'  | 2.19        | 0.43     |
| 23:BB:1946:U:H2'  | 23:BB:1947:C:C6   | 2.53        | 0.43     |
| 1:AA:747:A:H2'    | 1:AA:748:G:O4'    | 2.19        | 0.43     |
| 20:AB:22:TRP:CZ3  | 20:AB:24:PRO:HA   | 2.53        | 0.43     |
| 1:CA:425:G:H2'    | 1:CA:426:U:H6     | 1.83        | 0.43     |
| 41:BJ:12:LYS:O    | 41:BJ:13:ARG:HB2  | 2.18        | 0.43     |
| 23:BB:1426:G:H8   | 23:BB:1426:G:OP2  | 2.02        | 0.43     |
| 23:BB:1707:G:O2'  | 23:BB:1708:C:H5'  | 2.18        | 0.43     |
| 1:AA:1127:G:H5'   | 1:AA:1280:A:O2'   | 2.19        | 0.43     |
| 23:BB:519:U:H2'   | 23:BB:520:G:H8    | 1.83        | 0.43     |
| 38:DM:11:LYS:HD2  | 38:DM:86:LYS:HG2  | 1.99        | 0.43     |
| 23:BB:2649:C:H2'  | 23:BB:2650:U:C6   | 2.53        | 0.43     |
| 47:BF:121:PHE:O   | 47:BF:122:ASP:OD1 | 2.37        | 0.43     |
| 23:DB:1476:U:O2'  | 23:DB:1477:A:H8   | 2.02        | 0.43     |
| 23:DB:2821:A:OP2  | 23:DB:2822:G:OP2  | 2.37        | 0.43     |
| 23:DB:2821:A:OP2  | 42:DN:3:HIS:NE2   | 2.51        | 0.43     |
| 1:AA:642:A:H2'    | 1:AA:643:C:C6     | 2.54        | 0.43     |
| 23:BB:41:C:O2'    | 23:BB:42:A:H5'    | 2.18        | 0.43     |
| 23:BB:840:C:O2'   | 23:BB:841:G:H5'   | 2.19        | 0.43     |
| 23:BB:1385:A:O2'  | 23:BB:1396:U:H6   | 2.02        | 0.43     |
| 23:DB:1838:C:H4'  | 23:DB:1839:G:C8   | 2.54        | 0.43     |
| 23:BB:622:G:H2'   | 23:BB:623:C:C6    | 2.54        | 0.43     |
| 23:DB:2830:C:H1'  | 23:DB:2836:U:O4'  | 2.19        | 0.43     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 39:DX:15:ASN:ND2   | 39:DX:15:ASN:H     | 2.16        | 0.43     |
| 1:CA:1020:G:N3     | 1:CA:1020:G:H2'    | 2.33        | 0.43     |
| 23:DB:729:G:H2'    | 23:DB:1775:U:H1'   | 1.99        | 0.43     |
| 23:DB:1893:C:H2'   | 23:DB:1894:C:O4'   | 2.19        | 0.43     |
| 23:BB:1310:G:H1'   | 23:BB:1611:C:H5'   | 2.01        | 0.43     |
| 23:BB:2281:A:O2'   | 23:BB:2282:G:H5'   | 2.18        | 0.43     |
| 22:BA:57:A:OP2     | 22:BA:58:A:OP2     | 2.36        | 0.43     |
| 1:CA:914:A:O2'     | 1:CA:915:A:H5'     | 2.18        | 0.43     |
| 1:CA:916:U:H2'     | 1:CA:917:G:H8      | 1.84        | 0.43     |
| 23:BB:104:A:H2'    | 23:BB:105:C:O4'    | 2.17        | 0.43     |
| 52:BW:27:GLY:O     | 52:BW:63:ASP:HA    | 2.18        | 0.43     |
| 2:AC:178:ARG:HG2   | 2:AC:206:ILE:HA    | 2.00        | 0.43     |
| 28:DP:36:LYS:HA    | 28:DP:36:LYS:HD3   | 1.87        | 0.43     |
| 1:CA:1045:C:H2'    | 1:CA:1046:A:O4'    | 2.19        | 0.43     |
| 52:BW:59:PHE:O     | 52:BW:60:ALA:HB3   | 2.17        | 0.43     |
| 23:DB:2330:G:H1'   | 52:DW:38:ARG:CB    | 2.49        | 0.43     |
| 25:DC:106:PRO:O    | 25:DC:109:LEU:HD13 | 2.18        | 0.43     |
| 23:BB:19:A:OP1     | 44:BQ:22:GLY:N     | 2.52        | 0.43     |
| 40:BH:111:ALA:HB3  | 40:BH:114:GLU:HG2  | 2.00        | 0.43     |
| 40:BH:116:ARG:HH11 | 40:BH:116:ARG:HB2  | 1.83        | 0.43     |
| 16:CQ:6:THR:O      | 16:CQ:7:LEU:HD23   | 2.19        | 0.43     |
| 47:DF:65:LEU:CD2   | 47:DF:87:LYS:HD2   | 2.47        | 0.43     |
| 23:DB:855:G:C2     | 52:DW:23:LYS:HE3   | 2.53        | 0.43     |
| 44:DQ:63:ARG:NH2   | 44:DQ:96:ASP:CA    | 2.79        | 0.43     |
| 13:AN:60:ARG:HH21  | 13:AN:69:PRO:HD3   | 1.82        | 0.43     |
| 23:DB:2443:C:O2'   | 23:DB:2444:G:H5'   | 2.18        | 0.43     |
| 50:BT:47:VAL:HG12  | 50:BT:47:VAL:O     | 2.19        | 0.43     |
| 46:DU:85:ARG:NH1   | 46:DU:86:PHE:H     | 2.16        | 0.43     |
| 1:AA:947:G:OP1     | 12:AM:106:ARG:HB3  | 2.18        | 0.43     |
| 23:BB:346:A:H5'    | 23:BB:346:A:N3     | 2.33        | 0.43     |
| 1:AA:411:A:O2'     | 1:AA:412:A:N3      | 2.43        | 0.43     |
| 2:AC:76:ILE:HD13   | 2:AC:83:VAL:HG21   | 2.00        | 0.43     |
| 47:DF:106:ALA:N    | 47:DF:108:PRO:HD2  | 2.33        | 0.43     |
| 18:CS:42:ASN:ND2   | 18:CS:43:MET:N     | 2.67        | 0.43     |
| 29:DE:32:VAL:HG23  | 29:DE:33:VAL:N     | 2.33        | 0.43     |
| 23:DB:483:A:H5''   | 46:DU:46:LYS:HG3   | 2.01        | 0.43     |
| 45:DS:28:LYS:HB3   | 45:DS:29:VAL:H     | 1.42        | 0.43     |
| 45:DS:36:LEU:HB3   | 45:DS:48:LYS:HB2   | 2.01        | 0.43     |
| 25:BC:202:ARG:HH11 | 25:BC:213:ARG:NH2  | 2.17        | 0.43     |
| 29:DE:184:ASP:O    | 29:DE:185:LYS:HG3  | 2.19        | 0.43     |
| 29:DE:117:ARG:HA   | 29:DE:185:LYS:HE3  | 2.00        | 0.43     |
| 2:CC:120:THR:HA    | 2:CC:123:LEU:HD12  | 2.01        | 0.43     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 38:DM:47:GLU:O   | 38:DM:51:ARG:HG3   | 2.19        | 0.43     |
| 49:BR:3:ALA:HB1  | 49:BR:59:ILE:HD13  | 2.01        | 0.43     |
| 27:DK:99:ILE:H   | 27:DK:118:LEU:HD23 | 1.83        | 0.43     |
| 3:AD:121:ALA:O   | 3:AD:122:ILE:HD13  | 2.19        | 0.43     |
| 1:CA:279:A:H5'   | 1:CA:281:G:H5'     | 1.99        | 0.43     |
| 28:DP:3:ILE:HG23 | 28:DP:4:ILE:H      | 1.83        | 0.43     |
| 23:BB:1441:G:O2' | 23:BB:1442:U:H5'   | 2.19        | 0.43     |
| 38:BM:47:GLU:O   | 38:BM:51:ARG:HG3   | 2.19        | 0.43     |
| 1:AA:271:C:O2'   | 1:AA:272:C:H5'     | 2.19        | 0.43     |
| 5:AF:4:TYR:CE2   | 5:AF:71:ILE:HG21   | 2.53        | 0.43     |
| 1:CA:715:A:O2'   | 1:CA:716:A:H5'     | 2.18        | 0.43     |
| 23:DB:1131:G:H22 | 23:DB:2024:G:H21   | 1.65        | 0.43     |
| 1:AA:1097:C:H2'  | 1:AA:1098:C:C6     | 2.53        | 0.43     |
| 16:AQ:18:LYS:HD3 | 16:AQ:48:GLU:HG2   | 2.01        | 0.43     |
| 23:DB:2591:C:O2' | 23:DB:2592:G:H5'   | 2.19        | 0.43     |
| 28:BP:20:ARG:CG  | 28:BP:21:PRO:HD2   | 2.45        | 0.43     |
| 45:BS:6:LYS:HA   | 45:BS:50:VAL:HG11  | 2.01        | 0.43     |
| 1:CA:1460:C:H2'  | 1:CA:1461:G:H8     | 1.84        | 0.43     |
| 23:DB:1172:C:H2' | 23:DB:1173:U:O4'   | 2.18        | 0.43     |
| 6:CG:22:LEU:O    | 6:CG:25:PHE:HB3    | 2.19        | 0.43     |
| 23:BB:2578:G:O2' | 23:BB:2579:C:H5'   | 2.18        | 0.43     |
| 1:AA:796:C:H2'   | 1:AA:797:C:H6      | 1.84        | 0.43     |
| 1:CA:678:U:H4'   | 1:CA:778:G:OP1     | 2.19        | 0.43     |
| 2:CC:65:VAL:HG21 | 2:CC:90:VAL:HG11   | 2.01        | 0.43     |
| 43:DO:6:ALA:O    | 43:DO:10:ARG:HG3   | 2.19        | 0.43     |
| 20:AB:132:GLU:CD | 20:AB:136:ARG:HH21 | 2.21        | 0.43     |
| 23:BB:1260:A:H2' | 23:BB:1261:C:H6    | 1.83        | 0.43     |
| 43:BO:40:ILE:CG2 | 43:BO:44:GLY:HA2   | 2.49        | 0.43     |
| 43:BO:75:GLY:HA3 | 43:BO:106:LEU:HA   | 1.99        | 0.43     |
| 1:AA:1307:U:H2'  | 1:AA:1308:U:O4'    | 2.19        | 0.43     |
| 51:BZ:66:THR:O   | 51:BZ:70:GLU:HG3   | 2.19        | 0.43     |
| 9:AJ:65:TYR:C    | 13:AN:98:ALA:HB2   | 2.39        | 0.43     |
| 5:AF:81:ASN:O    | 5:AF:82:ASP:C      | 2.57        | 0.43     |
| 23:DB:708:G:H2'  | 23:DB:709:U:C6     | 2.53        | 0.43     |
| 46:BU:25:LYS:CE  | 46:BU:36:GLU:HG3   | 2.49        | 0.43     |
| 23:BB:962:G:H21  | 23:BB:2250:G:H1    | 1.63        | 0.43     |
| 40:DH:44:ILE:O   | 40:DH:48:GLU:HG2   | 2.19        | 0.43     |
| 43:DO:75:GLY:HA3 | 43:DO:106:LEU:HA   | 2.00        | 0.43     |
| 23:DB:1720:U:C2' | 23:DB:1721:G:H5'   | 2.49        | 0.43     |
| 1:AA:205:A:H2'   | 1:AA:206:C:O4'     | 2.19        | 0.43     |
| 1:AA:903:G:H2'   | 1:AA:904:U:C6      | 2.53        | 0.43     |
| 23:BB:1300:G:H5' | 23:BB:1301:A:N3    | 2.34        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 48:BG:154:GLU:O   | 48:BG:156:TYR:N    | 2.51        | 0.43     |
| 23:DB:79:C:HO2'   | 23:DB:346:A:H8     | 1.55        | 0.43     |
| 23:BB:208:C:H2'   | 23:BB:209:C:C6     | 2.53        | 0.43     |
| 23:DB:2771:C:H1'  | 26:DD:208:LYS:NZ   | 2.33        | 0.43     |
| 1:CA:177:G:N3     | 1:CA:177:G:O4'     | 2.52        | 0.43     |
| 1:AA:454:G:O2'    | 1:AA:455:G:H5'     | 2.19        | 0.43     |
| 2:AC:178:ARG:CG   | 2:AC:206:ILE:HA    | 2.49        | 0.43     |
| 1:AA:241:G:O2'    | 1:AA:242:G:H5'     | 2.18        | 0.43     |
| 14:CO:45:GLU:HB3  | 14:CO:46:HIS:HD1   | 1.84        | 0.43     |
| 23:DB:2533:U:H2'  | 23:DB:2534:A:O4'   | 2.18        | 0.43     |
| 9:CJ:41:PRO:O     | 9:CJ:42:LEU:HB2    | 2.18        | 0.43     |
| 26:BD:35:THR:N    | 26:BD:49:GLN:O     | 2.51        | 0.43     |
| 23:BB:1678:A:H2'  | 23:BB:1679:A:O4'   | 2.19        | 0.43     |
| 8:CI:118:ARG:HG2  | 8:CI:118:ARG:O     | 2.19        | 0.43     |
| 50:DT:7:LEU:O     | 50:DT:7:LEU:HD13   | 2.19        | 0.43     |
| 1:CA:138:G:C6     | 1:CA:226:G:C6      | 3.07        | 0.43     |
| 1:AA:932:C:H4'    | 6:AG:3:ARG:NH2     | 2.34        | 0.43     |
| 23:BB:1238:G:O2'  | 23:BB:1239:G:H5'   | 2.18        | 0.43     |
| 23:BB:1863:G:H2'  | 23:BB:1864:U:O4'   | 2.19        | 0.43     |
| 23:DB:1099:G:H4'  | 24:DI:4:VAL:HB     | 2.01        | 0.43     |
| 23:DB:947:A:O2'   | 23:DB:984:A:H2     | 2.02        | 0.43     |
| 44:DQ:33:VAL:O    | 44:DQ:37:ALA:N     | 2.51        | 0.43     |
| 47:DF:33:ILE:HG22 | 47:DF:34:THR:N     | 2.34        | 0.43     |
| 8:CI:51:LEU:HB3   | 8:CI:56:MET:HB2    | 2.01        | 0.43     |
| 41:DJ:17:VAL:CG2  | 41:DJ:137:PRO:HB2  | 2.33        | 0.43     |
| 47:DF:42:ALA:HB1  | 47:DF:46:LYS:NZ    | 2.34        | 0.43     |
| 43:DO:35:ILE:HG21 | 43:DO:71:ALA:HB1   | 2.01        | 0.43     |
| 43:DO:34:HIS:CE1  | 43:DO:65:THR:HG21  | 2.53        | 0.43     |
| 3:CD:29:THR:H     | 3:CD:33:ILE:HG22   | 1.83        | 0.43     |
| 46:DU:84:PHE:CD2  | 46:DU:93:ARG:HG2   | 2.54        | 0.43     |
| 23:BB:1203:U:C4'  | 37:BL:3:LEU:HD12   | 2.46        | 0.43     |
| 37:BL:42:SER:C    | 37:BL:44:GLY:N     | 2.67        | 0.43     |
| 47:BF:141:ASP:O   | 47:BF:142:TYR:C    | 2.58        | 0.43     |
| 42:DN:52:ILE:O    | 42:DN:55:ALA:HB3   | 2.19        | 0.43     |
| 42:DN:87:PHE:CE1  | 42:DN:116:VAL:HG12 | 2.54        | 0.43     |
| 40:DH:80:ILE:CD1  | 40:DH:146:VAL:HG13 | 2.46        | 0.43     |
| 49:DR:21:ARG:C    | 49:DR:22:LEU:HD23  | 2.39        | 0.43     |
| 1:AA:922:G:H2'    | 1:AA:923:A:H8      | 1.84        | 0.43     |
| 47:DF:134:GLN:C   | 47:DF:136:ILE:N    | 2.72        | 0.43     |
| 1:CA:15:G:H2'     | 1:CA:16:A:H8       | 1.84        | 0.43     |
| 18:CS:47:THR:HG23 | 18:CS:60:PHE:CE1   | 2.47        | 0.43     |
| 45:BS:17:VAL:C    | 45:BS:19:LEU:N     | 2.70        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 12:AM:79:LEU:HG   | 12:AM:79:LEU:H     | 1.59        | 0.43     |
| 16:AQ:62:GLU:HB2  | 16:AQ:72:TRP:CE2   | 2.54        | 0.43     |
| 23:BB:662:G:O4'   | 37:BL:14:LYS:HB2   | 2.19        | 0.43     |
| 23:BB:2807:U:H1'  | 23:BB:2892:G:N2    | 2.34        | 0.43     |
| 3:CD:172:VAL:HG23 | 3:CD:178:GLU:O     | 2.18        | 0.43     |
| 21:CU:3:ILE:HG23  | 21:CU:18:PHE:CD1   | 2.54        | 0.43     |
| 23:DB:550:C:OP1   | 41:DJ:2:LYS:HE3    | 2.19        | 0.43     |
| 23:BB:819:A:N6    | 23:BB:1189:A:H1'   | 2.33        | 0.43     |
| 45:BS:29:VAL:HG11 | 45:BS:55:ILE:CD1   | 2.49        | 0.43     |
| 23:DB:2886:A:H62  | 31:D0:39:ARG:CD    | 2.31        | 0.43     |
| 1:CA:1411:C:O2'   | 1:CA:1412:C:H5'    | 2.19        | 0.43     |
| 49:DR:4:VAL:HG23  | 49:DR:39:LEU:N     | 2.29        | 0.43     |
| 1:CA:311:C:O2'    | 1:CA:312:C:H5'     | 2.19        | 0.43     |
| 23:DB:776:G:H4'   | 23:DB:777:G:C5'    | 2.49        | 0.43     |
| 2:CC:119:ILE:HD11 | 2:CC:133:MET:HA    | 2.00        | 0.43     |
| 25:BC:207:ALA:O   | 25:BC:208:GLY:C    | 2.57        | 0.43     |
| 14:CO:24:SER:O    | 14:CO:25:THR:C     | 2.57        | 0.43     |
| 28:DP:50:ARG:O    | 28:DP:51:ASN:HB2   | 2.19        | 0.43     |
| 1:CA:491:G:O2'    | 1:CA:492:C:H5'     | 2.19        | 0.43     |
| 23:BB:719:C:O2'   | 23:BB:720:U:H5'    | 2.19        | 0.43     |
| 16:CQ:17:GLU:C    | 16:CQ:19:SER:H     | 2.22        | 0.43     |
| 29:BE:48:THR:HG23 | 29:BE:51:GLU:OE2   | 2.18        | 0.43     |
| 24:BI:83:ALA:N    | 24:BI:100:ILE:HD11 | 2.33        | 0.43     |
| 53:B6:137:LEU:O   | 53:B6:140:LEU:HB3  | 2.19        | 0.43     |
| 23:BB:1873:G:O2'  | 23:BB:1874:C:H5'   | 2.19        | 0.43     |
| 6:CG:14:ASP:O     | 6:CG:18:GLY:HA2    | 2.19        | 0.43     |
| 1:AA:1009:U:H1'   | 1:AA:1021:A:N1     | 2.34        | 0.43     |
| 20:CB:172:ILE:H   | 20:CB:172:ILE:HG13 | 1.69        | 0.43     |
| 40:BH:53:GLU:O    | 40:BH:54:LEU:HD23  | 2.19        | 0.43     |
| 23:DB:1683:U:H2'  | 23:DB:1684:G:H8    | 1.83        | 0.43     |
| 45:BS:83:LYS:O    | 45:BS:84:ARG:NE    | 2.51        | 0.43     |
| 9:CJ:10:LEU:HD11  | 9:CJ:25:ILE:CD1    | 2.48        | 0.43     |
| 2:CC:42:LEU:HD21  | 2:CC:90:VAL:HG22   | 2.01        | 0.43     |
| 26:DD:159:LYS:HZ2 | 26:DD:160:LYS:N    | 2.17        | 0.43     |
| 18:CS:14:LEU:HD22 | 18:CS:34:SER:OG    | 2.19        | 0.43     |
| 50:BT:48:GLN:CA   | 50:BT:48:GLN:HE21  | 2.27        | 0.43     |
| 22:BA:94:A:H2'    | 22:BA:95:U:O4'     | 2.18        | 0.43     |
| 37:BL:129:LYS:HA  | 37:BL:132:ARG:CD   | 2.49        | 0.43     |
| 37:BL:136:GLU:HA  | 37:BL:140:GLY:CA   | 2.48        | 0.43     |
| 2:CC:16:PRO:HG2   | 2:CC:53:ARG:HH22   | 1.84        | 0.43     |
| 9:AJ:87:LEU:N     | 9:AJ:87:LEU:HD13   | 2.33        | 0.43     |
| 1:AA:908:A:H2'    | 1:AA:909:A:H8      | 1.84        | 0.43     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 44:DQ:32:ARG:O     | 44:DQ:36:GLN:HG3  | 2.18        | 0.43     |
| 53:D6:150:SER:O    | 53:D6:151:GLU:C   | 2.57        | 0.43     |
| 23:BB:2249:U:H4'   | 23:BB:2275:C:C5   | 2.53        | 0.43     |
| 23:BB:2249:U:N3    | 23:BB:2253:G:OP2  | 2.52        | 0.43     |
| 23:BB:1749:A:H2'   | 23:BB:1750:G:H8   | 1.84        | 0.43     |
| 23:DB:132:G:O2'    | 23:DB:133:U:H5'   | 2.18        | 0.43     |
| 23:BB:1835:G:H2'   | 23:BB:1836:C:H6   | 1.82        | 0.43     |
| 1:CA:224:U:O2'     | 1:CA:225:C:H5'    | 2.18        | 0.43     |
| 26:BD:46:ARG:HH12  | 26:BD:88:GLU:CG   | 2.32        | 0.43     |
| 23:BB:218:A:H2'    | 23:BB:219:A:O4'   | 2.19        | 0.43     |
| 23:DB:351:C:H2'    | 23:DB:352:A:H8    | 1.84        | 0.43     |
| 23:DB:2436:G:N3    | 23:DB:2598:A:H2   | 2.16        | 0.43     |
| 1:AA:1406:U:H2'    | 1:AA:1407:C:H5'   | 2.00        | 0.43     |
| 1:CA:251:G:N2      | 1:CA:266:G:O6     | 2.51        | 0.43     |
| 20:CB:35:ASN:O     | 20:CB:37:VAL:HG12 | 2.19        | 0.43     |
| 5:CF:45:ARG:HH22   | 17:CR:25:ILE:HD13 | 1.83        | 0.43     |
| 23:BB:823:C:O2'    | 23:BB:824:U:H5'   | 2.19        | 0.43     |
| 23:BB:381:G:OP1    | 51:BZ:16:ASN:ND2  | 2.52        | 0.43     |
| 43:DO:56:LYS:HG2   | 43:DO:60:GLU:CG   | 2.49        | 0.43     |
| 23:DB:1862:G:O2'   | 23:DB:1863:G:H5'  | 2.18        | 0.43     |
| 23:BB:1239:G:H5"   | 57:BB:3606:HOH:O  | 2.18        | 0.43     |
| 23:DB:1304:A:H2'   | 23:DB:1305:C:C6   | 2.54        | 0.43     |
| 23:DB:242:G:H5"    | 34:D3:63:TYR:CE2  | 2.52        | 0.43     |
| 46:DU:94:PHE:HB3   | 46:DU:101:THR:HA  | 2.01        | 0.43     |
| 26:BD:182:ALA:O    | 26:BD:184:ARG:HG2 | 2.19        | 0.43     |
| 10:CK:108:ASN:HD21 | 21:CU:6:ARG:HG3   | 1.84        | 0.43     |
| 3:CD:150:LYS:HD3   | 3:CD:150:LYS:HA   | 1.89        | 0.43     |
| 23:BB:211:C:O2'    | 23:BB:212:G:H5'   | 2.19        | 0.43     |
| 23:DB:1678:A:H2'   | 23:DB:1679:A:O4'  | 2.19        | 0.43     |
| 23:BB:2329:U:H2'   | 23:BB:2330:G:H8   | 1.82        | 0.43     |
| 52:BW:19:ARG:O     | 52:BW:20:LEU:HD23 | 2.19        | 0.43     |
| 23:BB:1819:A:H1'   | 23:BB:1821:A:C6   | 2.53        | 0.43     |
| 23:DB:2327:A:N7    | 23:DB:2388:A:N6   | 2.66        | 0.43     |
| 25:DC:90:ILE:HD13  | 25:DC:103:ILE:C   | 2.39        | 0.43     |
| 48:BG:84:LYS:HG2   | 48:BG:85:LYS:N    | 2.25        | 0.43     |
| 47:BF:87:LYS:CG    | 47:BF:88:VAL:H    | 2.22        | 0.43     |
| 37:DL:143:GLU:CG   | 37:DL:144:GLU:N   | 2.79        | 0.43     |
| 48:DG:94:ARG:NH2   | 48:DG:104:LEU:HA  | 2.34        | 0.43     |
| 53:D6:73:GLN:O     | 53:D6:76:LEU:HB2  | 2.18        | 0.43     |
| 8:AI:21:LYS:HG3    | 8:AI:22:PRO:HD2   | 2.01        | 0.43     |
| 8:AI:35:GLU:HG3    | 8:AI:44:ARG:HD2   | 2.01        | 0.43     |
| 35:DV:62:THR:HG21  | 35:DV:71:LYS:NZ   | 2.34        | 0.43     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 13:CN:68:ARG:HH12  | 13:CN:71:GLY:N    | 2.16        | 0.43     |
| 13:CN:5:MET:O      | 13:CN:8:ARG:HB3   | 2.19        | 0.43     |
| 23:BB:996:A:H4'    | 44:BQ:91:ARG:HD2  | 2.01        | 0.43     |
| 49:BR:5:PHE:N      | 49:BR:5:PHE:CD1   | 2.87        | 0.43     |
| 47:DF:52:ALA:HA    | 47:DF:55:ASP:HB2  | 2.01        | 0.43     |
| 51:BZ:32:ASN:O     | 51:BZ:33:LEU:O    | 2.37        | 0.43     |
| 42:BN:8:ARG:NH2    | 42:BN:39:PRO:HA   | 2.34        | 0.43     |
| 1:AA:948:C:H2'     | 1:AA:949:A:H8     | 1.84        | 0.43     |
| 3:AD:29:THR:H      | 3:AD:33:ILE:HG22  | 1.84        | 0.43     |
| 46:DU:81:ARG:CD    | 46:DU:96:LYS:HG3  | 2.49        | 0.43     |
| 47:BF:102:LEU:HD13 | 47:BF:102:LEU:C   | 2.39        | 0.43     |
| 47:BF:113:PHE:HE1  | 47:BF:116:LEU:HB2 | 1.84        | 0.43     |
| 37:BL:78:ARG:NH2   | 37:BL:78:ARG:HB3  | 2.34        | 0.43     |
| 29:BE:154:ASP:C    | 29:BE:156:ASN:H   | 2.21        | 0.43     |
| 42:DN:79:LEU:HA    | 42:DN:83:LEU:HD11 | 2.00        | 0.43     |
| 1:CA:16:A:C2'      | 1:CA:17:U:H5'     | 2.49        | 0.43     |
| 4:CE:28:ARG:NH2    | 4:CE:30:PHE:HB3   | 2.34        | 0.43     |
| 3:AD:172:VAL:O     | 3:AD:172:VAL:HG13 | 2.19        | 0.43     |
| 23:BB:1245:G:OP1   | 37:BL:13:LYS:HE3  | 2.18        | 0.43     |
| 32:B4:8:LYS:O      | 32:B4:35:GLN:NE2  | 2.52        | 0.43     |
| 34:D3:32:LEU:HA    | 34:D3:35:LYS:HD2  | 2.01        | 0.43     |
| 23:DB:979:A:H2'    | 23:DB:982:C:N4    | 2.34        | 0.43     |
| 13:CN:19:TYR:HB3   | 13:CN:20:PHE:H    | 1.66        | 0.43     |
| 13:CN:50:LEU:H     | 13:CN:51:PRO:HD2  | 1.84        | 0.43     |
| 29:DE:146:VAL:HG12 | 29:DE:147:LEU:N   | 2.34        | 0.43     |
| 23:BB:28:A:N6      | 23:BB:512:G:O2'   | 2.51        | 0.43     |
| 1:CA:333:U:H2'     | 1:CA:334:C:C6     | 2.54        | 0.43     |
| 42:DN:34:ILE:HG22  | 42:DN:35:LYS:N    | 2.33        | 0.43     |
| 44:DQ:106:THR:O    | 44:DQ:109:VAL:HB  | 2.18        | 0.43     |
| 23:BB:10:A:N6      | 23:BB:2895:G:H1'  | 2.34        | 0.43     |
| 23:DB:1439:A:C5    | 23:DB:1552:A:N6   | 2.86        | 0.43     |
| 14:CO:33:THR:OG1   | 14:CO:85:LEU:HD23 | 2.19        | 0.43     |
| 46:BU:62:ALA:O     | 46:BU:63:ALA:HB3  | 2.19        | 0.43     |
| 1:AA:553:A:H2'     | 1:AA:554:A:C8     | 2.53        | 0.43     |
| 14:AO:24:SER:O     | 14:AO:25:THR:C    | 2.57        | 0.43     |
| 40:BH:44:ILE:HG13  | 40:BH:45:GLU:H    | 1.84        | 0.43     |
| 27:DK:87:LEU:HB2   | 27:DK:93:GLN:C    | 2.38        | 0.43     |
| 27:DK:87:LEU:HD12  | 27:DK:92:GLU:CA   | 2.48        | 0.43     |
| 23:BB:610:C:O2'    | 23:BB:611:C:H5'   | 2.18        | 0.43     |
| 6:AG:14:ASP:O      | 6:AG:18:GLY:HA2   | 2.18        | 0.43     |
| 6:AG:14:ASP:CB     | 6:AG:19:SER:H     | 2.31        | 0.43     |
| 23:DB:1174:U:H1'   | 23:DB:1176:U:O2   | 2.18        | 0.43     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:DB:1174:U:OP2   | 23:DB:1174:U:H6   | 2.02        | 0.43     |
| 34:D3:61:LEU:N     | 34:D3:62:PRO:HD3  | 2.34        | 0.43     |
| 34:D3:6:VAL:HG23   | 34:D3:60:CYS:O    | 2.19        | 0.43     |
| 23:DB:608:A:H2'    | 23:DB:609:A:H8    | 1.81        | 0.43     |
| 23:BB:327:G:O2'    | 23:BB:328:U:H5'   | 2.19        | 0.43     |
| 2:CC:111:ASP:HB3   | 2:CC:114:LEU:HD12 | 2.01        | 0.43     |
| 23:DB:544:C:O2'    | 23:DB:545:U:O4'   | 2.37        | 0.43     |
| 1:AA:708:C:O2'     | 1:AA:709:U:H5'    | 2.18        | 0.43     |
| 25:BC:245:THR:HG23 | 25:BC:249:VAL:O   | 2.19        | 0.43     |
| 9:AJ:91:ASP:C      | 9:AJ:92:LEU:HD13  | 2.39        | 0.43     |
| 53:D6:44:GLU:OE2   | 53:D6:47:GLY:N    | 2.52        | 0.43     |
| 23:BB:1047:G:O2'   | 23:BB:1048:A:OP2  | 2.36        | 0.43     |
| 23:BB:401:A:H2'    | 23:BB:402:A:H8    | 1.84        | 0.43     |
| 23:BB:1349:C:H2'   | 23:BB:1350:C:C6   | 2.53        | 0.43     |
| 14:CO:59:MET:HG2   | 14:CO:59:MET:H    | 1.50        | 0.43     |
| 1:AA:832:G:O2'     | 1:AA:833:G:H5'    | 2.19        | 0.43     |
| 23:BB:1506:U:H2'   | 23:BB:1507:C:C6   | 2.54        | 0.43     |
| 23:DB:2784:U:H2'   | 23:DB:2785:C:C6   | 2.54        | 0.43     |
| 34:B3:44:ARG:N     | 34:B3:45:PRO:CD   | 2.82        | 0.43     |
| 23:BB:521:U:H2'    | 23:BB:522:A:H8    | 1.81        | 0.43     |
| 23:DB:1745:A:H2'   | 23:DB:1746:A:O4'  | 2.19        | 0.43     |
| 49:DR:91:GLN:HG3   | 49:DR:92:TRP:N    | 2.33        | 0.43     |
| 29:BE:18:THR:HG22  | 29:BE:106:LYS:HE2 | 1.99        | 0.43     |
| 23:DB:1880:U:H2'   | 23:DB:1881:C:C6   | 2.54        | 0.43     |
| 23:DB:2553:G:H2'   | 23:DB:2554:U:H4'  | 1.99        | 0.43     |
| 23:BB:2301:C:O2'   | 23:BB:2302:U:H5'  | 2.19        | 0.43     |
| 23:DB:1300:G:H5'   | 23:DB:1301:A:N3   | 2.34        | 0.43     |
| 43:BO:100:HIS:C    | 43:BO:104:GLN:HB2 | 2.39        | 0.43     |
| 23:DB:1675:C:H2'   | 23:DB:1676:A:O4'  | 2.19        | 0.43     |
| 29:BE:1:MET:HB2    | 29:BE:16:GLU:HB2  | 2.01        | 0.43     |
| 33:B1:28:THR:C     | 33:B1:30:PRO:HD3  | 2.39        | 0.43     |
| 28:BP:13:LYS:HG2   | 28:BP:76:HIS:ND1  | 2.34        | 0.43     |
| 23:DB:2081:U:OP1   | 51:DZ:19:SER:HB3  | 2.18        | 0.43     |
| 23:DB:2208:C:H2'   | 23:DB:2209:G:H8   | 1.84        | 0.43     |
| 1:CA:970:C:N4      | 8:CI:128:LYS:HG2  | 2.33        | 0.43     |
| 23:BB:1845:G:C6    | 23:BB:1896:G:C6   | 3.07        | 0.43     |
| 38:BM:131:VAL:HG12 | 38:BM:132:THR:N   | 2.34        | 0.43     |
| 3:CD:73:ASN:O      | 3:CD:76:LYS:HB2   | 2.19        | 0.43     |
| 23:DB:699:A:H2'    | 23:DB:700:G:O4'   | 2.19        | 0.43     |
| 37:DL:81:ASP:O     | 37:DL:83:ALA:N    | 2.45        | 0.43     |
| 23:DB:1830:C:O2'   | 23:DB:1831:G:H5'  | 2.19        | 0.43     |
| 23:DB:1830:C:H2'   | 23:DB:1831:G:H8   | 1.83        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 5:CF:69:GLU:O     | 5:CF:73:GLU:HG3    | 2.19        | 0.43     |
| 23:BB:2208:C:H2'  | 23:BB:2209:G:C8    | 2.54        | 0.43     |
| 1:AA:874:G:O2'    | 1:AA:875:U:H5'     | 2.19        | 0.43     |
| 28:DP:86:LYS:HB3  | 28:DP:87:ARG:H     | 1.57        | 0.43     |
| 4:CE:59:ILE:H     | 4:CE:59:ILE:HG13   | 1.65        | 0.43     |
| 29:BE:4:VAL:HG12  | 29:BE:6:LYS:H      | 1.84        | 0.43     |
| 23:DB:2392:A:O3'  | 34:D3:26:ALA:HB1   | 2.18        | 0.43     |
| 23:BB:2361:G:O2'  | 23:BB:2362:C:H5'   | 2.19        | 0.43     |
| 40:BH:27:ARG:HE   | 51:BZ:64:ILE:HD11  | 1.83        | 0.42     |
| 1:AA:1526:G:O2'   | 1:AA:1527:U:H5'    | 2.19        | 0.42     |
| 21:AU:40:PRO:C    | 21:AU:42:THR:N     | 2.72        | 0.42     |
| 48:DG:94:ARG:HH21 | 48:DG:104:LEU:HA   | 1.83        | 0.42     |
| 48:DG:93:TYR:O    | 48:DG:94:ARG:HG3   | 2.19        | 0.42     |
| 52:DW:49:ASN:ND2  | 52:DW:50:VAL:N     | 2.67        | 0.42     |
| 47:DF:115:GLY:HA2 | 47:DF:177:ARG:NH1  | 2.34        | 0.42     |
| 1:CA:1250:A:C2    | 1:CA:1370:G:H1'    | 2.54        | 0.42     |
| 1:CA:1348:U:C4'   | 8:CI:121:ARG:HG3   | 2.31        | 0.42     |
| 44:DQ:87:VAL:HG12 | 44:DQ:89:ILE:HD13  | 2.01        | 0.42     |
| 41:DJ:58:ASN:O    | 41:DJ:59:ALA:HB3   | 2.19        | 0.42     |
| 23:DB:804:A:H5''  | 23:DB:805:G:OP1    | 2.19        | 0.42     |
| 51:BZ:36:HIS:HB3  | 51:BZ:38:PHE:CE2   | 2.54        | 0.42     |
| 51:BZ:5:CYS:O     | 51:BZ:6:GLN:HB3    | 2.19        | 0.42     |
| 24:DI:52:LEU:HD13 | 24:DI:81:LYS:NZ    | 2.34        | 0.42     |
| 23:BB:2305:U:C4   | 47:BF:151:LEU:HA   | 2.54        | 0.42     |
| 47:BF:116:LEU:HB3 | 47:BF:176:PHE:CA   | 2.49        | 0.42     |
| 29:BE:130:LYS:C   | 29:BE:132:LYS:N    | 2.71        | 0.42     |
| 40:DH:119:ASN:O   | 40:DH:121:VAL:HG22 | 2.19        | 0.42     |
| 1:CA:1079:G:C6    | 1:CA:1080:A:N6     | 2.86        | 0.42     |
| 1:CA:921:U:H2'    | 1:CA:922:G:O4'     | 2.19        | 0.42     |
| 29:DE:28:VAL:HG23 | 29:DE:29:HIS:N     | 2.34        | 0.42     |
| 32:B4:2:LYS:HG2   | 32:B4:4:ARG:HG3    | 2.01        | 0.42     |
| 32:B4:3:VAL:O     | 32:B4:4:ARG:O      | 2.37        | 0.42     |
| 6:AG:110:ARG:HE   | 6:AG:122:GLU:HB2   | 1.84        | 0.42     |
| 32:B4:5:ALA:HA    | 32:B4:37:GLN:NE2   | 2.34        | 0.42     |
| 38:DM:29:GLY:HA2  | 38:DM:106:ASP:HB2  | 2.01        | 0.42     |
| 46:BU:73:ASN:HB3  | 46:BU:95:PHE:CD2   | 2.54        | 0.42     |
| 8:AI:33:SER:CB    | 8:AI:36:GLN:HB2    | 2.42        | 0.42     |
| 13:CN:20:PHE:HD2  | 13:CN:54:SER:O     | 2.02        | 0.42     |
| 48:BG:147:LEU:O   | 48:BG:150:TYR:HB2  | 2.19        | 0.42     |
| 45:BS:22:ASP:HA   | 45:BS:25:ARG:HH12  | 1.80        | 0.42     |
| 23:BB:571:U:H3'   | 49:BR:80:ARG:CZ    | 2.47        | 0.42     |
| 38:BM:103:TYR:HB2 | 38:BM:117:PHE:CE1  | 2.54        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 49:DR:16:GLU:HG2  | 49:DR:101:ILE:CB   | 2.49        | 0.42     |
| 37:DL:82:LEU:O    | 37:DL:85:VAL:HG12  | 2.19        | 0.42     |
| 38:BM:55:ARG:HG3  | 38:BM:55:ARG:O     | 2.19        | 0.42     |
| 23:DB:2015:A:H2'  | 23:DB:2016:U:O4'   | 2.18        | 0.42     |
| 11:AL:20:VAL:HG12 | 11:AL:93:ARG:CB    | 2.47        | 0.42     |
| 4:AE:148:SER:OG   | 4:AE:151:MET:HB2   | 2.18        | 0.42     |
| 5:CF:99:ALA:O     | 5:CF:100:SER:CB    | 2.66        | 0.42     |
| 14:CO:71:LYS:HB2  | 14:CO:78:TYR:CD2   | 2.54        | 0.42     |
| 10:AK:80:ASN:ND2  | 10:AK:80:ASN:H     | 2.16        | 0.42     |
| 22:BA:116:G:H4'   | 43:BO:54:VAL:HG22  | 2.01        | 0.42     |
| 35:DV:29:ILE:HD12 | 35:DV:90:ASP:HA    | 2.01        | 0.42     |
| 23:DB:154:U:H2'   | 23:DB:155:A:H8     | 1.84        | 0.42     |
| 23:DB:1470:A:H3'  | 23:DB:1471:G:H8    | 1.84        | 0.42     |
| 23:BB:1824:G:H1'  | 25:BC:251:THR:HG21 | 2.00        | 0.42     |
| 45:DS:31:GLN:C    | 45:DS:33:LEU:N     | 2.71        | 0.42     |
| 20:CB:19:THR:HG23 | 20:CB:20:ARG:N     | 2.33        | 0.42     |
| 3:AD:2:ARG:HB3    | 3:AD:114:ARG:HH22  | 1.83        | 0.42     |
| 23:DB:2285:C:OP2  | 33:D1:5:ARG:HD3    | 2.19        | 0.42     |
| 23:DB:2457:U:H2'  | 23:DB:2458:G:H5'   | 2.01        | 0.42     |
| 40:BH:57:LYS:CG   | 40:BH:58:LEU:N     | 2.82        | 0.42     |
| 53:D6:33:ALA:HB1  | 53:D6:63:PRO:HA    | 2.00        | 0.42     |
| 23:BB:2450:A:O2'  | 23:BB:2451:A:H5'   | 2.18        | 0.42     |
| 23:BB:1404:C:O2'  | 23:BB:1405:U:H5'   | 2.19        | 0.42     |
| 1:AA:1460:C:H2'   | 1:AA:1461:G:H8     | 1.84        | 0.42     |
| 23:DB:2291:U:H2'  | 23:DB:2292:U:C6    | 2.54        | 0.42     |
| 23:DB:871:U:C2    | 23:DB:907:G:C6     | 3.07        | 0.42     |
| 5:AF:81:ASN:O     | 5:AF:83:ALA:N      | 2.52        | 0.42     |
| 23:BB:1535:A:H3'  | 23:BB:1536:C:C6    | 2.52        | 0.42     |
| 23:BB:2815:C:C2   | 23:BB:2816:G:C8    | 3.07        | 0.42     |
| 1:AA:283:U:H2'    | 1:AA:284:C:H6      | 1.84        | 0.42     |
| 23:DB:2376:A:N1   | 43:DO:92:PHE:HD2   | 2.17        | 0.42     |
| 26:DD:15:PHE:CD2  | 28:DP:77:SER:HA    | 2.54        | 0.42     |
| 22:DA:83:G:C6     | 22:DA:94:A:C6      | 3.07        | 0.42     |
| 1:AA:591:U:O2'    | 1:AA:592:G:H5'     | 2.19        | 0.42     |
| 5:AF:85:ILE:CG2   | 5:AF:86:ARG:H      | 2.32        | 0.42     |
| 1:CA:648:A:H2'    | 1:CA:649:A:C8      | 2.54        | 0.42     |
| 7:AH:17:GLN:NE2   | 7:AH:69:ALA:HB1    | 2.34        | 0.42     |
| 46:BU:13:LEU:HA   | 46:BU:18:LYS:HD3   | 2.01        | 0.42     |
| 1:CA:1234:C:H2'   | 1:CA:1235:U:C6     | 2.54        | 0.42     |
| 2:AC:117:ASP:OD2  | 2:AC:186:SER:HB3   | 2.19        | 0.42     |
| 23:BB:2757:A:H2   | 48:BG:63:GLN:HE22  | 1.67        | 0.42     |
| 48:BG:5:LYS:HE2   | 48:BG:61:TRP:CH2   | 2.54        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 29:DE:2:GLU:OE1   | 29:DE:11:ALA:HB1   | 2.19        | 0.42     |
| 1:CA:960:U:O2'    | 1:CA:1223:C:H4'    | 2.18        | 0.42     |
| 17:AR:25:ILE:HG13 | 17:AR:26:ALA:N     | 2.34        | 0.42     |
| 5:CF:46:GLN:HA    | 5:CF:46:GLN:NE2    | 2.33        | 0.42     |
| 23:BB:2181:U:H2'  | 23:BB:2182:U:O4'   | 2.19        | 0.42     |
| 23:BB:1923:U:H2'  | 23:BB:1924:C:C6    | 2.54        | 0.42     |
| 1:AA:1121:U:H2'   | 1:AA:1122:U:C6     | 2.54        | 0.42     |
| 40:DH:109:GLU:O   | 40:DH:110:VAL:HG12 | 2.18        | 0.42     |
| 1:AA:755:G:H2'    | 1:AA:756:C:H6      | 1.84        | 0.42     |
| 23:BB:1248:G:OP1  | 44:BQ:1:ALA:HB3    | 2.19        | 0.42     |
| 30:BY:3:THR:HB    | 30:BY:36:GLU:HG2   | 2.01        | 0.42     |
| 23:DB:253:C:P     | 34:D3:4:LYS:HZ2    | 2.42        | 0.42     |
| 53:D6:183:ILE:C   | 53:D6:185:GLY:H    | 2.21        | 0.42     |
| 43:BO:15:ARG:HH21 | 43:BO:95:SER:HB3   | 1.84        | 0.42     |
| 1:AA:792:A:C4     | 1:AA:794:A:C6      | 3.08        | 0.42     |
| 15:AP:36:VAL:HG13 | 15:AP:36:VAL:O     | 2.19        | 0.42     |
| 43:DO:61:GLN:HE21 | 43:DO:61:GLN:HB3   | 1.70        | 0.42     |
| 23:BB:308:G:H1'   | 23:BB:501:A:OP1    | 2.19        | 0.42     |
| 13:CN:47:LEU:O    | 13:CN:49:THR:N     | 2.52        | 0.42     |
| 43:BO:56:LYS:HG2  | 43:BO:60:GLU:CG    | 2.49        | 0.42     |
| 23:DB:2328:A:H2'  | 23:DB:2329:U:H6    | 1.77        | 0.42     |
| 52:DW:42:THR:O    | 52:DW:43:LYS:HE3   | 2.19        | 0.42     |
| 23:DB:1824:G:H1'  | 25:DC:251:THR:HG21 | 2.02        | 0.42     |
| 48:BG:93:TYR:HE1  | 48:BG:160:GLY:HA2  | 1.84        | 0.42     |
| 44:DQ:30:VAL:HG22 | 44:DQ:31:TYR:N     | 2.34        | 0.42     |
| 23:BB:2315:G:H2'  | 23:BB:2316:G:H8    | 1.84        | 0.42     |
| 16:CQ:74:LEU:HD13 | 16:CQ:74:LEU:C     | 2.40        | 0.42     |
| 47:DF:87:LYS:HG3  | 47:DF:88:VAL:N     | 2.21        | 0.42     |
| 53:B6:57:THR:HB   | 53:B6:69:GLN:O     | 2.18        | 0.42     |
| 41:DJ:33:ALA:O    | 41:DJ:34:ARG:C     | 2.57        | 0.42     |
| 20:CB:205:ALA:HB3 | 20:CB:208:ALA:HB3  | 2.01        | 0.42     |
| 8:AI:49:GLN:N     | 8:AI:50:PRO:HD2    | 2.34        | 0.42     |
| 48:DG:24:THR:OG1  | 48:DG:32:LEU:HD21  | 2.19        | 0.42     |
| 29:DE:60:TRP:CZ3  | 29:DE:62:GLN:HA    | 2.55        | 0.42     |
| 50:BT:54:GLU:H    | 50:BT:54:GLU:HG2   | 1.67        | 0.42     |
| 41:BJ:3:THR:O     | 41:BJ:4:PHE:O      | 2.36        | 0.42     |
| 46:BU:84:PHE:CD2  | 46:BU:93:ARG:HG2   | 2.53        | 0.42     |
| 47:BF:40:GLY:O    | 47:BF:41:GLU:C     | 2.57        | 0.42     |
| 47:BF:42:ALA:HB1  | 47:BF:46:LYS:NZ    | 2.34        | 0.42     |
| 47:BF:66:ILE:HD11 | 47:BF:83:PRO:CB    | 2.44        | 0.42     |
| 47:DF:2:LYS:CD    | 47:DF:100:GLU:HG2  | 2.49        | 0.42     |
| 10:AK:92:ARG:HE   | 21:AU:20:ARG:NH2   | 2.14        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 18:AS:50:VAL:O    | 18:AS:56:HIS:HA   | 2.20        | 0.42     |
| 37:DL:30:THR:O    | 37:DL:31:GLY:C    | 2.57        | 0.42     |
| 21:CU:3:ILE:HG21  | 21:CU:19:LYS:CG   | 2.45        | 0.42     |
| 1:AA:1251:A:O2'   | 1:AA:1252:A:H5'   | 2.19        | 0.42     |
| 1:AA:313:A:O2'    | 1:AA:314:C:H5'    | 2.18        | 0.42     |
| 23:DB:1723:G:N7   | 23:DB:1737:G:N2   | 2.61        | 0.42     |
| 1:CA:908:A:H2'    | 1:CA:909:A:H8     | 1.84        | 0.42     |
| 27:DK:119:ALA:O   | 27:DK:120:PRO:O   | 2.37        | 0.42     |
| 23:BB:2146:C:H1'  | 23:BB:2147:A:C4'  | 2.48        | 0.42     |
| 23:DB:784:G:H5''  | 25:DC:225:ASN:OD1 | 2.19        | 0.42     |
| 28:BP:6:GLN:HE21  | 28:BP:7:LEU:N     | 2.17        | 0.42     |
| 23:DB:557:C:H2'   | 23:DB:558:U:H6    | 1.83        | 0.42     |
| 23:BB:193:U:O3'   | 23:BB:803:U:H4'   | 2.20        | 0.42     |
| 4:AE:39:GLY:CA    | 4:AE:116:VAL:HB   | 2.46        | 0.42     |
| 4:AE:45:VAL:O     | 4:AE:70:MET:HB3   | 2.19        | 0.42     |
| 39:BX:20:ASN:HA   | 39:BX:24:GLU:OE1  | 2.20        | 0.42     |
| 4:CE:82:HIS:CD2   | 7:CH:95:MET:HG3   | 2.54        | 0.42     |
| 4:AE:52:ALA:N     | 4:AE:58:ALA:HB2   | 2.34        | 0.42     |
| 23:BB:2419:U:OP2  | 34:B3:32:LEU:HD13 | 2.19        | 0.42     |
| 49:BR:19:THR:CB   | 49:BR:97:LYS:HA   | 2.45        | 0.42     |
| 23:DB:125:A:H2    | 36:D2:9:VAL:HG22  | 1.84        | 0.42     |
| 22:BA:13:G:C5     | 22:BA:70:C:H4'    | 2.55        | 0.42     |
| 23:DB:118:A:N3    | 23:DB:178:G:H1'   | 2.34        | 0.42     |
| 1:CA:1477:U:H2'   | 1:CA:1478:U:H6    | 1.81        | 0.42     |
| 23:DB:1374:G:H2'  | 23:DB:1375:U:H6   | 1.82        | 0.42     |
| 9:CJ:24:GLU:CD    | 9:CJ:90:LEU:HD11  | 2.39        | 0.42     |
| 1:AA:1009:U:O2    | 1:AA:1009:U:C2'   | 2.67        | 0.42     |
| 43:DO:7:ARG:HA    | 43:DO:10:ARG:NE   | 2.34        | 0.42     |
| 23:DB:2538:C:O2'  | 23:DB:2539:C:H5'  | 2.18        | 0.42     |
| 23:BB:1114:C:H2'  | 23:BB:1115:G:O4'  | 2.19        | 0.42     |
| 1:AA:378:G:H2'    | 1:AA:379:C:C6     | 2.53        | 0.42     |
| 23:BB:1258:U:H4'  | 29:BE:79:ARG:HD2  | 2.02        | 0.42     |
| 23:BB:2876:G:H2'  | 23:BB:2877:G:O4'  | 2.19        | 0.42     |
| 42:BN:59:SER:C    | 42:BN:61:ALA:N    | 2.71        | 0.42     |
| 23:BB:2291:U:H2'  | 23:BB:2292:U:C6   | 2.53        | 0.42     |
| 43:BO:6:ALA:CB    | 43:BO:10:ARG:HH11 | 2.32        | 0.42     |
| 37:BL:135:ILE:CG2 | 37:BL:136:GLU:N   | 2.82        | 0.42     |
| 23:BB:707:G:O2'   | 23:BB:708:G:H5'   | 2.19        | 0.42     |
| 23:DB:493:G:H2'   | 23:DB:494:G:O4'   | 2.19        | 0.42     |
| 26:DD:70:LYS:C    | 26:DD:70:LYS:HD3  | 2.39        | 0.42     |
| 1:CA:327:A:O2'    | 1:CA:328:C:O4'    | 2.32        | 0.42     |
| 23:BB:520:G:O2'   | 23:BB:521:U:H5'   | 2.18        | 0.42     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:592:G:O2'     | 1:CA:593:U:H5'    | 2.19        | 0.42     |
| 34:B3:7:ARG:O      | 34:B3:8:GLY:C     | 2.57        | 0.42     |
| 38:BM:102:LEU:HD22 | 38:BM:102:LEU:N   | 2.34        | 0.42     |
| 23:DB:408:G:H2'    | 23:DB:409:G:H8    | 1.84        | 0.42     |
| 23:BB:1900:A:N1    | 23:BB:1970:A:C5   | 2.87        | 0.42     |
| 34:D3:7:ARG:O      | 34:D3:8:GLY:C     | 2.57        | 0.42     |
| 47:DF:119:LYS:C    | 47:DF:121:PHE:H   | 2.22        | 0.42     |
| 4:AE:87:VAL:HG21   | 4:AE:92:ARG:HD2   | 2.01        | 0.42     |
| 23:DB:1077:A:H4'   | 24:DI:93:ASN:OD1  | 2.19        | 0.42     |
| 23:DB:1271:G:C2    | 23:DB:1617:C:H4'  | 2.54        | 0.42     |
| 20:CB:13:VAL:CG1   | 20:CB:207:ARG:HG2 | 2.48        | 0.42     |
| 23:DB:2302:U:O2'   | 23:DB:2303:G:H5'  | 2.19        | 0.42     |
| 1:AA:37:U:H2'      | 1:AA:38:G:H8      | 1.84        | 0.42     |
| 23:BB:838:C:H2'    | 23:BB:839:U:H6    | 1.84        | 0.42     |
| 1:CA:537:G:H2'     | 1:CA:538:G:C8     | 2.54        | 0.42     |
| 23:BB:927:A:O2'    | 23:BB:928:A:H5'   | 2.18        | 0.42     |
| 15:AP:10:GLY:HA3   | 15:AP:15:PRO:HA   | 1.99        | 0.42     |
| 1:CA:65:A:C5       | 1:CA:381:C:N3     | 2.87        | 0.42     |
| 23:BB:787:C:H3'    | 23:BB:791:C:H41   | 1.84        | 0.42     |
| 36:D2:1:MET:HG2    | 36:D2:2:LYS:H     | 1.84        | 0.42     |
| 5:CF:55:HIS:O      | 5:CF:56:LYS:HG3   | 2.19        | 0.42     |
| 1:CA:1165:U:H2'    | 1:CA:1166:G:O4'   | 2.19        | 0.42     |
| 23:DB:603:A:H4'    | 23:DB:604:G:O5'   | 2.19        | 0.42     |
| 14:CO:64:ARG:NH2   | 14:CO:88:ARG:NH1  | 2.67        | 0.42     |
| 23:DB:809:G:O2'    | 23:DB:810:U:H5'   | 2.19        | 0.42     |
| 43:BO:30:ARG:HG3   | 43:BO:30:ARG:HH11 | 1.84        | 0.42     |
| 1:AA:397:A:N3      | 1:AA:397:A:H3'    | 2.34        | 0.42     |
| 46:BU:45:GLN:HE21  | 46:BU:45:GLN:HB3  | 1.57        | 0.42     |
| 23:BB:699:A:H2'    | 23:BB:700:G:O4'   | 2.18        | 0.42     |
| 43:DO:14:ALA:C     | 43:DO:16:ARG:H    | 2.22        | 0.42     |
| 23:DB:760:G:C2'    | 23:DB:761:A:H5'   | 2.49        | 0.42     |
| 5:AF:74:LEU:HA     | 5:AF:77:THR:OG1   | 2.19        | 0.42     |
| 1:AA:1206:G:C4'    | 2:AC:192:TYR:HA   | 2.38        | 0.42     |
| 25:BC:131:MET:HE1  | 25:BC:189:ALA:HB2 | 2.01        | 0.42     |
| 23:DB:1818:U:HO2'  | 23:DB:1819:A:P    | 2.41        | 0.42     |
| 25:DC:121:ALA:HB3  | 25:DC:129:LEU:CD1 | 2.49        | 0.42     |
| 25:DC:140:VAL:O    | 25:DC:141:HIS:HB2 | 2.20        | 0.42     |
| 53:B6:52:LEU:CD1   | 53:B6:58:VAL:HG23 | 2.48        | 0.42     |
| 40:BH:89:LYS:HB3   | 40:BH:89:LYS:NZ   | 2.34        | 0.42     |
| 40:BH:90:LEU:HD23  | 40:BH:123:ARG:HG2 | 2.01        | 0.42     |
| 8:CI:46:VAL:HG23   | 8:CI:47:VAL:N     | 2.34        | 0.42     |
| 41:DJ:6:ALA:HB3    | 41:DJ:45:THR:CB   | 2.49        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:AI:38:PHE:HB3   | 8:AI:43:ALA:HB3   | 2.01        | 0.42     |
| 8:AI:50:PRO:HD3   | 8:AI:79:ARG:CG    | 2.49        | 0.42     |
| 47:DF:42:ALA:O    | 47:DF:45:ASP:N    | 2.52        | 0.42     |
| 48:DG:26:LYS:HA   | 48:DG:32:LEU:N    | 2.35        | 0.42     |
| 23:DB:2358:A:H2'  | 23:DB:2359:C:H6   | 1.84        | 0.42     |
| 23:DB:672:C:H2'   | 23:DB:673:C:H6    | 1.83        | 0.42     |
| 23:DB:674:G:O3'   | 29:DE:60:TRP:CZ2  | 2.71        | 0.42     |
| 44:BQ:81:GLY:C    | 44:BQ:83:LYS:N    | 2.73        | 0.42     |
| 23:BB:994:C:O2'   | 49:BR:10:LYS:HE2  | 2.19        | 0.42     |
| 44:BQ:90:ASP:C    | 49:BR:11:GLN:HE22 | 2.22        | 0.42     |
| 46:BU:84:PHE:HB3  | 46:BU:91:LYS:HG3  | 2.01        | 0.42     |
| 53:B6:129:ILE:HA  | 53:B6:132:ILE:CD1 | 2.37        | 0.42     |
| 25:BC:90:ILE:HD11 | 25:BC:102:TYR:HB3 | 2.00        | 0.42     |
| 1:AA:429:U:H3'    | 3:AD:8:LEU:CD2    | 2.45        | 0.42     |
| 3:AD:30:LYS:N     | 3:AD:30:LYS:HD3   | 2.34        | 0.42     |
| 23:BB:1204:A:N1   | 23:BB:1241:A:N1   | 2.66        | 0.42     |
| 42:BN:52:ILE:HD13 | 42:BN:87:PHE:CE2  | 2.54        | 0.42     |
| 23:BB:2311:A:O2'  | 47:BF:84:ILE:HG21 | 2.19        | 0.42     |
| 12:CM:52:ILE:HD12 | 12:CM:55:LEU:CD1  | 2.49        | 0.42     |
| 1:AA:1278:G:H4'   | 1:AA:1279:G:H5'   | 2.01        | 0.42     |
| 23:BB:322:A:C2    | 23:BB:340:A:C6    | 3.06        | 0.42     |
| 23:BB:1458:U:O3'  | 23:BB:1459:G:O4'  | 2.37        | 0.42     |
| 40:DH:95:GLY:H    | 40:DH:98:ASP:HB2  | 1.83        | 0.42     |
| 1:CA:15:G:H2'     | 1:CA:16:A:C8      | 2.54        | 0.42     |
| 1:CA:1081:A:OP1   | 4:CE:22:LYS:HA    | 2.19        | 0.42     |
| 1:CA:1320:C:N4    | 18:CS:36:ARG:HE   | 2.16        | 0.42     |
| 1:AA:1314:C:H2'   | 1:AA:1315:U:H6    | 1.80        | 0.42     |
| 18:AS:36:ARG:H    | 18:AS:36:ARG:HG2  | 1.59        | 0.42     |
| 10:CK:86:LYS:HB2  | 10:CK:113:THR:HA  | 2.01        | 0.42     |
| 23:DB:137:U:O2    | 50:DT:1:MET:N     | 2.43        | 0.42     |
| 23:DB:2472:G:O6   | 23:DB:2476:A:H4'  | 2.19        | 0.42     |
| 11:CL:89:LEU:HD22 | 11:CL:89:LEU:N    | 2.34        | 0.42     |
| 39:DX:28:LEU:HB3  | 39:DX:43:LEU:HD21 | 2.01        | 0.42     |
| 45:BS:36:LEU:HB3  | 45:BS:48:LYS:HB2  | 2.00        | 0.42     |
| 53:D6:143:LEU:HA  | 53:D6:146:GLU:HG2 | 2.01        | 0.42     |
| 23:BB:26:G:H2'    | 23:BB:27:G:C1'    | 2.48        | 0.42     |
| 1:CA:1336:C:H4'   | 1:CA:1337:G:O5'   | 2.20        | 0.42     |
| 31:D0:41:HIS:O    | 31:D0:42:ILE:O    | 2.36        | 0.42     |
| 49:BR:38:VAL:HG22 | 49:BR:40:MET:H    | 1.84        | 0.42     |
| 1:AA:1390:U:O2'   | 1:AA:1391:U:H5'   | 2.19        | 0.42     |
| 28:DP:1:SER:H1    | 28:DP:4:ILE:HD12  | 1.84        | 0.42     |
| 44:DQ:9:ALA:O     | 44:DQ:11:ALA:N    | 2.52        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:116:C:C2'   | 23:BB:117:G:H5'   | 2.50        | 0.42     |
| 23:BB:1439:A:C8   | 23:BB:1440:U:C6   | 3.08        | 0.42     |
| 23:BB:1444:G:H2'  | 23:BB:1445:G:C8   | 2.53        | 0.42     |
| 20:AB:147:LEU:O   | 20:AB:151:LYS:N   | 2.52        | 0.42     |
| 38:BM:46:ILE:CG1  | 38:BM:47:GLU:N    | 2.81        | 0.42     |
| 29:BE:42:GLY:O    | 29:BE:43:THR:O    | 2.38        | 0.42     |
| 40:DH:113:SER:C   | 40:DH:115:VAL:H   | 2.22        | 0.42     |
| 9:AJ:5:ARG:HD3    | 9:AJ:79:PRO:HG3   | 2.00        | 0.42     |
| 3:CD:196:GLU:O    | 3:CD:200:VAL:HG13 | 2.19        | 0.42     |
| 1:CA:958:A:C6     | 1:CA:959:A:N1     | 2.87        | 0.42     |
| 1:CA:554:A:H5'    | 11:CL:25:ALA:HB1  | 2.00        | 0.42     |
| 23:BB:560:C:H3'   | 23:BB:561:G:C8    | 2.54        | 0.42     |
| 15:AP:40:ASN:HD21 | 15:AP:43:ALA:CA   | 2.31        | 0.42     |
| 23:BB:1222:U:P    | 49:BR:90:ARG:HH12 | 2.42        | 0.42     |
| 6:AG:104:VAL:HG12 | 6:AG:108:ARG:HD2  | 2.01        | 0.42     |
| 23:BB:2087:G:H2'  | 23:BB:2088:A:H8   | 1.84        | 0.42     |
| 35:BV:55:GLU:CD   | 35:BV:55:GLU:H    | 2.22        | 0.42     |
| 1:CA:1028:C:H2'   | 1:CA:1028:C:O2    | 2.18        | 0.42     |
| 1:CA:56:U:H2'     | 1:CA:57:G:H8      | 1.85        | 0.42     |
| 23:DB:1902:C:H4'  | 25:DC:241:LYS:O   | 2.19        | 0.42     |
| 1:AA:392:C:H2'    | 1:AA:393:A:C8     | 2.54        | 0.42     |
| 23:DB:520:G:O2'   | 23:DB:521:U:H5'   | 2.19        | 0.42     |
| 38:BM:69:PRO:HA   | 38:BM:94:ALA:CA   | 2.49        | 0.42     |
| 23:BB:1372:U:H2'  | 23:BB:1373:A:H8   | 1.84        | 0.42     |
| 1:CA:1143:G:O2'   | 1:CA:1144:G:H5'   | 2.19        | 0.42     |
| 9:CJ:80:THR:HG21  | 9:CJ:82:LYS:HZ1   | 1.84        | 0.42     |
| 23:DB:1948:G:C6   | 23:DB:1959:G:C6   | 3.08        | 0.42     |
| 23:DB:2689:U:H4'  | 23:DB:2690:U:OP2  | 2.19        | 0.42     |
| 1:CA:1308:U:H2'   | 1:CA:1309:G:H8    | 1.83        | 0.42     |
| 35:DV:49:ASN:ND2  | 35:DV:49:ASN:N    | 2.65        | 0.42     |
| 23:BB:1316:U:H2'  | 23:BB:1317:G:C8   | 2.54        | 0.42     |
| 23:BB:1745:A:O2'  | 23:BB:1746:A:H5'  | 2.19        | 0.42     |
| 23:DB:681:G:H2'   | 23:DB:682:G:H8    | 1.84        | 0.42     |
| 23:BB:2812:G:H2'  | 23:BB:2813:A:O4'  | 2.19        | 0.42     |
| 50:BT:14:PRO:HA   | 50:BT:32:LEU:CB   | 2.49        | 0.42     |
| 4:AE:55:VAL:N     | 4:AE:56:PRO:CD    | 2.82        | 0.42     |
| 23:DB:1848:A:H2'  | 23:DB:1849:G:H8   | 1.84        | 0.42     |
| 23:BB:234:U:O2'   | 23:BB:235:U:H5'   | 2.19        | 0.42     |
| 1:AA:665:A:H2'    | 1:AA:725:G:N2     | 2.34        | 0.42     |
| 1:CA:106:C:H2'    | 1:CA:107:G:C8     | 2.54        | 0.42     |
| 23:DB:1952:A:C6   | 23:DB:1953:A:N1   | 2.88        | 0.42     |
| 42:BN:9:GLN:C     | 42:BN:17:ARG:HD3  | 2.38        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:110:G:O2'   | 23:DB:111:A:H5'    | 2.19        | 0.42     |
| 1:CA:1354:U:H2'   | 1:CA:1355:G:C8     | 2.53        | 0.42     |
| 23:BB:1664:A:H1'  | 23:BB:2726:A:C2    | 2.55        | 0.42     |
| 1:AA:1426:G:H2'   | 1:AA:1427:C:H6     | 1.84        | 0.42     |
| 23:BB:1891:G:H2'  | 23:BB:1892:C:H6    | 1.85        | 0.42     |
| 23:BB:2408:U:O2'  | 23:BB:2409:G:H5'   | 2.20        | 0.42     |
| 43:DO:15:ARG:HH21 | 43:DO:95:SER:HB3   | 1.84        | 0.42     |
| 1:AA:538:G:OP2    | 11:AL:111:GLN:HB2  | 2.19        | 0.42     |
| 23:BB:158:U:H2'   | 23:BB:159:G:O4'    | 2.18        | 0.42     |
| 44:BQ:54:ARG:HB3  | 44:BQ:58:GLN:HE22  | 1.85        | 0.42     |
| 26:BD:18:ASP:OD1  | 26:BD:19:GLY:N     | 2.52        | 0.42     |
| 9:CJ:6:ILE:O      | 9:CJ:75:ASP:HA     | 2.19        | 0.42     |
| 49:DR:57:GLY:HA2  | 49:DR:102:SER:O    | 2.19        | 0.42     |
| 23:DB:820:A:H2'   | 23:DB:821:A:O4'    | 2.19        | 0.42     |
| 53:B6:179:LYS:HA  | 53:B6:179:LYS:HD3  | 1.90        | 0.42     |
| 36:B2:12:ARG:NH2  | 36:B2:12:ARG:HG3   | 2.34        | 0.42     |
| 23:DB:2110:G:H8   | 23:DB:2110:G:OP2   | 2.02        | 0.42     |
| 23:DB:2873:A:O4'  | 42:DN:6:SER:HB3    | 2.20        | 0.42     |
| 52:DW:28:GLU:HG3  | 52:DW:29:SER:H     | 1.84        | 0.42     |
| 25:DC:102:TYR:O   | 25:DC:103:ILE:HG13 | 2.19        | 0.42     |
| 25:DC:23:LEU:HD21 | 25:DC:89:ASN:OD1   | 2.19        | 0.42     |
| 48:BG:88:LEU:O    | 48:BG:88:LEU:HD12  | 2.19        | 0.42     |
| 23:DB:2751:G:OP2  | 48:DG:2:ARG:HD2    | 2.19        | 0.42     |
| 48:DG:89:VAL:HG12 | 48:DG:90:GLY:H     | 1.84        | 0.42     |
| 40:BH:143:ILE:O   | 40:BH:144:VAL:HG23 | 2.19        | 0.42     |
| 8:CI:37:TYR:HE2   | 8:CI:74:GLN:HG2    | 1.85        | 0.42     |
| 1:CA:1287:A:H2'   | 1:CA:1288:A:H8     | 1.83        | 0.42     |
| 41:BJ:16:TYR:CD2  | 41:BJ:140:LEU:HD12 | 2.54        | 0.42     |
| 8:AI:43:ALA:O     | 8:AI:46:VAL:HG22   | 2.19        | 0.42     |
| 50:BT:1:MET:HG3   | 50:BT:2:ILE:N      | 2.32        | 0.42     |
| 47:DF:42:ALA:O    | 47:DF:44:ALA:N     | 2.52        | 0.42     |
| 47:DF:45:ASP:C    | 47:DF:47:LYS:H     | 2.21        | 0.42     |
| 47:DF:78:ILE:HA   | 47:DF:79:ARG:HE    | 1.84        | 0.42     |
| 1:AA:598:U:H4'    | 7:AH:85:TYR:CD2    | 2.55        | 0.42     |
| 23:DB:2733:A:C3'  | 23:DB:2733:A:C8    | 3.01        | 0.42     |
| 1:CA:981:U:H2'    | 1:CA:982:U:C5      | 2.54        | 0.42     |
| 41:BJ:44:TYR:CZ   | 44:BQ:59:LEU:HD11  | 2.54        | 0.42     |
| 23:BB:2307:G:O6   | 47:BF:40:GLY:HA3   | 2.19        | 0.42     |
| 1:AA:864:A:H2'    | 1:AA:865:A:C8      | 2.54        | 0.42     |
| 47:DF:116:LEU:HB3 | 47:DF:176:PHE:HA   | 2.02        | 0.42     |
| 10:AK:109:ILE:HB  | 21:AU:16:ARG:HH12  | 1.84        | 0.42     |
| 45:BS:76:VAL:HA   | 45:BS:102:HIS:O    | 2.19        | 0.42     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 12:AM:39:ALA:HB3   | 12:AM:42:VAL:HG13  | 2.00        | 0.42     |
| 12:AM:44:ILE:HD12  | 12:AM:45:SER:N     | 2.34        | 0.42     |
| 53:D6:171:LYS:O    | 53:D6:174:GLN:HB3  | 2.19        | 0.42     |
| 23:BB:662:G:O3'    | 37:BL:16:GLY:HA2   | 2.19        | 0.42     |
| 23:DB:819:A:N6     | 23:DB:1189:A:H1'   | 2.35        | 0.42     |
| 23:BB:2267:A:C8    | 23:BB:2267:A:C4'   | 3.02        | 0.42     |
| 13:CN:30:ILE:O     | 13:CN:32:ASP:N     | 2.47        | 0.42     |
| 22:DA:75:G:H2'     | 22:DA:76:G:C8      | 2.55        | 0.42     |
| 27:BK:19:VAL:HG12  | 27:BK:43:ILE:HA    | 2.00        | 0.42     |
| 26:DD:169:ARG:O    | 26:DD:170:VAL:O    | 2.37        | 0.42     |
| 45:DS:59:GLU:OE2   | 45:DS:66:ILE:HG23  | 2.19        | 0.42     |
| 11:CL:28:GLN:HA    | 11:CL:81:ILE:O     | 2.20        | 0.42     |
| 49:BR:16:GLU:HG2   | 49:BR:101:ILE:CG1  | 2.48        | 0.42     |
| 27:DK:115:ILE:HG23 | 27:DK:116:ILE:H    | 1.84        | 0.42     |
| 49:DR:49:ILE:HB    | 49:DR:53:PHE:O     | 2.20        | 0.42     |
| 53:B6:114:LEU:CG   | 53:B6:183:ILE:HD11 | 2.50        | 0.42     |
| 1:AA:83:C:O3'      | 1:AA:84:U:C6       | 2.73        | 0.42     |
| 36:B2:10:LEU:O     | 36:B2:14:ARG:HG2   | 2.19        | 0.42     |
| 34:D3:23:HIS:O     | 34:D3:46:LYS:HB3   | 2.18        | 0.42     |
| 1:AA:1343:G:H1'    | 8:AI:122:ARG:NH1   | 2.34        | 0.42     |
| 45:DS:43:ALA:O     | 45:DS:46:LEU:HB2   | 2.19        | 0.42     |
| 45:DS:73:LYS:HD2   | 45:DS:73:LYS:HA    | 1.80        | 0.42     |
| 1:CA:1057:G:H2'    | 1:CA:1058:G:O4'    | 2.19        | 0.42     |
| 1:CA:1103:C:H5''   | 20:CB:96:LEU:HD12  | 2.00        | 0.42     |
| 1:AA:1057:G:H5''   | 2:AC:153:SER:CB    | 2.49        | 0.42     |
| 23:DB:558:U:OP1    | 41:DJ:114:LEU:N    | 2.52        | 0.42     |
| 23:BB:2723:C:H5''  | 42:BN:1:MET:CE     | 2.49        | 0.42     |
| 27:BK:87:LEU:HD12  | 27:BK:92:GLU:CA    | 2.49        | 0.42     |
| 50:BT:81:LYS:HG3   | 50:BT:82:LYS:N     | 2.34        | 0.42     |
| 41:BJ:110:PRO:O    | 41:BJ:115:GLY:HA3  | 2.19        | 0.42     |
| 23:BB:1584:U:H3'   | 23:BB:1585:C:H5'   | 2.00        | 0.42     |
| 23:BB:2347:C:O2'   | 33:B1:20:TYR:OH    | 2.34        | 0.42     |
| 6:AG:46:LEU:HG     | 6:AG:57:GLU:HB3    | 2.02        | 0.42     |
| 29:DE:48:THR:C     | 29:DE:50:ALA:N     | 2.72        | 0.42     |
| 1:CA:620:C:O2      | 3:CD:131:ILE:HG21  | 2.18        | 0.42     |
| 28:BP:31:VAL:HG13  | 28:BP:32:VAL:N     | 2.34        | 0.42     |
| 23:BB:1432:G:O2'   | 23:BB:1433:A:H5'   | 2.19        | 0.42     |
| 30:BY:47:ILE:O     | 30:BY:48:ASN:C     | 2.58        | 0.42     |
| 23:DB:1432:G:O2'   | 23:DB:1433:A:H5'   | 2.20        | 0.42     |
| 12:CM:28:ARG:CZ    | 12:CM:62:PHE:HB2   | 2.49        | 0.42     |
| 39:BX:52:ARG:O     | 39:BX:55:THR:HB    | 2.19        | 0.42     |
| 23:DB:1811:G:O2'   | 23:DB:1812:U:H5'   | 2.18        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:366:A:O2'    | 1:AA:367:U:P       | 2.78        | 0.42     |
| 22:DA:116:G:H4'   | 43:DO:54:VAL:HG22  | 2.01        | 0.42     |
| 43:DO:6:ALA:CB    | 43:DO:10:ARG:HH11  | 2.33        | 0.42     |
| 2:AC:70:ALA:HA    | 2:AC:105:VAL:HG22  | 2.01        | 0.42     |
| 22:BA:7:G:O2'     | 22:BA:8:C:H5'      | 2.19        | 0.42     |
| 23:DB:1930:G:H22  | 23:DB:1969:A:P     | 2.41        | 0.42     |
| 43:DO:83:LEU:HA   | 43:DO:83:LEU:HD12  | 1.83        | 0.42     |
| 22:BA:94:A:C2'    | 22:BA:95:U:H5'     | 2.50        | 0.42     |
| 23:BB:325:G:H2'   | 23:BB:326:G:C8     | 2.54        | 0.42     |
| 1:AA:584:G:H2'    | 1:AA:585:G:H8      | 1.84        | 0.42     |
| 23:BB:2815:C:H2'  | 23:BB:2816:G:C8    | 2.51        | 0.42     |
| 43:DO:40:ILE:CG2  | 43:DO:44:GLY:HA2   | 2.49        | 0.42     |
| 21:AU:9:GLU:OE2   | 2:CC:108:PRO:HG3   | 2.20        | 0.42     |
| 23:DB:577:G:O2'   | 23:DB:1254:A:OP1   | 2.36        | 0.42     |
| 41:DJ:101:ILE:O   | 41:DJ:105:VAL:HG22 | 2.20        | 0.42     |
| 53:D6:149:LEU:HB2 | 53:D6:154:THR:HG22 | 2.02        | 0.42     |
| 1:AA:327:A:H1'    | 1:AA:329:A:O4'     | 2.18        | 0.42     |
| 23:DB:39:G:H2'    | 23:DB:40:U:C6      | 2.54        | 0.42     |
| 3:CD:147:LYS:H    | 3:CD:147:LYS:HG3   | 1.66        | 0.42     |
| 36:D2:13:ASN:C    | 36:D2:15:SER:H     | 2.21        | 0.42     |
| 3:CD:19:PHE:HB3   | 3:CD:22:SER:OG     | 2.19        | 0.42     |
| 33:B1:29:LYS:HE2  | 33:B1:31:GLU:OE1   | 2.20        | 0.42     |
| 47:DF:122:ASP:HB3 | 47:DF:123:GLY:H    | 1.65        | 0.42     |
| 23:BB:738:G:H2'   | 23:BB:739:A:C8     | 2.53        | 0.42     |
| 23:DB:67:U:H2'    | 23:DB:68:G:C8      | 2.54        | 0.42     |
| 37:BL:118:THR:HA  | 37:BL:119:PRO:HD3  | 1.91        | 0.42     |
| 6:AG:16:LYS:HD3   | 6:AG:17:PHE:CE1    | 2.54        | 0.42     |
| 48:DG:5:LYS:HE2   | 48:DG:61:TRP:CH2   | 2.54        | 0.42     |
| 1:CA:93:U:H2'     | 1:CA:94:G:H5'      | 2.00        | 0.42     |
| 1:CA:160:A:H1'    | 1:CA:344:A:C5      | 2.54        | 0.42     |
| 23:DB:2256:G:H2'  | 23:DB:2257:U:C6    | 2.54        | 0.42     |
| 6:AG:10:LYS:HA    | 6:AG:10:LYS:NZ     | 2.33        | 0.42     |
| 1:CA:1229:A:H2'   | 1:CA:1230:C:H6     | 1.84        | 0.42     |
| 23:BB:1360:G:H2'  | 23:BB:1361:G:C5'   | 2.49        | 0.42     |
| 2:AC:50:SER:O     | 2:AC:114:LEU:HD21  | 2.20        | 0.42     |
| 23:BB:2256:G:H2'  | 23:BB:2257:U:C6    | 2.54        | 0.42     |
| 23:BB:1336:A:H3'  | 23:BB:1337:G:H8    | 1.84        | 0.42     |
| 40:BH:40:THR:N    | 40:BH:43:ASN:ND2   | 2.68        | 0.42     |
| 23:DB:1322:A:H2'  | 23:DB:1323:C:H5'   | 2.00        | 0.42     |
| 23:DB:1238:G:O2'  | 23:DB:1239:G:H5'   | 2.19        | 0.42     |
| 23:DB:800:A:H4'   | 23:DB:801:G:O5'    | 2.19        | 0.42     |
| 20:AB:80:LYS:HE3  | 20:AB:80:LYS:HB2   | 1.83        | 0.42     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 22:DA:67:G:O2'     | 22:DA:68:C:H5'     | 2.19        | 0.42     |
| 2:CC:178:ARG:CG    | 2:CC:206:ILE:HA    | 2.49        | 0.42     |
| 5:AF:69:GLU:O      | 5:AF:73:GLU:HG3    | 2.18        | 0.42     |
| 25:DC:140:VAL:CG2  | 25:DC:163:ILE:HG12 | 2.49        | 0.42     |
| 25:DC:169:ALA:O    | 25:DC:185:ALA:HB3  | 2.18        | 0.42     |
| 21:CU:42:THR:CB    | 21:CU:46:ARG:HH21  | 2.32        | 0.42     |
| 22:BA:42:C:C6      | 47:BF:65:LEU:HD22  | 2.55        | 0.42     |
| 48:DG:47:ASN:CG    | 48:DG:48:THR:N     | 2.73        | 0.42     |
| 41:BJ:55:ILE:CG2   | 41:BJ:123:LYS:HB2  | 2.49        | 0.42     |
| 8:AI:55:ASP:CB     | 8:AI:59:LYS:HG3    | 2.49        | 0.42     |
| 35:DV:4:ILE:N      | 35:DV:62:THR:O     | 2.52        | 0.42     |
| 26:DD:54:ALA:N     | 26:DD:76:GLY:HA2   | 2.34        | 0.42     |
| 7:AH:86:LYS:HG3    | 7:AH:124:ILE:HD11  | 2.01        | 0.42     |
| 25:DC:114:GLN:HE21 | 25:DC:114:GLN:HB3  | 1.61        | 0.42     |
| 51:BZ:77:LYS:CD    | 51:BZ:78:TYR:H     | 2.30        | 0.42     |
| 23:BB:335:C:O2'    | 23:BB:336:C:H5'    | 2.19        | 0.42     |
| 46:BU:84:PHE:O     | 46:BU:85:ARG:CB    | 2.53        | 0.42     |
| 46:BU:5:ARG:HH22   | 46:BU:93:ARG:HD3   | 1.85        | 0.42     |
| 47:BF:4:HIS:O      | 47:BF:7:TYR:HB3    | 2.19        | 0.42     |
| 29:BE:146:VAL:HG12 | 29:BE:147:LEU:N    | 2.34        | 0.42     |
| 1:AA:924:C:H5'     | 1:AA:1399:C:OP2    | 2.20        | 0.42     |
| 24:BI:37:PHE:HB2   | 24:BI:66:PHE:CZ    | 2.55        | 0.42     |
| 1:CA:19:A:OP1      | 4:CE:134:ASN:ND2   | 2.51        | 0.42     |
| 1:CA:865:A:C2      | 1:CA:918:A:H4'     | 2.54        | 0.42     |
| 18:AS:66:VAL:C     | 18:AS:68:HIS:H     | 2.22        | 0.42     |
| 1:AA:972:C:O2'     | 9:AJ:57:VAL:HA     | 2.19        | 0.42     |
| 50:DT:57:VAL:O     | 50:DT:85:VAL:O     | 2.37        | 0.42     |
| 50:DT:29:THR:H     | 50:DT:91:GLN:NE2   | 2.17        | 0.42     |
| 25:DC:203:VAL:O    | 25:DC:204:LEU:HB2  | 2.20        | 0.42     |
| 53:D6:173:ASP:O    | 53:D6:174:GLN:C    | 2.58        | 0.42     |
| 37:BL:30:THR:O     | 37:BL:31:GLY:C     | 2.58        | 0.42     |
| 38:DM:30:SER:OG    | 38:DM:106:ASP:HA   | 2.20        | 0.42     |
| 13:AN:50:LEU:H     | 13:AN:51:PRO:HD2   | 1.84        | 0.42     |
| 23:DB:2848:G:N3    | 23:DB:2849:U:H5    | 2.18        | 0.42     |
| 28:DP:99:LEU:HD22  | 28:DP:99:LEU:HA    | 1.89        | 0.42     |
| 13:CN:27:LYS:O     | 13:CN:32:ASP:HB2   | 2.19        | 0.42     |
| 1:AA:1251:A:H1'    | 1:AA:1370:G:O4'    | 2.20        | 0.42     |
| 29:DE:166:LYS:O    | 29:DE:167:VAL:HB   | 2.18        | 0.42     |
| 1:CA:1413:A:O2'    | 1:CA:1414:U:H5'    | 2.19        | 0.42     |
| 40:BH:141:LYS:N    | 40:BH:141:LYS:CD   | 2.83        | 0.42     |
| 35:BV:77:VAL:HG23  | 35:BV:89:ILE:CG2   | 2.50        | 0.42     |
| 1:CA:313:A:O2'     | 1:CA:314:C:H5'     | 2.19        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:842:U:H4'    | 1:AA:846:G:C2     | 2.54        | 0.42     |
| 26:DD:152:PRO:C   | 26:DD:154:LYS:H   | 2.22        | 0.42     |
| 23:BB:1729:U:H2'  | 23:BB:1730:C:H5'  | 2.01        | 0.42     |
| 44:DQ:7:VAL:HG23  | 44:DQ:8:ILE:N     | 2.35        | 0.42     |
| 44:DQ:8:ILE:HG23  | 44:DQ:9:ALA:N     | 2.34        | 0.42     |
| 26:BD:152:PRO:C   | 26:BD:154:LYS:H   | 2.23        | 0.42     |
| 2:CC:156:LEU:HD12 | 2:CC:163:ARG:HG3  | 2.00        | 0.42     |
| 23:DB:193:U:O3'   | 23:DB:803:U:H4'   | 2.19        | 0.42     |
| 1:AA:974:A:H8     | 1:AA:974:A:OP1    | 2.02        | 0.42     |
| 35:BV:42:LEU:CD2  | 35:BV:42:LEU:H    | 2.20        | 0.42     |
| 3:AD:100:VAL:HG21 | 3:AD:136:VAL:CG2  | 2.49        | 0.42     |
| 11:AL:115:LYS:O   | 11:AL:116:TYR:HB2 | 2.19        | 0.42     |
| 8:CI:9:GLY:CA     | 8:CI:80:HIS:HB3   | 2.49        | 0.42     |
| 23:BB:118:A:H5'   | 23:BB:119:A:H8    | 1.84        | 0.42     |
| 23:DB:2842:G:O2'  | 23:DB:2843:G:H5'  | 2.19        | 0.42     |
| 23:BB:2228:G:H2'  | 23:BB:2229:U:C6   | 2.55        | 0.42     |
| 23:DB:1353:A:C8   | 23:DB:1378:A:N6   | 2.88        | 0.42     |
| 19:CT:38:ILE:HG13 | 19:CT:82:ILE:HG22 | 2.02        | 0.42     |
| 23:DB:931:U:O4    | 23:DB:1166:G:N2   | 2.53        | 0.42     |
| 23:DB:2199:A:H5'' | 23:DB:2200:C:H5   | 1.85        | 0.42     |
| 1:AA:676:A:O2'    | 1:AA:677:U:H5'    | 2.19        | 0.42     |
| 1:AA:373:A:C1'    | 1:AA:481:G:H1'    | 2.49        | 0.42     |
| 28:DP:105:LYS:HA  | 28:DP:108:ARG:NE  | 2.35        | 0.42     |
| 23:BB:2276:G:O2'  | 23:BB:2277:G:H5'  | 2.20        | 0.42     |
| 26:BD:125:TRP:NE1 | 26:BD:161:MET:N   | 2.67        | 0.42     |
| 23:DB:2757:A:N3   | 23:DB:2757:A:H2'  | 2.34        | 0.42     |
| 26:DD:125:TRP:HE1 | 26:DD:161:MET:H   | 1.68        | 0.42     |
| 2:AC:19:SER:HB3   | 2:AC:21:TRP:HE1   | 1.84        | 0.42     |
| 22:BA:39:A:H2     | 22:BA:46:A:N6     | 2.15        | 0.42     |
| 1:CA:591:U:OP2    | 7:CH:30:LYS:HD2   | 2.20        | 0.42     |
| 23:DB:2636:C:O5'  | 26:DD:81:GLU:HB2  | 2.19        | 0.42     |
| 23:BB:1856:U:C2'  | 23:BB:1857:G:H5'  | 2.50        | 0.42     |
| 23:BB:2730:C:H4'  | 26:BD:174:SER:HB3 | 2.01        | 0.42     |
| 24:BI:14:ALA:CB   | 24:BI:50:LYS:HA   | 2.49        | 0.42     |
| 23:BB:2301:C:H2'  | 23:BB:2302:U:H6   | 1.85        | 0.42     |
| 23:DB:2729:G:H2'  | 23:DB:2730:C:H6   | 1.83        | 0.42     |
| 1:CA:469:C:O2'    | 1:CA:470:C:H5'    | 2.20        | 0.42     |
| 23:BB:1275:A:H2'  | 23:BB:1276:A:O4'  | 2.20        | 0.42     |
| 26:BD:40:LEU:HA   | 26:BD:45:TYR:N    | 2.35        | 0.42     |
| 23:DB:79:C:HO2'   | 23:DB:346:A:C1'   | 2.32        | 0.42     |
| 23:DB:1835:G:H2'  | 23:DB:1836:C:H6   | 1.83        | 0.42     |
| 23:DB:2322:A:N6   | 23:DB:2333:A:H62  | 2.17        | 0.42     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:2655:G:H1'   | 23:BB:2656:U:H5    | 1.84        | 0.42     |
| 23:DB:245:G:O2'    | 23:DB:246:C:H5'    | 2.19        | 0.42     |
| 23:DB:516:C:H2'    | 23:DB:517:C:C6     | 2.54        | 0.42     |
| 23:DB:438:G:H2'    | 23:DB:439:A:C8     | 2.55        | 0.42     |
| 14:CO:58:ARG:HH21  | 14:CO:62:GLN:HE22  | 1.67        | 0.42     |
| 23:BB:1435:G:H2'   | 23:BB:1436:G:C8    | 2.54        | 0.42     |
| 23:DB:2081:U:H2'   | 23:DB:2082:A:H8    | 1.85        | 0.42     |
| 1:CA:1241:G:H2'    | 1:CA:1242:G:H8     | 1.84        | 0.42     |
| 23:BB:1830:C:O2'   | 23:BB:1831:G:H5'   | 2.19        | 0.42     |
| 1:CA:1420:U:H2'    | 1:CA:1421:G:C8     | 2.55        | 0.42     |
| 23:BB:1449:G:O2'   | 23:BB:1450:G:H5'   | 2.19        | 0.42     |
| 53:B6:11:ARG:O     | 53:B6:15:GLN:HB2   | 2.19        | 0.42     |
| 23:DB:2838:G:H2'   | 23:DB:2839:G:H8    | 1.84        | 0.42     |
| 11:AL:65:TYR:HB3   | 11:AL:95:HIS:CD2   | 2.54        | 0.42     |
| 23:BB:1207:C:H2'   | 23:BB:1208:C:H6    | 1.83        | 0.42     |
| 3:CD:202:LEU:O     | 3:CD:202:LEU:HD12  | 2.20        | 0.42     |
| 15:AP:48:GLU:HG3   | 15:AP:49:GLY:H     | 1.83        | 0.42     |
| 24:BI:15:GLY:O     | 24:BI:16:MET:HB2   | 2.19        | 0.42     |
| 16:AQ:47:ASP:OD2   | 16:AQ:51:GLU:HG2   | 2.19        | 0.42     |
| 2:CC:125:ARG:HB3   | 2:CC:127:VAL:HG13  | 2.01        | 0.42     |
| 52:BW:59:PHE:CD2   | 52:BW:60:ALA:N     | 2.88        | 0.42     |
| 25:DC:121:ALA:HB3  | 25:DC:129:LEU:HD11 | 2.02        | 0.42     |
| 48:BG:106:LEU:O    | 48:BG:108:PHE:N    | 2.47        | 0.42     |
| 37:DL:121:THR:HG22 | 37:DL:141:LYS:CB   | 2.50        | 0.42     |
| 20:AB:187:ASP:O    | 20:AB:189:ASN:N    | 2.53        | 0.42     |
| 53:D6:84:ARG:HD2   | 53:D6:92:PRO:CG    | 2.50        | 0.42     |
| 53:B6:65:THR:CG2   | 53:B6:66:LEU:N     | 2.82        | 0.42     |
| 40:BH:80:ILE:CD1   | 40:BH:144:VAL:HG22 | 2.40        | 0.42     |
| 40:BH:82:SER:O     | 40:BH:92:GLY:N     | 2.50        | 0.42     |
| 8:CI:29:ILE:HG12   | 8:CI:64:ILE:HB     | 2.01        | 0.42     |
| 8:CI:78:ILE:O      | 8:CI:82:ILE:HG13   | 2.20        | 0.42     |
| 20:CB:202:ASN:HD22 | 20:CB:204:ASP:H    | 1.62        | 0.42     |
| 26:DD:4:LEU:HD12   | 26:DD:32:ASN:CB    | 2.50        | 0.42     |
| 47:DF:79:ARG:NE    | 47:DF:79:ARG:N     | 2.68        | 0.42     |
| 23:DB:2359:C:O3'   | 34:D3:50:SER:HB3   | 2.19        | 0.42     |
| 30:DY:47:ILE:O     | 30:DY:48:ASN:C     | 2.57        | 0.42     |
| 3:CD:160:LEU:HA    | 3:CD:163:GLN:CG    | 2.50        | 0.42     |
| 3:CD:25:ARG:HB2    | 3:CD:25:ARG:NH1    | 2.33        | 0.42     |
| 23:DB:1062:G:H2'   | 23:DB:1063:G:H8    | 1.84        | 0.42     |
| 1:AA:921:U:H2'     | 1:AA:922:G:O4'     | 2.20        | 0.42     |
| 12:CM:109:LYS:HB2  | 12:CM:113:LYS:NZ   | 2.34        | 0.42     |
| 1:CA:1221:G:OP1    | 18:CS:35:ARG:HD2   | 2.20        | 0.42     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:AA:1270:G:H4'    | 1:AA:1313:U:O2'   | 2.20        | 0.42     |
| 11:AL:49:ARG:HH12  | 11:AL:88:ASP:HB2  | 1.83        | 0.42     |
| 40:BH:106:ALA:O    | 40:BH:108:VAL:N   | 2.53        | 0.42     |
| 23:DB:850:U:O3'    | 30:DY:22:THR:HG22 | 2.20        | 0.42     |
| 1:AA:1250:A:H2     | 1:AA:1370:G:H1'   | 1.83        | 0.42     |
| 15:CP:52:LEU:CD2   | 15:CP:75:ILE:HA   | 2.50        | 0.42     |
| 45:BS:32:ALA:O     | 45:BS:36:LEU:HD23 | 2.19        | 0.42     |
| 45:BS:59:GLU:OE2   | 45:BS:66:ILE:HG23 | 2.20        | 0.42     |
| 23:BB:729:G:OP1    | 25:BC:12:ARG:HB2  | 2.19        | 0.42     |
| 49:BR:101:ILE:HG22 | 49:BR:101:ILE:O   | 2.20        | 0.42     |
| 49:DR:39:LEU:O     | 49:DR:49:ILE:HG12 | 2.20        | 0.42     |
| 24:DI:105:LEU:HD11 | 24:DI:139:VAL:CG2 | 2.44        | 0.42     |
| 26:BD:148:GLN:O    | 26:BD:149:ASN:CB  | 2.67        | 0.42     |
| 20:AB:103:TRP:CZ3  | 20:AB:107:ARG:HD2 | 2.55        | 0.42     |
| 48:DG:115:GLN:CD   | 48:DG:115:GLN:N   | 2.62        | 0.42     |
| 23:DB:2102:G:O2'   | 23:DB:2103:C:H5'  | 2.19        | 0.42     |
| 11:AL:28:GLN:HA    | 11:AL:81:ILE:O    | 2.19        | 0.42     |
| 1:CA:1299:A:H2'    | 1:CA:1301:U:C1'   | 2.44        | 0.42     |
| 1:AA:108:G:H5'     | 1:AA:109:A:C5'    | 2.45        | 0.42     |
| 5:CF:40:GLU:OE1    | 5:CF:100:SER:HB2  | 2.20        | 0.42     |
| 23:BB:182:A:H2'    | 23:BB:183:C:H6    | 1.84        | 0.42     |
| 41:DJ:120:ARG:HB3  | 41:DJ:120:ARG:HE  | 1.69        | 0.42     |
| 5:AF:40:GLU:OE1    | 5:AF:100:SER:HB2  | 2.20        | 0.42     |
| 23:DB:2846:G:OP1   | 28:DP:52:ARG:NH1  | 2.52        | 0.42     |
| 26:BD:113:SER:OG   | 26:BD:114:LYS:N   | 2.51        | 0.42     |
| 3:AD:96:ARG:O      | 3:AD:99:ASN:HB3   | 2.19        | 0.42     |
| 23:DB:322:A:H5'    | 23:DB:340:A:C1'   | 2.48        | 0.42     |
| 7:AH:4:ASP:OD1     | 7:AH:7:ALA:HB2    | 2.19        | 0.42     |
| 1:CA:1121:U:H2'    | 1:CA:1122:U:C6    | 2.54        | 0.42     |
| 29:BE:48:THR:N     | 29:BE:51:GLU:HG3  | 2.34        | 0.42     |
| 23:DB:647:G:H2'    | 23:DB:648:G:C8    | 2.54        | 0.42     |
| 34:B3:61:LEU:N     | 34:B3:62:PRO:HD3  | 2.34        | 0.42     |
| 28:BP:50:ARG:HB3   | 28:BP:57:ALA:H    | 1.84        | 0.42     |
| 23:DB:1591:A:H2'   | 23:DB:1592:C:O4'  | 2.19        | 0.42     |
| 23:BB:2231:U:H2'   | 23:BB:2232:C:H6   | 1.83        | 0.42     |
| 1:AA:1161:C:O2'    | 1:AA:1162:C:H5'   | 2.20        | 0.42     |
| 23:DB:1041:G:C2    | 23:DB:1042:G:N7   | 2.88        | 0.42     |
| 1:AA:1225:A:OP1    | 12:AM:100:ARG:HA  | 2.20        | 0.42     |
| 23:DB:12:U:H1'     | 23:DB:2627:G:OP1  | 2.20        | 0.42     |
| 42:DN:13:ASN:C     | 42:DN:15:SER:H    | 2.22        | 0.42     |
| 1:CA:373:A:H5'     | 1:CA:373:A:H8     | 1.84        | 0.42     |
| 23:DB:2578:G:H2'   | 23:DB:2579:C:H6   | 1.84        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1949:G:H2'  | 23:BB:1950:G:C8    | 2.54        | 0.42     |
| 1:CA:389:A:C6     | 1:CA:390:U:H1'     | 2.54        | 0.42     |
| 41:DJ:13:ARG:HB3  | 41:DJ:53:TYR:CD2   | 2.54        | 0.42     |
| 37:BL:23:ILE:H    | 37:BL:23:ILE:CD1   | 2.30        | 0.42     |
| 41:BJ:41:LYS:O    | 44:BQ:66:ALA:HB1   | 2.19        | 0.42     |
| 48:DG:137:LYS:O   | 48:DG:140:ILE:HG13 | 2.20        | 0.42     |
| 23:BB:2250:G:O5'  | 23:BB:2250:G:H8    | 2.03        | 0.42     |
| 1:AA:1152:A:H2'   | 1:AA:1153:G:C8     | 2.54        | 0.42     |
| 23:DB:576:U:H2'   | 23:DB:577:G:H8     | 1.84        | 0.42     |
| 19:CT:31:ILE:O    | 19:CT:34:VAL:HG23  | 2.20        | 0.42     |
| 22:DA:93:C:H2'    | 22:DA:94:A:H8      | 1.84        | 0.42     |
| 37:DL:135:ILE:CG2 | 37:DL:136:GLU:N    | 2.81        | 0.42     |
| 23:BB:2299:U:H2'  | 23:BB:2300:C:C6    | 2.55        | 0.42     |
| 1:CA:1015:G:H2'   | 1:CA:1016:A:C8     | 2.53        | 0.42     |
| 23:DB:428:A:O2'   | 23:DB:429:A:H5'    | 2.18        | 0.42     |
| 23:BB:1252:G:H1'  | 44:BQ:32:ARG:NH2   | 2.34        | 0.42     |
| 48:DG:154:GLU:O   | 48:DG:156:TYR:N    | 2.52        | 0.42     |
| 23:DB:349:U:O2    | 23:DB:349:U:H2'    | 2.19        | 0.42     |
| 23:BB:1675:C:H2'  | 23:BB:1676:A:O4'   | 2.19        | 0.42     |
| 49:BR:15:SER:OG   | 49:BR:18:GLN:HG2   | 2.20        | 0.42     |
| 23:DB:840:C:O2'   | 23:DB:841:G:H5'    | 2.20        | 0.42     |
| 23:DB:1370:C:H2'  | 23:DB:1371:G:O4'   | 2.20        | 0.42     |
| 23:DB:797:G:OP2   | 29:DE:57:LYS:HB2   | 2.20        | 0.42     |
| 23:DB:619:G:H3'   | 23:DB:620:G:H21    | 1.85        | 0.42     |
| 1:AA:106:C:HO2'   | 1:AA:107:G:H5'     | 1.85        | 0.42     |
| 1:CA:655:A:H2'    | 1:CA:656:G:O4'     | 2.20        | 0.42     |
| 3:CD:43:ARG:NH1   | 3:CD:43:ARG:HB3    | 2.34        | 0.42     |
| 23:BB:769:U:H2'   | 23:BB:770:G:H8     | 1.85        | 0.42     |
| 1:CA:1229:A:OP2   | 12:CM:112:ARG:HD2  | 2.19        | 0.42     |
| 23:BB:103:A:H2'   | 23:BB:104:A:C8     | 2.55        | 0.42     |
| 26:BD:2:ILE:H     | 26:BD:2:ILE:HG13   | 1.73        | 0.42     |
| 1:CA:515:G:O2'    | 1:CA:516:U:H5'     | 2.19        | 0.42     |
| 1:CA:1429:A:O2'   | 1:CA:1430:A:H5'    | 2.20        | 0.42     |
| 1:AA:1159:U:O4'   | 1:AA:1182:G:N2     | 2.53        | 0.42     |
| 23:BB:1908:C:O2'  | 23:BB:1909:C:H5'   | 2.19        | 0.42     |
| 1:AA:63:C:H2'     | 1:AA:64:G:H5'      | 2.02        | 0.42     |
| 10:AK:101:ALA:C   | 10:AK:103:GLY:H    | 2.23        | 0.42     |
| 23:BB:586:A:H5'   | 29:BE:84:THR:OG1   | 2.19        | 0.42     |
| 31:D0:56:LYS:O    | 31:D0:56:LYS:HD3   | 2.20        | 0.42     |
| 23:DB:1107:G:O2'  | 23:DB:1108:U:H5'   | 2.18        | 0.42     |
| 23:DB:2234:G:O2'  | 23:DB:2235:G:H5'   | 2.19        | 0.42     |
| 28:BP:48:ALA:HB3  | 28:BP:59:THR:CB    | 2.50        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 21:AU:33:ARG:NE   | 21:AU:34:ARG:HG2  | 2.34        | 0.42     |
| 23:DB:2355:G:H4'  | 52:DW:20:LEU:HD13 | 2.00        | 0.42     |
| 23:DB:2354:C:H2'  | 23:DB:2355:G:H8   | 1.83        | 0.42     |
| 25:DC:120:ASP:O   | 25:DC:121:ALA:C   | 2.58        | 0.42     |
| 48:BG:91:VAL:O    | 48:BG:93:TYR:N    | 2.51        | 0.42     |
| 47:BF:31:GLU:O    | 47:BF:32:LYS:O    | 2.38        | 0.42     |
| 48:DG:9:VAL:N     | 48:DG:48:THR:HB   | 2.34        | 0.42     |
| 52:DW:50:VAL:HG23 | 52:DW:61:LYS:CE   | 2.50        | 0.42     |
| 8:CI:56:MET:C     | 8:CI:58:GLU:N     | 2.73        | 0.42     |
| 8:AI:93:LEU:HD13  | 8:AI:97:LEU:HD11  | 2.02        | 0.42     |
| 35:BV:93:ARG:HH11 | 35:BV:93:ARG:HG3  | 1.84        | 0.42     |
| 29:DE:60:TRP:HB3  | 29:DE:61:ARG:H    | 1.42        | 0.42     |
| 50:BT:55:VAL:HG22 | 50:BT:87:LEU:CD2  | 2.50        | 0.42     |
| 23:BB:77:G:O2'    | 23:BB:78:U:H5'    | 2.20        | 0.42     |
| 3:AD:160:LEU:HD23 | 3:AD:164:ARG:HH21 | 1.85        | 0.42     |
| 42:BN:81:ASN:O    | 42:BN:85:PRO:HD2  | 2.19        | 0.42     |
| 24:DI:112:LYS:HB2 | 24:DI:116:MET:SD  | 2.60        | 0.42     |
| 47:BF:79:ARG:NE   | 47:BF:79:ARG:N    | 2.67        | 0.42     |
| 1:AA:1277:C:H1'   | 1:AA:1282:C:C2    | 2.55        | 0.42     |
| 46:DU:73:ASN:HD22 | 46:DU:73:ASN:N    | 2.17        | 0.42     |
| 47:BF:52:ALA:HA   | 47:BF:55:ASP:HB2  | 2.01        | 0.42     |
| 23:DB:1169:A:H2'  | 23:DB:1170:C:H6   | 1.85        | 0.42     |
| 1:CA:955:U:H1'    | 1:CA:1227:A:H62   | 1.84        | 0.42     |
| 4:CE:131:ASN:HD22 | 4:CE:134:ASN:H    | 1.68        | 0.42     |
| 4:CE:136:VAL:HG13 | 4:CE:137:ARG:H    | 1.81        | 0.42     |
| 18:CS:43:MET:O    | 18:CS:61:VAL:HB   | 2.20        | 0.42     |
| 42:DN:101:GLY:HA2 | 42:DN:109:PRO:HA  | 2.01        | 0.42     |
| 23:DB:668:A:H2'   | 23:DB:670:A:H62   | 1.85        | 0.42     |
| 12:AM:79:LEU:HA   | 12:AM:82:LEU:HB2  | 2.02        | 0.42     |
| 29:BE:33:VAL:HA   | 29:BE:36:ALA:HB3  | 2.00        | 0.42     |
| 46:BU:71:ILE:HD11 | 46:BU:81:ARG:O    | 2.19        | 0.42     |
| 37:DL:19:LEU:HD23 | 37:DL:31:GLY:O    | 2.20        | 0.42     |
| 23:DB:850:U:O2'   | 30:DY:22:THR:HA   | 2.19        | 0.42     |
| 48:BG:152:ARG:HG3 | 48:BG:153:PRO:HD2 | 2.01        | 0.42     |
| 31:D0:37:HIS:CD2  | 31:D0:43:THR:HG22 | 2.55        | 0.42     |
| 44:BQ:105:PHE:HA  | 44:BQ:108:LEU:CD1 | 2.49        | 0.42     |
| 49:BR:16:GLU:HG2  | 49:BR:101:ILE:CB  | 2.50        | 0.42     |
| 26:BD:10:GLY:O    | 26:BD:11:MET:HB2  | 2.19        | 0.42     |
| 1:CA:1390:U:O2'   | 1:CA:1391:U:H5'   | 2.20        | 0.42     |
| 20:CB:161:PHE:HA  | 20:CB:183:PHE:O   | 2.19        | 0.42     |
| 20:CB:67:LEU:HD22 | 20:CB:91:VAL:HG23 | 2.02        | 0.42     |
| 23:BB:116:C:N4    | 23:BB:117:G:C6    | 2.88        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 20:CB:148:GLY:O   | 20:CB:151:LYS:HG2  | 2.19        | 0.42     |
| 1:CA:999:C:H2'    | 1:CA:1000:A:H8     | 1.84        | 0.42     |
| 49:DR:63:VAL:O    | 49:DR:63:VAL:HG23  | 2.20        | 0.42     |
| 37:BL:100:ILE:O   | 37:BL:100:ILE:HG12 | 2.19        | 0.42     |
| 29:DE:157:LEU:HG  | 29:DE:169:VAL:HG11 | 2.02        | 0.42     |
| 23:DB:62:U:H2'    | 23:DB:63:A:H5'     | 1.98        | 0.42     |
| 46:DU:24:VAL:HA   | 46:DU:35:VAL:HA    | 2.01        | 0.42     |
| 31:D0:30:ASP:HB3  | 31:D0:33:SER:O     | 2.19        | 0.42     |
| 23:DB:188:G:OP1   | 51:DZ:14:THR:HG23  | 2.20        | 0.42     |
| 23:BB:2747:G:H8   | 23:BB:2747:G:O5'   | 2.03        | 0.42     |
| 42:BN:92:GLY:HA2  | 42:BN:94:TYR:CZ    | 2.54        | 0.42     |
| 7:CH:66:GLN:HB3   | 7:CH:67:GLY:H      | 1.74        | 0.42     |
| 29:DE:41:GLN:O    | 29:DE:42:GLY:C     | 2.58        | 0.42     |
| 39:DX:5:GLU:OE2   | 39:DX:5:GLU:HA     | 2.19        | 0.42     |
| 23:BB:1998:A:H2'  | 23:BB:1999:C:C6    | 2.52        | 0.42     |
| 23:DB:703:U:H2'   | 23:DB:704:G:O4'    | 2.19        | 0.42     |
| 49:DR:2:TYR:HB2   | 49:DR:42:ALA:CB    | 2.48        | 0.42     |
| 41:BJ:101:ILE:O   | 41:BJ:105:VAL:HG22 | 2.19        | 0.42     |
| 1:CA:366:A:O2'    | 1:CA:367:U:P       | 2.77        | 0.42     |
| 1:AA:1511:G:O2'   | 1:AA:1512:U:H5'    | 2.18        | 0.42     |
| 2:AC:105:VAL:HG23 | 2:AC:105:VAL:O     | 2.20        | 0.42     |
| 1:AA:1028:C:H2'   | 1:AA:1028:C:O2     | 2.19        | 0.42     |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:O4'    | 2.20        | 0.42     |
| 1:CA:1127:G:H5'   | 1:CA:1280:A:O2'    | 2.20        | 0.42     |
| 1:AA:835:U:O2'    | 1:AA:836:G:H5'     | 2.20        | 0.42     |
| 23:DB:754:U:H2'   | 23:DB:755:U:H6     | 1.84        | 0.42     |
| 3:AD:16:THR:CG2   | 3:AD:17:ASP:N      | 2.83        | 0.42     |
| 23:DB:2803:G:O2'  | 23:DB:2804:U:H5'   | 2.20        | 0.42     |
| 14:AO:36:ILE:HD11 | 14:AO:59:MET:HB2   | 2.01        | 0.42     |
| 23:BB:2553:G:H2'  | 23:BB:2554:U:H4'   | 2.00        | 0.42     |
| 26:BD:70:LYS:HD3  | 26:BD:70:LYS:C     | 2.39        | 0.42     |
| 1:CA:766:A:H2'    | 1:CA:767:A:H8      | 1.84        | 0.42     |
| 1:CA:1508:A:H2'   | 1:CA:1509:C:H6     | 1.84        | 0.42     |
| 23:DB:40:U:H2'    | 23:DB:41:C:C6      | 2.55        | 0.42     |
| 46:DU:14:THR:O    | 46:DU:18:LYS:HA    | 2.19        | 0.42     |
| 23:DB:928:A:O2'   | 30:DY:37:ARG:HD3   | 2.20        | 0.42     |
| 1:AA:543:U:H2'    | 1:AA:544:G:H8      | 1.85        | 0.42     |
| 9:CJ:26:VAL:O     | 9:CJ:30:LYS:HG3    | 2.18        | 0.42     |
| 23:BB:552:U:H2'   | 23:BB:553:G:H8     | 1.84        | 0.42     |
| 10:CK:82:GLU:HG2  | 10:CK:108:ASN:HB2  | 2.02        | 0.42     |
| 23:DB:95:A:H1'    | 39:DX:40:SER:OG    | 2.19        | 0.42     |
| 1:AA:1481:U:H2'   | 1:AA:1482:G:C8     | 2.55        | 0.42     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1522:A:H4'   | 23:DB:1524:G:C8    | 2.55        | 0.42     |
| 1:AA:1404:C:H2'    | 1:AA:1405:G:C8     | 2.54        | 0.42     |
| 23:DB:1099:G:OP2   | 24:DI:2:LYS:O      | 2.37        | 0.42     |
| 50:DT:4:GLU:OE2    | 50:DT:5:GLU:HG2    | 2.19        | 0.42     |
| 23:BB:20:C:O2'     | 23:BB:21:A:H5'     | 2.20        | 0.42     |
| 44:BQ:30:VAL:HG22  | 44:BQ:31:TYR:N     | 2.35        | 0.42     |
| 48:DG:10:VAL:HG13  | 48:DG:14:VAL:HB    | 2.01        | 0.42     |
| 37:BL:125:LEU:HB2  | 37:BL:143:GLU:OE2  | 2.19        | 0.42     |
| 26:BD:32:ASN:HD22  | 26:BD:50:VAL:HG21  | 1.85        | 0.42     |
| 53:D6:57:THR:O     | 53:D6:68:VAL:HA    | 2.20        | 0.42     |
| 44:DQ:73:ILE:HG13  | 44:DQ:74:SER:N     | 2.35        | 0.42     |
| 44:DQ:94:LEU:C     | 44:DQ:96:ASP:H     | 2.22        | 0.42     |
| 51:DZ:6:GLN:HE22   | 51:DZ:77:LYS:CE    | 2.32        | 0.42     |
| 51:DZ:77:LYS:CG    | 51:DZ:78:TYR:N     | 2.82        | 0.42     |
| 25:BC:128:THR:CG2  | 25:BC:190:THR:HG22 | 2.49        | 0.42     |
| 37:DL:78:ARG:NH2   | 37:DL:78:ARG:HB3   | 2.35        | 0.42     |
| 42:DN:39:PRO:C     | 42:DN:41:ALA:H     | 2.23        | 0.42     |
| 30:BY:11:SER:OG    | 30:BY:13:ILE:HG13  | 2.19        | 0.42     |
| 47:DF:137:PHE:O    | 47:DF:138:PRO:C    | 2.58        | 0.42     |
| 4:CE:33:THR:HG22   | 4:CE:51:LYS:HB3    | 2.02        | 0.42     |
| 13:AN:26:LEU:HD23  | 13:AN:27:LYS:N     | 2.35        | 0.42     |
| 23:DB:135:U:O2'    | 23:DB:136:G:H5'    | 2.20        | 0.42     |
| 23:DB:1789:A:O2'   | 23:DB:1790:C:H5'   | 2.20        | 0.42     |
| 53:D6:15:GLN:HB3   | 53:D6:16:LYS:NZ    | 2.35        | 0.42     |
| 29:BE:29:HIS:O     | 29:BE:32:VAL:HG22  | 2.19        | 0.42     |
| 11:CL:42:LYS:HD2   | 11:CL:43:LYS:HG2   | 2.02        | 0.42     |
| 15:AP:52:LEU:CD2   | 15:AP:75:ILE:HA    | 2.50        | 0.42     |
| 23:DB:851:C:H4'    | 30:DY:46:MET:HA    | 2.02        | 0.42     |
| 23:DB:2742:G:OP1   | 32:D4:36:ARG:HD3   | 2.20        | 0.42     |
| 23:BB:974:G:P      | 49:BR:78:ARG:HD3   | 2.60        | 0.42     |
| 23:BB:2547:A:H2'   | 23:BB:2548:U:H6    | 1.80        | 0.42     |
| 32:D4:3:VAL:HG23   | 32:D4:4:ARG:N      | 2.29        | 0.42     |
| 23:BB:1199:U:C5'   | 44:BQ:4:LYS:HD3    | 2.49        | 0.42     |
| 44:BQ:7:VAL:HG23   | 44:BQ:8:ILE:N      | 2.33        | 0.42     |
| 49:DR:101:ILE:HG22 | 49:DR:101:ILE:O    | 2.18        | 0.42     |
| 49:DR:38:VAL:O     | 49:DR:53:PHE:HB3   | 2.19        | 0.42     |
| 27:BK:98:ARG:C     | 27:BK:99:ILE:HD12  | 2.40        | 0.42     |
| 35:BV:30:ILE:HA    | 35:BV:91:PHE:O     | 2.19        | 0.42     |
| 1:AA:279:A:H5'     | 1:AA:281:G:H5'     | 2.01        | 0.42     |
| 36:D2:34:ARG:O     | 36:D2:38:GLY:N     | 2.53        | 0.42     |
| 23:BB:2743:U:H3'   | 23:BB:2744:G:H5''  | 2.01        | 0.42     |
| 23:BB:2653:U:H3'   | 23:BB:2654:A:H2'   | 2.01        | 0.42     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 45:DS:51:LEU:HD12  | 45:DS:105:VAL:HG11 | 2.01        | 0.42     |
| 45:DS:44:ALA:C     | 45:DS:46:LEU:N     | 2.72        | 0.42     |
| 9:AJ:76:ILE:H      | 9:AJ:76:ILE:HG13   | 1.71        | 0.42     |
| 4:CE:104:ILE:HD11  | 4:CE:111:ARG:HA    | 2.02        | 0.42     |
| 1:AA:552:U:H2'     | 1:AA:553:A:H8      | 1.84        | 0.42     |
| 2:AC:129:PHE:CG    | 2:AC:130:ARG:N     | 2.88        | 0.42     |
| 23:DB:1372:U:H1'   | 23:DB:2214:C:C4    | 2.55        | 0.42     |
| 25:BC:30:ALA:O     | 25:BC:32:LEU:N     | 2.50        | 0.42     |
| 20:AB:161:PHE:HA   | 20:AB:183:PHE:O    | 2.19        | 0.42     |
| 39:BX:1:MET:HB3    | 39:BX:5:GLU:OE1    | 2.20        | 0.42     |
| 1:AA:167:A:H2'     | 1:AA:168:G:H8      | 1.85        | 0.42     |
| 1:CA:499:A:H1'     | 1:CA:500:G:C8      | 2.54        | 0.42     |
| 1:CA:503:C:O2'     | 1:CA:504:C:H5'     | 2.20        | 0.42     |
| 49:DR:19:THR:CB    | 49:DR:97:LYS:HA    | 2.48        | 0.42     |
| 23:DB:519:U:H2'    | 23:DB:520:G:H8     | 1.84        | 0.42     |
| 19:AT:43:LYS:HB3   | 19:AT:85:LEU:HD21  | 2.02        | 0.42     |
| 23:DB:543:G:N2     | 23:DB:545:U:H5'    | 2.35        | 0.42     |
| 20:AB:160:LEU:HD21 | 20:AB:182:VAL:HG22 | 2.01        | 0.42     |
| 23:BB:635:C:O2'    | 23:BB:636:G:H5'    | 2.19        | 0.42     |
| 6:AG:6:ILE:HB      | 6:AG:7:GLY:H       | 1.54        | 0.42     |
| 1:CA:880:C:O2'     | 1:CA:881:G:H5'     | 2.20        | 0.42     |
| 1:CA:1200:C:O5'    | 1:CA:1201:A:H3'    | 2.20        | 0.42     |
| 9:CJ:87:LEU:N      | 9:CJ:87:LEU:HD13   | 2.34        | 0.42     |
| 23:DB:2000:C:O2'   | 23:DB:2001:C:H5'   | 2.19        | 0.42     |
| 23:BB:1063:G:O2'   | 23:BB:1064:C:H5'   | 2.20        | 0.42     |
| 23:BB:816:C:O2'    | 23:BB:817:C:H5'    | 2.20        | 0.42     |
| 37:BL:136:GLU:HA   | 37:BL:140:GLY:N    | 2.35        | 0.42     |
| 23:BB:1683:U:H2'   | 23:BB:1684:G:H8    | 1.83        | 0.42     |
| 1:AA:130:A:H1'     | 1:AA:263:A:O2'     | 2.20        | 0.42     |
| 23:DB:325:G:H2'    | 23:DB:326:G:C8     | 2.55        | 0.42     |
| 1:CA:586:C:C5'     | 7:CH:81:GLY:HA2    | 2.48        | 0.42     |
| 5:CF:18:VAL:N      | 5:CF:19:PRO:HD2    | 2.35        | 0.42     |
| 29:BE:106:LYS:O    | 29:BE:110:SER:HB2  | 2.20        | 0.42     |
| 25:BC:221:GLY:O    | 25:BC:223:ALA:N    | 2.51        | 0.42     |
| 7:AH:29:SER:O      | 7:AH:30:LYS:C      | 2.58        | 0.42     |
| 37:BL:61:LEU:N     | 37:BL:61:LEU:HD12  | 2.35        | 0.42     |
| 23:BB:1720:U:C2'   | 23:BB:1721:G:H5'   | 2.49        | 0.42     |
| 38:DM:102:LEU:N    | 38:DM:102:LEU:HD22 | 2.35        | 0.42     |
| 4:CE:92:ARG:HB3    | 4:CE:92:ARG:NH1    | 2.35        | 0.42     |
| 23:DB:1397:U:H5''  | 23:DB:1398:C:H5    | 1.85        | 0.42     |
| 1:CA:103:U:H1'     | 1:CA:171:A:N1      | 2.35        | 0.42     |
| 23:BB:1846:G:N2    | 23:BB:1848:A:N6    | 2.68        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:77:G:H2'    | 23:DB:78:U:H6     | 1.85        | 0.42     |
| 23:DB:1748:C:H2'  | 23:DB:1749:A:C8   | 2.55        | 0.42     |
| 23:DB:337:C:H2'   | 23:DB:338:G:O4'   | 2.20        | 0.42     |
| 6:CG:120:ALA:HA   | 6:CG:123:LEU:HD12 | 2.02        | 0.42     |
| 9:AJ:21:ALA:O     | 9:AJ:25:ILE:HG13  | 2.19        | 0.42     |
| 23:BB:841:G:H2'   | 23:BB:842:U:C6    | 2.55        | 0.42     |
| 19:CT:14:GLU:O    | 19:CT:17:ARG:HB3  | 2.19        | 0.42     |
| 5:CF:45:ARG:NH2   | 17:CR:25:ILE:HD13 | 2.35        | 0.42     |
| 23:BB:285:G:H2'   | 23:BB:286:U:H6    | 1.84        | 0.42     |
| 23:BB:787:C:H5''  | 23:BB:788:A:H5'   | 2.02        | 0.42     |
| 1:AA:185:U:H2'    | 1:AA:186:C:C6     | 2.55        | 0.42     |
| 23:DB:957:C:N4    | 23:DB:2459:A:C8   | 2.88        | 0.42     |
| 32:D4:30:GLU:HA   | 32:D4:31:PRO:HD3  | 1.91        | 0.42     |
| 23:BB:1932:A:H2'  | 23:BB:1933:G:O4'  | 2.20        | 0.42     |
| 23:BB:88:G:C2'    | 23:BB:89:A:H5'    | 2.50        | 0.42     |
| 51:DZ:27:ARG:H    | 51:DZ:27:ARG:HG3  | 1.68        | 0.42     |
| 23:DB:1751:U:H2'  | 23:DB:1752:C:C5   | 2.54        | 0.42     |
| 23:BB:1410:G:H2'  | 23:BB:1411:U:C6   | 2.54        | 0.42     |
| 52:BW:50:VAL:HG23 | 52:BW:61:LYS:CE   | 2.49        | 0.42     |
| 25:DC:152:GLN:HA  | 25:DC:155:ARG:CD  | 2.49        | 0.42     |
| 25:DC:144:GLU:OE2 | 25:DC:188:ARG:HG3 | 2.20        | 0.42     |
| 1:CA:1093:A:P     | 6:CG:3:ARG:HH12   | 2.42        | 0.42     |
| 53:D6:80:GLU:CD   | 53:D6:99:LEU:HD13 | 2.40        | 0.42     |
| 53:D6:80:GLU:HA   | 53:D6:83:ILE:CG1  | 2.43        | 0.42     |
| 53:D6:89:GLY:O    | 53:D6:90:LEU:HG   | 2.20        | 0.42     |
| 53:B6:38:LEU:HD21 | 53:B6:88:LEU:HD22 | 2.02        | 0.42     |
| 23:DB:1420:A:C2'  | 23:DB:2211:A:H62  | 2.15        | 0.42     |
| 8:CI:21:LYS:HG3   | 8:CI:22:PRO:HD2   | 2.01        | 0.42     |
| 53:B6:76:LEU:HG   | 53:B6:94:ASN:OD1  | 2.19        | 0.42     |
| 41:BJ:26:GLY:C    | 41:BJ:28:LEU:N    | 2.74        | 0.42     |
| 41:DJ:34:ARG:O    | 41:DJ:38:GLY:N    | 2.53        | 0.42     |
| 1:AA:1148:U:H2'   | 1:AA:1149:C:O4'   | 2.20        | 0.42     |
| 8:AI:25:GLY:HA3   | 8:AI:57:VAL:HA    | 2.02        | 0.42     |
| 8:AI:56:MET:C     | 8:AI:58:GLU:N     | 2.73        | 0.42     |
| 8:AI:51:LEU:HB3   | 8:AI:56:MET:HB2   | 2.02        | 0.42     |
| 8:AI:6:TYR:C      | 8:AI:85:ALA:HB2   | 2.40        | 0.42     |
| 47:DF:40:GLY:O    | 47:DF:41:GLU:C    | 2.57        | 0.42     |
| 1:AA:599:C:O2'    | 1:AA:600:A:H5'    | 2.20        | 0.42     |
| 44:BQ:91:ARG:NH2  | 49:BR:11:GLN:O    | 2.53        | 0.42     |
| 51:BZ:51:VAL:HG12 | 51:BZ:52:SER:N    | 2.35        | 0.42     |
| 13:AN:68:ARG:HH12 | 13:AN:71:GLY:N    | 2.18        | 0.42     |
| 46:BU:85:ARG:HH11 | 46:BU:86:PHE:N    | 2.15        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BC:64:VAL:O    | 25:BC:102:TYR:O    | 2.38        | 0.42     |
| 43:BO:35:ILE:C    | 43:BO:36:TYR:HD2   | 2.23        | 0.42     |
| 47:BF:29:ARG:HH11 | 47:BF:29:ARG:HB2   | 1.85        | 0.42     |
| 40:DH:90:LEU:HD11 | 40:DH:146:VAL:HG11 | 2.01        | 0.42     |
| 40:DH:90:LEU:HD12 | 40:DH:90:LEU:N     | 2.21        | 0.42     |
| 25:BC:199:HIS:C   | 25:BC:201:LEU:H    | 2.23        | 0.42     |
| 45:BS:13:SER:HG   | 45:BS:16:LYS:HB2   | 1.85        | 0.42     |
| 29:BE:60:TRP:HB3  | 29:BE:61:ARG:H     | 1.42        | 0.42     |
| 23:DB:1187:G:OP1  | 49:DR:85:LYS:NZ    | 2.51        | 0.42     |
| 11:CL:49:ARG:HH12 | 11:CL:88:ASP:CB    | 2.33        | 0.42     |
| 23:DB:2267:A:C8   | 23:DB:2267:A:C4'   | 3.03        | 0.42     |
| 13:CN:80:ARG:HG2  | 13:CN:80:ARG:HH11  | 1.85        | 0.42     |
| 23:BB:546:U:H4'   | 23:BB:547:A:OP2    | 2.19        | 0.42     |
| 1:AA:1324:A:H2'   | 1:AA:1325:C:H6     | 1.84        | 0.42     |
| 23:BB:512:G:P     | 23:BB:1215:G:N2    | 2.92        | 0.42     |
| 11:CL:21:PRO:HG2  | 11:CL:94:TYR:OH    | 2.20        | 0.42     |
| 27:DK:99:ILE:HG12 | 27:DK:115:ILE:HG13 | 2.00        | 0.42     |
| 23:DB:2346:A:O4'  | 23:DB:2383:G:O4'   | 2.38        | 0.42     |
| 34:B3:23:HIS:ND1  | 34:B3:24:LYS:N     | 2.68        | 0.42     |
| 20:CB:103:TRP:CZ3 | 20:CB:107:ARG:HD2  | 2.53        | 0.42     |
| 4:AE:82:HIS:CD2   | 7:AH:95:MET:HG3    | 2.54        | 0.42     |
| 1:CA:109:A:H2'    | 1:CA:326:G:N2      | 2.35        | 0.42     |
| 2:CC:129:PHE:CE2  | 2:CC:156:LEU:HD13  | 2.55        | 0.42     |
| 2:CC:184:ASN:ND2  | 2:CC:185:THR:H     | 2.18        | 0.42     |
| 14:CO:81:LEU:O    | 14:CO:85:LEU:HD13  | 2.20        | 0.42     |
| 27:DK:73:ASP:OD2  | 27:DK:75:SER:HB3   | 2.19        | 0.42     |
| 19:CT:70:LYS:HA   | 19:CT:73:ARG:CZ    | 2.50        | 0.42     |
| 16:AQ:17:GLU:O    | 16:AQ:18:LYS:HB2   | 2.20        | 0.42     |
| 12:AM:2:ARG:HG3   | 12:AM:5:GLY:HA2    | 2.02        | 0.42     |
| 4:AE:61:LYS:NZ    | 4:AE:61:LYS:HB3    | 2.35        | 0.42     |
| 23:DB:1727:C:H2'  | 23:DB:1728:C:O4'   | 2.20        | 0.42     |
| 37:DL:47:ARG:NH2  | 37:DL:47:ARG:HB3   | 2.35        | 0.42     |
| 1:CA:1026:G:O2'   | 1:CA:1027:C:H5'    | 2.20        | 0.42     |
| 1:AA:408:A:OP1    | 3:AD:109:THR:OG1   | 2.36        | 0.42     |
| 39:BX:13:GLU:OE2  | 39:BX:13:GLU:HA    | 2.20        | 0.42     |
| 23:BB:96:C:H4'    | 39:BX:41:HIS:ND1   | 2.35        | 0.42     |
| 2:AC:65:VAL:HG21  | 2:AC:90:VAL:HG11   | 2.02        | 0.42     |
| 2:CC:49:ALA:O     | 2:CC:50:SER:HB2    | 2.20        | 0.42     |
| 19:AT:56:ILE:O    | 19:AT:60:GLN:HG2   | 2.20        | 0.42     |
| 52:BW:44:PHE:HB3  | 52:BW:78:PHE:CE1   | 2.54        | 0.42     |
| 23:BB:1927:A:H2'  | 23:BB:1928:A:C8    | 2.55        | 0.42     |
| 1:AA:481:G:O2'    | 1:AA:482:A:H8      | 2.03        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:877:A:N6    | 23:DB:898:C:C2    | 2.88        | 0.42     |
| 31:D0:8:THR:HG23  | 31:D0:10:SER:HB3  | 2.02        | 0.42     |
| 1:AA:828:U:O2'    | 20:AB:24:PRO:HB3  | 2.18        | 0.42     |
| 23:BB:1318:U:H2'  | 23:BB:1319:C:C6   | 2.55        | 0.42     |
| 23:BB:1213:A:C6   | 23:BB:1237:A:H1'  | 2.53        | 0.42     |
| 23:BB:1237:A:H2'  | 23:BB:1237:A:N3   | 2.35        | 0.42     |
| 34:D3:44:ARG:N    | 34:D3:45:PRO:CD   | 2.83        | 0.42     |
| 27:BK:70:ARG:CB   | 27:BK:70:ARG:HH11 | 2.33        | 0.42     |
| 23:DB:690:G:N3    | 25:DC:42:ARG:NH2  | 2.68        | 0.42     |
| 5:CF:81:ASN:O     | 5:CF:83:ALA:N     | 2.53        | 0.42     |
| 23:DB:2737:G:H2'  | 23:DB:2738:A:H8   | 1.83        | 0.42     |
| 23:DB:1047:G:O2'  | 23:DB:1109:C:N4   | 2.53        | 0.42     |
| 24:DI:140:GLU:CD  | 24:DI:140:GLU:H   | 2.23        | 0.42     |
| 28:BP:104:GLY:O   | 28:BP:106:ALA:N   | 2.45        | 0.42     |
| 5:CF:18:VAL:HG21  | 5:CF:58:HIS:CE1   | 2.54        | 0.42     |
| 29:BE:102:ARG:NH2 | 29:BE:102:ARG:HG3 | 2.35        | 0.42     |
| 38:DM:77:PRO:O    | 38:DM:78:LEU:O    | 2.38        | 0.42     |
| 1:AA:728:A:H2'    | 1:AA:729:A:C8     | 2.55        | 0.42     |
| 5:AF:18:VAL:N     | 5:AF:19:PRO:HD2   | 2.35        | 0.42     |
| 23:DB:1674:G:N2   | 23:DB:1677:A:N1   | 2.67        | 0.42     |
| 19:AT:14:GLU:O    | 19:AT:17:ARG:HB3  | 2.20        | 0.42     |
| 23:BB:2530:A:H3'  | 48:BG:156:TYR:OH  | 2.20        | 0.42     |
| 1:AA:993:G:H2'    | 1:AA:995:C:H41    | 1.84        | 0.42     |
| 23:DB:70:G:O4'    | 23:DB:73:A:H1'    | 2.19        | 0.42     |
| 9:AJ:26:VAL:O     | 9:AJ:30:LYS:HG3   | 2.19        | 0.42     |
| 41:BJ:75:TYR:HD1  | 41:BJ:86:GLN:HB3  | 1.84        | 0.42     |
| 20:CB:130:LYS:H   | 20:CB:130:LYS:HG2 | 1.51        | 0.42     |
| 48:DG:28:LYS:HB2  | 48:DG:28:LYS:HE2  | 1.91        | 0.42     |
| 23:DB:1891:G:H2'  | 23:DB:1892:C:H6   | 1.85        | 0.42     |
| 23:DB:1359:A:H2'  | 23:DB:1360:G:O4'  | 2.20        | 0.42     |
| 2:AC:111:ASP:O    | 2:AC:115:VAL:HG23 | 2.20        | 0.42     |
| 2:AC:114:LEU:O    | 2:AC:115:VAL:C    | 2.58        | 0.42     |
| 1:AA:894:G:H2'    | 1:AA:895:G:H8     | 1.85        | 0.42     |
| 1:CA:1262:C:H2'   | 1:CA:1263:C:O4'   | 2.20        | 0.42     |
| 8:AI:112:ARG:HH22 | 9:AJ:64:GLN:HE22  | 1.67        | 0.42     |
| 1:AA:582:C:O2'    | 1:AA:583:A:H5'    | 2.19        | 0.42     |
| 52:DW:12:GLY:O    | 52:DW:13:ARG:HB2  | 2.19        | 0.42     |
| 1:CA:775:G:O2'    | 1:CA:776:G:H5'    | 2.19        | 0.42     |
| 23:DB:566:U:H2'   | 23:DB:567:U:C6    | 2.55        | 0.42     |
| 1:CA:1119:C:OP2   | 8:CI:10:ARG:NH2   | 2.52        | 0.42     |
| 44:DQ:78:PHE:CZ   | 44:DQ:82:LEU:HD11 | 2.55        | 0.42     |
| 23:BB:2434:A:H2'  | 23:BB:2434:A:H8   | 1.72        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 46:DU:23:LYS:H    | 46:DU:23:LYS:HD2   | 1.85        | 0.42     |
| 8:AI:30:ASN:HD22  | 8:AI:65:THR:HA     | 1.84        | 0.42     |
| 3:CD:102:TYR:HE1  | 3:CD:108:ALA:O     | 2.02        | 0.42     |
| 52:DW:28:GLU:HB2  | 52:DW:31:LEU:HD21  | 2.02        | 0.42     |
| 48:DG:93:TYR:HE1  | 48:DG:160:GLY:HA2  | 1.84        | 0.42     |
| 16:CQ:7:LEU:O     | 16:CQ:60:ILE:HD13  | 2.20        | 0.42     |
| 53:D6:61:PRO:CD   | 53:D6:66:LEU:HA    | 2.48        | 0.42     |
| 22:DA:42:C:O2'    | 47:DF:91:ARG:NH1   | 2.53        | 0.42     |
| 41:DJ:41:LYS:O    | 44:DQ:66:ALA:HB1   | 2.20        | 0.42     |
| 49:DR:5:PHE:CD1   | 49:DR:5:PHE:N      | 2.88        | 0.42     |
| 8:AI:56:MET:O     | 8:AI:58:GLU:N      | 2.45        | 0.42     |
| 8:AI:37:TYR:HE2   | 8:AI:74:GLN:HG2    | 1.85        | 0.42     |
| 41:DJ:59:ALA:C    | 41:DJ:61:LYS:N     | 2.73        | 0.42     |
| 47:DF:42:ALA:HB1  | 47:DF:46:LYS:HZ3   | 1.85        | 0.42     |
| 47:DF:78:ILE:N    | 47:DF:78:ILE:CD1   | 2.83        | 0.42     |
| 41:BJ:43:GLU:O    | 41:BJ:44:TYR:C     | 2.57        | 0.42     |
| 23:BB:2200:C:OP1  | 51:BZ:37:ARG:N     | 2.53        | 0.42     |
| 51:BZ:32:ASN:C    | 51:BZ:33:LEU:HD12  | 2.41        | 0.42     |
| 25:BC:109:LEU:N   | 25:BC:109:LEU:CD2  | 2.82        | 0.42     |
| 33:B1:8:ILE:CG2   | 33:B1:51:ALA:HA    | 2.50        | 0.42     |
| 23:DB:1060:U:H5   | 24:DI:131:THR:HG22 | 1.82        | 0.42     |
| 23:BB:1059:G:H2'  | 23:BB:1060:U:C6    | 2.54        | 0.42     |
| 47:BF:134:GLN:C   | 47:BF:136:ILE:N    | 2.73        | 0.42     |
| 42:DN:55:ALA:HA   | 42:DN:80:PHE:CD1   | 2.55        | 0.42     |
| 1:CA:947:G:OP1    | 12:CM:106:ARG:HB3  | 2.20        | 0.42     |
| 4:CE:35:LEU:HD22  | 4:CE:133:ILE:HA    | 2.02        | 0.42     |
| 18:AS:50:VAL:HG22 | 18:AS:70:LEU:HD23  | 2.01        | 0.42     |
| 32:B4:2:LYS:CG    | 32:B4:4:ARG:HE     | 2.23        | 0.42     |
| 9:AJ:51:VAL:HG22  | 13:AN:80:ARG:HB2   | 1.99        | 0.42     |
| 53:D6:177:GLU:O   | 53:D6:180:GLU:HB3  | 2.19        | 0.42     |
| 53:D6:18:LEU:HD21 | 53:D6:171:LYS:CG   | 2.50        | 0.42     |
| 23:DB:972:A:C3'   | 23:DB:973:A:H5"    | 2.38        | 0.42     |
| 23:DB:974:G:P     | 49:DR:78:ARG:HD3   | 2.59        | 0.42     |
| 32:B4:36:ARG:O    | 32:B4:37:GLN:C     | 2.58        | 0.42     |
| 1:AA:1288:A:H2    | 1:AA:1371:G:N3     | 2.17        | 0.42     |
| 35:DV:40:ILE:N    | 35:DV:40:ILE:CD1   | 2.83        | 0.42     |
| 9:CJ:5:ARG:HD3    | 9:CJ:79:PRO:HG3    | 2.02        | 0.42     |
| 43:BO:67:ASN:H    | 43:BO:70:ALA:HB3   | 1.85        | 0.42     |
| 42:DN:69:ARG:H    | 42:DN:69:ARG:HD3   | 1.84        | 0.42     |
| 49:BR:4:VAL:HG23  | 49:BR:39:LEU:N     | 2.31        | 0.42     |
| 7:AH:45:ILE:HD13  | 7:AH:60:LEU:HD11   | 2.02        | 0.42     |
| 23:BB:1428:C:H2'  | 23:BB:1569:A:OP2   | 2.20        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:88:U:O2'     | 1:AA:89:U:C6      | 2.72        | 0.42     |
| 23:BB:116:C:C4    | 23:BB:117:G:C5    | 3.08        | 0.42     |
| 34:B3:31:ILE:HD11 | 34:B3:34:LYS:CD   | 2.47        | 0.42     |
| 1:AA:34:C:H2'     | 1:AA:35:G:C8      | 2.54        | 0.42     |
| 1:CA:191:G:H2'    | 1:CA:192:A:C8     | 2.54        | 0.42     |
| 10:AK:30:ILE:HG13 | 10:AK:30:ILE:O    | 2.18        | 0.42     |
| 43:BO:52:SER:C    | 43:BO:54:VAL:H    | 2.23        | 0.42     |
| 23:DB:1139:G:H2'  | 23:DB:1140:C:H6   | 1.85        | 0.42     |
| 3:CD:104:MET:HE3  | 3:CD:170:LEU:HD13 | 2.02        | 0.42     |
| 23:BB:2343:U:H2'  | 23:BB:2344:U:C6   | 2.55        | 0.42     |
| 39:BX:18:LEU:O    | 39:BX:22:LEU:HB3  | 2.20        | 0.42     |
| 37:BL:47:ARG:HB3  | 37:BL:47:ARG:NH2  | 2.35        | 0.42     |
| 1:CA:782:A:N6     | 1:CA:801:U:C5     | 2.87        | 0.42     |
| 1:CA:832:G:O2'    | 1:CA:833:G:H5'    | 2.19        | 0.42     |
| 23:DB:1176:U:O5'  | 23:DB:1176:U:H6   | 2.03        | 0.42     |
| 23:DB:2135:A:H61  | 23:DB:2156:G:C2'  | 2.33        | 0.42     |
| 50:DT:54:GLU:HG2  | 50:DT:90:GLY:HA3  | 2.02        | 0.42     |
| 45:DS:83:LYS:O    | 45:DS:84:ARG:NE   | 2.52        | 0.42     |
| 47:DF:19:PHE:CZ   | 47:DF:164:GLU:HG2 | 2.54        | 0.42     |
| 23:BB:377:G:O2'   | 23:BB:378:C:H5'   | 2.20        | 0.42     |
| 10:CK:110:THR:CG2 | 21:CU:4:LYS:HA    | 2.48        | 0.42     |
| 50:DT:73:ARG:HB3  | 50:DT:73:ARG:NH2  | 2.34        | 0.42     |
| 1:AA:370:C:H2'    | 1:AA:371:A:H8     | 1.85        | 0.42     |
| 23:BB:1064:C:C4'  | 24:BI:90:GLY:HA2  | 2.49        | 0.42     |
| 25:BC:61:TYR:CA   | 25:BC:85:ASN:HD21 | 2.31        | 0.42     |
| 23:DB:2231:U:H2'  | 23:DB:2232:C:C6   | 2.55        | 0.42     |
| 23:DB:508:A:O2'   | 23:DB:509:C:OP1   | 2.34        | 0.42     |
| 51:BZ:65:ASP:O    | 51:BZ:69:ALA:N    | 2.52        | 0.42     |
| 43:BO:9:ARG:HG3   | 43:BO:10:ARG:H    | 1.85        | 0.42     |
| 25:BC:53:ILE:O    | 25:BC:53:ILE:HG23 | 2.20        | 0.42     |
| 23:BB:818:G:C6    | 23:BB:1187:G:H2'  | 2.55        | 0.42     |
| 1:CA:747:A:H2'    | 1:CA:748:G:O4'    | 2.19        | 0.42     |
| 23:BB:2411:A:H2'  | 23:BB:2412:A:C8   | 2.55        | 0.42     |
| 1:CA:692:U:O4     | 10:CK:53:GLY:HA2  | 2.19        | 0.42     |
| 23:DB:2512:C:OP2  | 26:DD:128:ARG:HD2 | 2.20        | 0.42     |
| 1:AA:1508:A:H2'   | 1:AA:1509:C:C6    | 2.55        | 0.42     |
| 22:DA:49:C:OP1    | 43:DO:101:GLY:HA3 | 2.19        | 0.42     |
| 23:DB:2815:C:H2'  | 23:DB:2816:G:C8   | 2.53        | 0.42     |
| 23:DB:1745:A:H2'  | 23:DB:1746:A:C8   | 2.55        | 0.42     |
| 24:DI:99:LYS:HB2  | 24:DI:140:GLU:OE1 | 2.19        | 0.42     |
| 23:BB:1476:U:O2'  | 23:BB:1477:A:H8   | 2.02        | 0.42     |
| 23:BB:1883:U:H2'  | 23:BB:1884:G:C1'  | 2.50        | 0.42     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1013:C:H2'  | 23:BB:1014:A:C8    | 2.55        | 0.42     |
| 6:CG:152:HIS:O    | 6:CG:153:TYR:C     | 2.58        | 0.42     |
| 22:BA:35:C:H2'    | 22:BA:36:C:H5'     | 2.00        | 0.42     |
| 23:BB:564:C:H1'   | 44:BQ:36:GLN:OE1   | 2.20        | 0.42     |
| 23:DB:423:A:H5''  | 23:DB:424:G:C5'    | 2.50        | 0.42     |
| 6:AG:71:THR:O     | 6:AG:89:GLU:HA     | 2.20        | 0.42     |
| 46:BU:14:THR:O    | 46:BU:18:LYS:HA    | 2.20        | 0.42     |
| 23:DB:2653:U:H3'  | 23:DB:2654:A:H2'   | 2.02        | 0.42     |
| 17:AR:22:TYR:CE1  | 17:AR:23:LYS:HG3   | 2.55        | 0.42     |
| 23:BB:1313:U:H4'  | 23:BB:1332:G:H4'   | 2.02        | 0.42     |
| 23:BB:1249:U:H4'  | 44:BQ:3:VAL:HG11   | 2.02        | 0.42     |
| 28:DP:44:GLY:HA3  | 28:DP:60:VAL:HG12  | 2.02        | 0.42     |
| 23:DB:246:C:C2'   | 23:DB:247:G:H5'    | 2.50        | 0.42     |
| 23:BB:553:G:C2'   | 23:BB:554:U:H5'    | 2.50        | 0.42     |
| 1:CA:771:G:H2'    | 1:CA:772:U:C6      | 2.55        | 0.42     |
| 23:BB:2508:G:O3'  | 23:BB:2555:U:H5'   | 2.20        | 0.42     |
| 23:BB:2514:U:H2'  | 23:BB:2515:C:C6    | 2.55        | 0.42     |
| 26:BD:35:THR:OG1  | 26:BD:49:GLN:HG2   | 2.20        | 0.42     |
| 43:BO:56:LYS:O    | 43:BO:60:GLU:HG2   | 2.20        | 0.42     |
| 23:BB:1516:G:O2'  | 23:BB:1517:G:H5'   | 2.19        | 0.42     |
| 1:CA:197:A:H1'    | 1:CA:198:G:C1'     | 2.50        | 0.42     |
| 23:BB:389:G:O2'   | 23:BB:390:U:H5'    | 2.20        | 0.42     |
| 28:BP:36:LYS:HD3  | 28:BP:36:LYS:HA    | 1.85        | 0.42     |
| 23:DB:2614:A:O4'  | 31:D0:1:ALA:HB3    | 2.20        | 0.42     |
| 46:BU:23:LYS:HD2  | 46:BU:23:LYS:H     | 1.85        | 0.42     |
| 14:AO:17:ARG:HA   | 14:AO:17:ARG:NH1   | 2.35        | 0.42     |
| 16:CQ:82:VAL:HG13 | 16:CQ:82:VAL:O     | 2.19        | 0.42     |
| 23:BB:502:A:N6    | 23:BB:505:A:N1     | 2.67        | 0.42     |
| 5:AF:72:ASP:HA    | 5:AF:75:GLU:OE1    | 2.19        | 0.42     |
| 48:DG:50:THR:HG22 | 48:DG:51:PHE:N     | 2.35        | 0.41     |
| 41:DJ:43:GLU:O    | 41:DJ:44:TYR:C     | 2.57        | 0.41     |
| 44:DQ:84:LYS:O    | 44:DQ:86:SER:N     | 2.53        | 0.41     |
| 23:DB:825:A:O2'   | 37:DL:54:GLN:NE2   | 2.52        | 0.41     |
| 24:DI:108:ILE:CG2 | 24:DI:128:ILE:HD13 | 2.49        | 0.41     |
| 47:BF:2:LYS:CD    | 47:BF:100:GLU:HG2  | 2.48        | 0.41     |
| 25:BC:180:MET:HB2 | 25:BC:268:ARG:H    | 1.85        | 0.41     |
| 1:CA:813:U:O2     | 1:CA:813:U:H2'     | 2.20        | 0.41     |
| 45:BS:13:SER:HB3  | 45:BS:16:LYS:HE3   | 2.01        | 0.41     |
| 20:CB:46:VAL:N    | 20:CB:47:PRO:CD    | 2.83        | 0.41     |
| 1:AA:1320:C:C2    | 18:AS:71:GLY:HA3   | 2.55        | 0.41     |
| 23:BB:674:G:H5''  | 29:BE:71:GLY:N     | 2.34        | 0.41     |
| 23:DB:2893:A:H4'  | 23:DB:2894:G:H5'   | 2.01        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 38:DM:64:TRP:HE3   | 38:DM:104:GLU:O    | 2.03        | 0.41     |
| 31:B0:41:HIS:O     | 31:B0:42:ILE:O     | 2.38        | 0.41     |
| 23:DB:2848:G:N3    | 23:DB:2849:U:C5    | 2.88        | 0.41     |
| 22:DA:75:G:H2'     | 22:DA:76:G:H8      | 1.85        | 0.41     |
| 23:BB:2768:U:H2'   | 23:BB:2769:U:O4'   | 2.20        | 0.41     |
| 45:BS:73:LYS:HA    | 45:BS:73:LYS:HD2   | 1.83        | 0.41     |
| 25:BC:210:ALA:O    | 25:BC:213:ARG:HB3  | 2.20        | 0.41     |
| 23:BB:844:A:C2     | 23:BB:845:A:N1     | 2.88        | 0.41     |
| 31:D0:48:TYR:CZ    | 31:D0:49:ARG:HG3   | 2.55        | 0.41     |
| 37:DL:101:ILE:HG22 | 37:DL:102:GLY:N    | 2.35        | 0.41     |
| 26:DD:69:ALA:CA    | 26:DD:73:VAL:HB    | 2.50        | 0.41     |
| 29:DE:132:LYS:O    | 29:DE:135:ALA:HB3  | 2.19        | 0.41     |
| 29:DE:157:LEU:HD12 | 29:DE:157:LEU:O    | 2.20        | 0.41     |
| 2:CC:133:MET:HE1   | 2:CC:165:GLU:HG3   | 2.02        | 0.41     |
| 23:DB:362:A:H3'    | 23:DB:363:G:H8     | 1.85        | 0.41     |
| 23:DB:182:A:H2'    | 23:DB:183:C:C6     | 2.54        | 0.41     |
| 5:AF:98:GLU:HG2    | 5:AF:99:ALA:H      | 1.81        | 0.41     |
| 25:DC:30:ALA:O     | 25:DC:32:LEU:N     | 2.51        | 0.41     |
| 23:BB:1795:C:O2'   | 23:BB:1796:U:H5'   | 2.20        | 0.41     |
| 11:AL:107:LYS:HD2  | 11:AL:107:LYS:O    | 2.20        | 0.41     |
| 11:AL:98:ARG:HB2   | 11:AL:116:TYR:HA   | 2.01        | 0.41     |
| 35:DV:31:TYR:CB    | 35:DV:37:PRO:HG3   | 2.48        | 0.41     |
| 36:D2:10:LEU:O     | 36:D2:14:ARG:HG2   | 2.20        | 0.41     |
| 39:DX:44:LYS:HA    | 39:DX:44:LYS:HD2   | 1.87        | 0.41     |
| 1:CA:549:C:H2'     | 1:CA:550:G:H8      | 1.84        | 0.41     |
| 40:DH:62:LEU:HG    | 40:DH:66:ASN:HD22  | 1.83        | 0.41     |
| 2:AC:78:LYS:HG3    | 2:AC:81:GLU:HB3    | 2.01        | 0.41     |
| 23:DB:1685:C:H2'   | 23:DB:1686:C:H6    | 1.85        | 0.41     |
| 1:CA:1009:U:C2'    | 1:CA:1009:U:O2     | 2.68        | 0.41     |
| 23:BB:2028:U:H2'   | 23:BB:2029:G:O4'   | 2.20        | 0.41     |
| 2:CC:52:SER:HB3    | 2:CC:114:LEU:HG    | 2.02        | 0.41     |
| 23:BB:509:C:H5''   | 23:BB:510:C:OP2    | 2.20        | 0.41     |
| 23:BB:1562:U:H2'   | 23:BB:1563:U:H6    | 1.84        | 0.41     |
| 23:BB:1563:U:O2'   | 23:BB:1564:C:H5'   | 2.20        | 0.41     |
| 43:BO:28:VAL:HG12  | 43:BO:93:ASP:O     | 2.20        | 0.41     |
| 23:BB:1686:C:H2'   | 23:BB:1687:G:O4'   | 2.19        | 0.41     |
| 4:AE:56:PRO:HG2    | 4:AE:57:ALA:H      | 1.85        | 0.41     |
| 23:DB:2376:A:H1'   | 43:DO:111:ARG:HH12 | 1.84        | 0.41     |
| 23:BB:2527:C:O4'   | 32:B4:1:MET:N      | 2.52        | 0.41     |
| 23:BB:577:G:O2'    | 23:BB:1254:A:OP1   | 2.36        | 0.41     |
| 23:DB:2569:G:C2    | 23:DB:2570:G:C8    | 3.07        | 0.41     |
| 23:BB:2730:C:H2'   | 23:BB:2731:G:C8    | 2.55        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:1115:U:H1'   | 13:CN:100:TRP:O    | 2.20        | 0.41     |
| 23:BB:779:U:H2'   | 23:BB:780:G:H8     | 1.84        | 0.41     |
| 23:DB:107:G:C2    | 23:DB:108:G:C8     | 3.09        | 0.41     |
| 23:DB:1639:C:O2'  | 23:DB:1640:A:H5'   | 2.20        | 0.41     |
| 1:AA:628:G:H2'    | 1:AA:629:A:H8      | 1.83        | 0.41     |
| 1:AA:818:G:H3'    | 1:AA:819:A:C5'     | 2.50        | 0.41     |
| 23:BB:814:C:H2'   | 23:BB:815:C:H6     | 1.85        | 0.41     |
| 2:CC:10:ARG:HG3   | 2:CC:10:ARG:HH11   | 1.85        | 0.41     |
| 1:CA:543:U:H2'    | 1:CA:544:G:H8      | 1.84        | 0.41     |
| 1:AA:811:C:H4'    | 1:AA:900:A:H62     | 1.83        | 0.41     |
| 17:AR:22:TYR:HA   | 17:AR:57:ALA:HB1   | 2.02        | 0.41     |
| 9:AJ:10:LEU:HD23  | 9:AJ:98:VAL:HG12   | 2.00        | 0.41     |
| 23:DB:2322:A:N6   | 23:DB:2333:A:N6    | 2.68        | 0.41     |
| 23:DB:208:C:H2'   | 23:DB:209:C:C6     | 2.54        | 0.41     |
| 23:DB:1693:U:H1'  | 25:DC:13:ARG:NH2   | 2.35        | 0.41     |
| 23:DB:553:G:C2'   | 23:DB:554:U:H5'    | 2.50        | 0.41     |
| 23:DB:823:C:H2'   | 23:DB:824:U:C6     | 2.55        | 0.41     |
| 22:BA:54:G:O2'    | 22:BA:55:U:H5'     | 2.20        | 0.41     |
| 23:BB:2745:C:H1'  | 48:BG:142:GLN:OE1  | 2.19        | 0.41     |
| 10:AK:108:ASN:ND2 | 21:AU:6:ARG:HB2    | 2.35        | 0.41     |
| 23:DB:1764:C:H2'  | 23:DB:1765:U:H6    | 1.86        | 0.41     |
| 23:BB:2046:G:H1'  | 31:B0:18:HIS:CD2   | 2.55        | 0.41     |
| 23:DB:2863:C:O2'  | 23:DB:2864:G:H5'   | 2.19        | 0.41     |
| 1:AA:1047:G:H21   | 1:AA:1215:G:C4'    | 2.33        | 0.41     |
| 4:AE:36:THR:O     | 4:AE:48:GLY:N      | 2.52        | 0.41     |
| 23:DB:1098:A:H3'  | 24:DI:3:LYS:HB3    | 2.01        | 0.41     |
| 52:BW:67:LYS:O    | 52:BW:68:PHE:CB    | 2.61        | 0.41     |
| 25:BC:121:ALA:HB3 | 25:BC:129:LEU:HG   | 2.02        | 0.41     |
| 52:DW:17:ALA:O    | 52:DW:18:LYS:HD2   | 2.19        | 0.41     |
| 23:DB:1823:G:O2'  | 23:DB:1824:G:H5'   | 2.19        | 0.41     |
| 25:DC:109:LEU:H   | 25:DC:109:LEU:HD23 | 1.85        | 0.41     |
| 48:DG:42:VAL:HA   | 48:DG:50:THR:O     | 2.20        | 0.41     |
| 47:DF:92:GLY:O    | 47:DF:95:MET:HB3   | 2.20        | 0.41     |
| 8:CI:26:LYS:HB2   | 8:CI:61:ASP:CB     | 2.49        | 0.41     |
| 41:DJ:6:ALA:CB    | 41:DJ:45:THR:HG21  | 2.50        | 0.41     |
| 20:CB:187:ASP:O   | 20:CB:189:ASN:N    | 2.53        | 0.41     |
| 35:DV:61:LEU:HD11 | 35:DV:74:ALA:HB2   | 2.02        | 0.41     |
| 29:DE:62:GLN:HG2  | 29:DE:63:LYS:HG3   | 2.02        | 0.41     |
| 23:DB:2674:G:H2'  | 23:DB:2675:A:C8    | 2.55        | 0.41     |
| 50:BT:53:VAL:HG12 | 50:BT:54:GLU:N     | 2.35        | 0.41     |
| 41:BJ:4:PHE:O     | 41:BJ:44:TYR:CZ    | 2.73        | 0.41     |
| 44:BQ:94:LEU:C    | 44:BQ:96:ASP:H     | 2.22        | 0.41     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 3:CD:160:LEU:HA    | 3:CD:163:GLN:HG3  | 2.03        | 0.41     |
| 51:BZ:77:LYS:CG    | 51:BZ:78:TYR:N    | 2.83        | 0.41     |
| 3:AD:29:THR:HG22   | 3:AD:30:LYS:HD3   | 2.01        | 0.41     |
| 30:BY:16:LEU:HD23  | 30:BY:19:HIS:CD2  | 2.55        | 0.41     |
| 46:DU:73:ASN:O     | 46:DU:75:ALA:N    | 2.53        | 0.41     |
| 1:CA:948:C:H2'     | 1:CA:949:A:H8     | 1.85        | 0.41     |
| 18:CS:36:ARG:H     | 18:CS:36:ARG:HG2  | 1.60        | 0.41     |
| 18:CS:48:ILE:HD11  | 18:CS:61:VAL:HG23 | 2.02        | 0.41     |
| 1:AA:1318:A:H5''   | 1:AA:1319:A:OP2   | 2.20        | 0.41     |
| 18:AS:48:ILE:HD11  | 18:AS:61:VAL:HG23 | 2.01        | 0.41     |
| 10:CK:34:THR:HB    | 10:CK:40:ALA:CA   | 2.37        | 0.41     |
| 8:AI:87:MET:O      | 8:AI:87:MET:HE2   | 2.19        | 0.41     |
| 29:BE:58:LYS:CE    | 29:BE:58:LYS:H    | 2.33        | 0.41     |
| 10:CK:113:THR:HG21 | 21:CU:28:LEU:HD12 | 2.02        | 0.41     |
| 23:BB:1179:G:H2'   | 23:BB:1180:U:H6   | 1.84        | 0.41     |
| 3:CD:172:VAL:HG13  | 3:CD:172:VAL:O    | 2.20        | 0.41     |
| 15:AP:66:THR:HG22  | 15:AP:67:ILE:N    | 2.36        | 0.41     |
| 3:CD:138:PRO:C     | 3:CD:140:ASP:H    | 2.24        | 0.41     |
| 13:CN:26:LEU:HD23  | 13:CN:27:LYS:N    | 2.35        | 0.41     |
| 23:BB:45:G:H2'     | 23:BB:215:G:C5    | 2.55        | 0.41     |
| 22:DA:106:G:H2'    | 22:DA:107:G:O4'   | 2.20        | 0.41     |
| 22:DA:77:U:O2'     | 22:DA:78:A:H5'    | 2.20        | 0.41     |
| 27:BK:19:VAL:C     | 27:BK:41:ILE:HD11 | 2.40        | 0.41     |
| 42:BN:33:ILE:HA    | 42:BN:113:ILE:O   | 2.20        | 0.41     |
| 42:DN:65:LEU:HD11  | 42:DN:69:ARG:NH1  | 2.33        | 0.41     |
| 42:DN:33:ILE:HA    | 42:DN:113:ILE:O   | 2.19        | 0.41     |
| 40:BH:73:ASN:HD22  | 40:BH:74:ALA:N    | 2.13        | 0.41     |
| 49:DR:3:ALA:HB1    | 49:DR:59:ILE:HD13 | 2.01        | 0.41     |
| 1:CA:465:A:N3      | 1:CA:465:A:O4'    | 2.53        | 0.41     |
| 7:AH:49:LYS:HB3    | 7:AH:59:GLU:CB    | 2.42        | 0.41     |
| 26:DD:8:LYS:O      | 26:DD:9:VAL:HB    | 2.20        | 0.41     |
| 40:DH:70:GLU:OE1   | 40:DH:71:LYS:HG3  | 2.20        | 0.41     |
| 36:D2:39:ARG:HG3   | 36:D2:39:ARG:HH11 | 1.85        | 0.41     |
| 23:BB:1438:U:O2'   | 23:BB:1439:A:H5'  | 2.19        | 0.41     |
| 25:DC:157:ALA:HA   | 25:DC:194:VAL:CG2 | 2.50        | 0.41     |
| 20:AB:98:GLY:HA2   | 20:AB:101:THR:CG2 | 2.50        | 0.41     |
| 46:DU:10:VAL:HA    | 46:DU:70:ALA:O    | 2.21        | 0.41     |
| 40:DH:115:VAL:HB   | 40:DH:132:PHE:HD1 | 1.81        | 0.41     |
| 26:BD:114:LYS:HG2  | 26:BD:114:LYS:H   | 1.53        | 0.41     |
| 3:AD:96:ARG:HH12   | 3:AD:133:SER:CB   | 2.32        | 0.41     |
| 23:BB:718:A:H3'    | 23:BB:719:C:H6    | 1.85        | 0.41     |
| 23:BB:265:A:N6     | 23:BB:427:U:O2'   | 2.53        | 0.41     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 34:B3:32:LEU:HA    | 34:B3:35:LYS:HD2  | 2.01        | 0.41     |
| 35:DV:21:ARG:HE    | 35:DV:87:GLN:HB3  | 1.85        | 0.41     |
| 23:BB:275:C:H2'    | 23:BB:276:U:H5'   | 2.02        | 0.41     |
| 1:AA:489:C:O2'     | 1:AA:490:C:H5'    | 2.20        | 0.41     |
| 23:DB:1386:C:H1'   | 23:DB:1470:A:H1'  | 2.01        | 0.41     |
| 20:CB:185:ILE:HG23 | 20:CB:199:ILE:O   | 2.21        | 0.41     |
| 1:AA:8:A:O4'       | 4:AE:106:ALA:C    | 2.59        | 0.41     |
| 23:DB:2876:G:H2'   | 23:DB:2877:G:O4'  | 2.20        | 0.41     |
| 1:CA:499:A:O4'     | 1:CA:547:A:N6     | 2.53        | 0.41     |
| 23:BB:754:U:H2'    | 23:BB:755:U:H6    | 1.85        | 0.41     |
| 25:DC:115:ILE:HA   | 25:DC:127:ASN:OD1 | 2.20        | 0.41     |
| 23:BB:2376:A:H2'   | 23:BB:2377:A:O4'  | 2.20        | 0.41     |
| 52:BW:77:LYS:HB2   | 52:BW:77:LYS:HZ3  | 1.83        | 0.41     |
| 1:AA:448:A:H2'     | 1:AA:449:G:H8     | 1.83        | 0.41     |
| 1:CA:283:U:H2'     | 1:CA:284:C:H6     | 1.83        | 0.41     |
| 29:DE:1:MET:HB2    | 29:DE:16:GLU:HB2  | 2.02        | 0.41     |
| 1:AA:720:C:H5''    | 17:AR:40:PRO:HA   | 2.01        | 0.41     |
| 42:DN:59:SER:C     | 42:DN:61:ALA:N    | 2.72        | 0.41     |
| 1:CA:817:C:C2      | 1:CA:819:A:O4'    | 2.73        | 0.41     |
| 22:DA:17:C:H2'     | 22:DA:18:G:H8     | 1.85        | 0.41     |
| 23:BB:1505:A:H2'   | 23:BB:1506:U:H6   | 1.85        | 0.41     |
| 23:DB:528:A:H3'    | 23:DB:528:A:C8    | 2.54        | 0.41     |
| 23:DB:2812:G:H2'   | 23:DB:2813:A:O4'  | 2.20        | 0.41     |
| 23:DB:903:C:H2'    | 23:DB:904:G:C8    | 2.55        | 0.41     |
| 1:CA:665:A:H2'     | 1:CA:732:C:O2     | 2.21        | 0.41     |
| 23:BB:2889:C:H2'   | 23:BB:2890:G:C8   | 2.55        | 0.41     |
| 1:AA:691:G:H1'     | 1:AA:696:A:N6     | 2.35        | 0.41     |
| 4:CE:87:VAL:HG21   | 4:CE:92:ARG:HD2   | 2.01        | 0.41     |
| 23:BB:235:U:H2'    | 23:BB:236:C:H6    | 1.83        | 0.41     |
| 23:BB:2543:G:H8    | 23:BB:2543:G:H5'  | 1.84        | 0.41     |
| 46:BU:13:LEU:HD12  | 46:BU:68:ASN:C    | 2.40        | 0.41     |
| 48:BG:154:GLU:HB3  | 48:BG:158:GLY:H   | 1.85        | 0.41     |
| 23:DB:77:G:H2'     | 23:DB:78:U:C6     | 2.55        | 0.41     |
| 23:DB:1332:G:HO2'  | 23:DB:1609:A:H2   | 1.64        | 0.41     |
| 23:BB:1773:A:H2'   | 23:BB:1774:C:O4'  | 2.19        | 0.41     |
| 1:AA:251:G:N2      | 1:AA:266:G:O6     | 2.52        | 0.41     |
| 33:D1:28:THR:C     | 33:D1:30:PRO:HD3  | 2.40        | 0.41     |
| 23:DB:2010:G:O2'   | 23:DB:2011:U:H5'  | 2.20        | 0.41     |
| 6:AG:15:PRO:HG2    | 6:AG:16:LYS:H     | 1.85        | 0.41     |
| 1:AA:435:A:N3      | 1:AA:435:A:H2'    | 2.33        | 0.41     |
| 48:BG:28:LYS:HE2   | 48:BG:28:LYS:HB2  | 1.88        | 0.41     |
| 23:DB:1183:U:H2'   | 23:DB:1184:U:C6   | 2.56        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 49:DR:29:THR:HG23 | 49:DR:65:ALA:HA    | 2.02        | 0.41     |
| 23:DB:2903:U:O2   | 23:DB:2903:U:H2'   | 2.21        | 0.41     |
| 17:CR:25:ILE:HG13 | 17:CR:26:ALA:N     | 2.34        | 0.41     |
| 23:BB:1159:U:O2'  | 23:BB:1160:G:H5'   | 2.19        | 0.41     |
| 50:DT:7:LEU:C     | 50:DT:9:LYS:HD3    | 2.41        | 0.41     |
| 43:BO:15:ARG:HH21 | 43:BO:95:SER:CB    | 2.33        | 0.41     |
| 23:DB:1322:A:C2'  | 23:DB:1323:C:H5'   | 2.50        | 0.41     |
| 2:CC:178:ARG:HG2  | 2:CC:206:ILE:HA    | 2.02        | 0.41     |
| 15:AP:48:GLU:HG3  | 15:AP:49:GLY:N     | 2.35        | 0.41     |
| 2:CC:85:LYS:O     | 2:CC:89:VAL:HG23   | 2.19        | 0.41     |
| 1:AA:61:G:H2'     | 1:AA:62:U:C6       | 2.55        | 0.41     |
| 23:DB:1330:C:H2'  | 23:DB:1331:G:H8    | 1.85        | 0.41     |
| 1:AA:1401:G:H2'   | 1:AA:1402:C:O4'    | 2.19        | 0.41     |
| 23:DB:1084:A:H1'  | 23:DB:1106:G:H5'   | 2.01        | 0.41     |
| 14:AO:31:LEU:O    | 14:AO:34:ALA:HB3   | 2.19        | 0.41     |
| 33:D1:25:ASN:OD1  | 33:D1:27:ARG:HB2   | 2.20        | 0.41     |
| 1:CA:687:A:C2     | 1:CA:704:A:C5      | 3.08        | 0.41     |
| 1:CA:528:C:H41    | 11:CL:45:ASN:CG    | 2.23        | 0.41     |
| 23:DB:2779:U:OP1  | 23:DB:2780:G:H2'   | 2.20        | 0.41     |
| 1:AA:1262:C:H2'   | 1:AA:1263:C:O4'    | 2.20        | 0.41     |
| 1:AA:1173:U:H2'   | 1:AA:1174:G:C8     | 2.54        | 0.41     |
| 23:BB:2452:C:H2'  | 23:BB:2453:A:C8    | 2.54        | 0.41     |
| 25:BC:131:MET:C   | 25:BC:133:ASN:N    | 2.73        | 0.41     |
| 48:BG:10:VAL:CG2  | 48:BG:49:LEU:HD13  | 2.51        | 0.41     |
| 48:DG:96:ALA:O    | 48:DG:97:VAL:HB    | 2.21        | 0.41     |
| 26:BD:51:THR:HG22 | 26:BD:52:THR:H     | 1.83        | 0.41     |
| 53:D6:43:VAL:HG11 | 53:D6:79:ILE:HA    | 2.03        | 0.41     |
| 53:B6:68:VAL:CG2  | 53:B6:99:LEU:HD12  | 2.50        | 0.41     |
| 40:BH:90:LEU:HD22 | 40:BH:123:ARG:HA   | 2.03        | 0.41     |
| 1:CA:1287:A:N6    | 1:CA:1288:A:N6     | 2.67        | 0.41     |
| 41:BJ:32:LEU:HD22 | 41:BJ:122:LEU:HD11 | 2.02        | 0.41     |
| 23:DB:996:A:O3'   | 44:DQ:91:ARG:HG3   | 2.20        | 0.41     |
| 41:DJ:16:TYR:CD2  | 41:DJ:140:LEU:HD12 | 2.55        | 0.41     |
| 43:DO:35:ILE:O    | 43:DO:35:ILE:HG22  | 2.19        | 0.41     |
| 30:DY:7:THR:O     | 30:DY:54:VAL:HG12  | 2.20        | 0.41     |
| 50:BT:41:ALA:C    | 50:BT:43:ILE:N     | 2.73        | 0.41     |
| 41:BJ:34:ARG:O    | 41:BJ:38:GLY:N     | 2.53        | 0.41     |
| 12:CM:17:ALA:CB   | 12:CM:44:ILE:HG12  | 2.50        | 0.41     |
| 46:DU:73:ASN:HB3  | 46:DU:95:PHE:CD2   | 2.56        | 0.41     |
| 47:BF:141:ASP:O   | 47:BF:143:ASP:N    | 2.53        | 0.41     |
| 47:BF:3:LEU:HD11  | 47:BF:172:PHE:CE1  | 2.55        | 0.41     |
| 37:BL:79:LEU:CG   | 37:BL:112:LEU:HA   | 2.35        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 21:AU:3:ILE:CD1   | 21:AU:19:LYS:HA    | 2.47        | 0.41     |
| 31:B0:21:LEU:HB3  | 45:BS:23:LEU:HD21  | 2.03        | 0.41     |
| 23:DB:136:G:H2'   | 23:DB:137:U:C6     | 2.56        | 0.41     |
| 23:BB:811:U:C4    | 37:BL:21:ARG:NH2   | 2.88        | 0.41     |
| 38:DM:23:GLY:HA3  | 38:DM:66:ARG:NH1   | 2.35        | 0.41     |
| 1:AA:719:C:H2'    | 17:AR:38:ILE:HD13  | 2.02        | 0.41     |
| 17:AR:38:ILE:HG22 | 17:AR:58:ILE:HD13  | 2.00        | 0.41     |
| 23:DB:1032:A:OP1  | 32:D4:8:LYS:HG3    | 2.20        | 0.41     |
| 29:BE:188:MET:CE  | 29:BE:193:VAL:HG22 | 2.50        | 0.41     |
| 23:DB:981:A:H2'   | 23:DB:982:C:C5'    | 2.50        | 0.41     |
| 23:BB:2061:G:H5'' | 23:BB:2503:A:C2    | 2.55        | 0.41     |
| 17:CR:38:ILE:CG2  | 17:CR:58:ILE:HD13  | 2.51        | 0.41     |
| 26:DD:114:LYS:HE3 | 26:DD:116:LYS:CE   | 2.51        | 0.41     |
| 27:DK:72:PRO:O    | 27:DK:74:GLY:N     | 2.53        | 0.41     |
| 38:BM:64:TRP:O    | 38:BM:103:TYR:HA   | 2.21        | 0.41     |
| 31:D0:48:TYR:O    | 31:D0:50:GLY:N     | 2.52        | 0.41     |
| 27:BK:71:ARG:HD2  | 27:BK:106:GLU:OE2  | 2.19        | 0.41     |
| 11:CL:29:LYS:CB   | 11:CL:56:LEU:HD22  | 2.51        | 0.41     |
| 44:BQ:111:LYS:HE3 | 49:BR:48:LYS:NZ    | 2.36        | 0.41     |
| 44:DQ:105:PHE:HA  | 44:DQ:108:LEU:HD12 | 2.01        | 0.41     |
| 47:BF:163:GLU:O   | 47:BF:166:ARG:HB2  | 2.20        | 0.41     |
| 7:AH:47:ASP:CG    | 7:AH:48:PHE:N      | 2.70        | 0.41     |
| 36:B2:39:ARG:HH11 | 36:B2:39:ARG:HG3   | 1.86        | 0.41     |
| 36:D2:31:LEU:O    | 36:D2:34:ARG:N     | 2.53        | 0.41     |
| 46:BU:26:ASN:ND2  | 46:BU:34:ILE:HD12  | 2.33        | 0.41     |
| 9:AJ:5:ARG:N      | 9:AJ:76:ILE:O      | 2.53        | 0.41     |
| 23:BB:2621:G:OP1  | 26:BD:124:ARG:NH2  | 2.53        | 0.41     |
| 14:AO:71:LYS:HB2  | 14:AO:78:TYR:CD2   | 2.55        | 0.41     |
| 13:CN:3:GLN:OE1   | 13:CN:3:GLN:HA     | 2.21        | 0.41     |
| 16:CQ:17:GLU:O    | 16:CQ:18:LYS:HB2   | 2.21        | 0.41     |
| 6:AG:96:ASN:O     | 6:AG:100:MET:HG3   | 2.20        | 0.41     |
| 23:BB:297:G:H2'   | 23:BB:298:G:C8     | 2.55        | 0.41     |
| 1:CA:1314:C:N4    | 18:CS:3:SER:CB     | 2.83        | 0.41     |
| 23:DB:1867:G:O2'  | 23:DB:1868:C:H5'   | 2.21        | 0.41     |
| 23:DB:1402:U:H2'  | 23:DB:1403:A:O5'   | 2.20        | 0.41     |
| 43:DO:6:ALA:HB1   | 43:DO:10:ARG:HH11  | 1.86        | 0.41     |
| 43:DO:9:ARG:HA    | 43:DO:12:THR:OG1   | 2.20        | 0.41     |
| 23:DB:269:C:C2    | 23:DB:270:A:C8     | 3.08        | 0.41     |
| 50:BT:68:LYS:O    | 50:BT:74:ILE:HD12  | 2.20        | 0.41     |
| 23:DB:2064:C:H2'  | 23:DB:2065:C:H6    | 1.84        | 0.41     |
| 23:DB:1998:A:H2'  | 23:DB:1999:C:C6    | 2.54        | 0.41     |
| 40:DH:141:LYS:H   | 40:DH:141:LYS:CD   | 2.34        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:BB:1064:C:C1'  | 24:BI:90:GLY:HA2  | 2.50        | 0.41     |
| 53:B6:5:GLU:O     | 53:B6:8:ALA:HB3   | 2.20        | 0.41     |
| 23:DB:1152:C:H4'  | 44:DQ:76:SER:HA   | 2.02        | 0.41     |
| 43:BO:79:ALA:HB2  | 43:BO:110:ALA:HB1 | 2.02        | 0.41     |
| 34:B3:7:ARG:HH11  | 34:B3:7:ARG:CG    | 2.33        | 0.41     |
| 23:DB:237:C:O2'   | 23:DB:238:C:H5'   | 2.20        | 0.41     |
| 49:BR:58:VAL:O    | 49:BR:58:VAL:HG22 | 2.19        | 0.41     |
| 9:AJ:86:ALA:C     | 9:AJ:87:LEU:HD13  | 2.39        | 0.41     |
| 1:AA:152:A:H2'    | 1:AA:153:C:O4'    | 2.20        | 0.41     |
| 4:AE:98:ALA:HB3   | 4:AE:121:ASN:C    | 2.41        | 0.41     |
| 1:AA:908:A:O2'    | 1:AA:909:A:H5'    | 2.21        | 0.41     |
| 1:AA:1115:U:H1'   | 13:AN:100:TRP:O   | 2.20        | 0.41     |
| 23:BB:2195:U:O2'  | 23:BB:2196:C:H5'  | 2.21        | 0.41     |
| 23:DB:2096:C:H2'  | 23:DB:2096:C:O2   | 2.21        | 0.41     |
| 23:DB:256:A:H2'   | 23:DB:257:C:H6    | 1.84        | 0.41     |
| 23:BB:1748:C:H2'  | 23:BB:1749:A:C8   | 2.55        | 0.41     |
| 25:DC:226:PRO:HD3 | 25:DC:233:GLY:H   | 1.85        | 0.41     |
| 23:DB:1313:U:H4'  | 23:DB:1332:G:H4'  | 2.01        | 0.41     |
| 37:DL:118:THR:HA  | 37:DL:119:PRO:HD3 | 1.91        | 0.41     |
| 23:DB:2818:U:H4'  | 23:DB:2837:A:C4'  | 2.50        | 0.41     |
| 1:CA:266:G:O2'    | 1:CA:267:C:H3'    | 2.21        | 0.41     |
| 23:DB:111:A:O2'   | 23:DB:112:U:H5'   | 2.21        | 0.41     |
| 1:AA:207:C:O2'    | 1:AA:208:U:H5'    | 2.21        | 0.41     |
| 5:AF:45:ARG:NH2   | 17:AR:25:ILE:HD13 | 2.35        | 0.41     |
| 23:DB:729:G:C8    | 25:DC:206:LYS:HE3 | 2.55        | 0.41     |
| 14:CO:69:TYR:HA   | 14:CO:72:ARG:NH1  | 2.36        | 0.41     |
| 15:CP:8:ARG:CZ    | 15:CP:15:PRO:HB3  | 2.50        | 0.41     |
| 23:DB:765:C:H2'   | 23:DB:766:U:C6    | 2.55        | 0.41     |
| 1:AA:291:U:H2'    | 1:AA:292:G:C8     | 2.55        | 0.41     |
| 23:DB:1764:C:O2'  | 23:DB:1765:U:H5'  | 2.20        | 0.41     |
| 23:DB:95:A:H4'    | 39:DX:38:GLN:O    | 2.21        | 0.41     |
| 1:CA:1159:U:O4'   | 1:CA:1182:G:N2    | 2.53        | 0.41     |
| 2:AC:85:LYS:O     | 2:AC:89:VAL:HG23  | 2.19        | 0.41     |
| 1:AA:382:A:H2'    | 1:AA:383:A:C8     | 2.55        | 0.41     |
| 11:AL:35:ARG:HH21 | 11:AL:36:VAL:HG22 | 1.85        | 0.41     |
| 5:CF:72:ASP:HA    | 5:CF:75:GLU:OE1   | 2.21        | 0.41     |
| 49:BR:57:GLY:HA2  | 49:BR:102:SER:O   | 2.21        | 0.41     |
| 23:BB:2049:G:O2'  | 23:BB:2050:C:H5'  | 2.19        | 0.41     |
| 27:DK:21:CYS:HB2  | 27:DK:39:ILE:HG21 | 2.01        | 0.41     |
| 23:DB:2856:A:H2'  | 23:DB:2857:G:C8   | 2.55        | 0.41     |
| 23:BB:2901:C:H2'  | 23:BB:2901:C:O2   | 2.20        | 0.41     |
| 38:BM:90:GLU:HA   | 38:BM:90:GLU:OE1  | 2.19        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:282:A:N3     | 1:AA:282:A:H2'     | 2.36        | 0.41     |
| 38:BM:20:LEU:N    | 38:BM:20:LEU:HD22  | 2.35        | 0.41     |
| 17:CR:52:ARG:HG3  | 17:CR:52:ARG:HH11  | 1.86        | 0.41     |
| 23:DB:1932:A:H2'  | 23:DB:1933:G:O4'   | 2.20        | 0.41     |
| 23:DB:1758:U:O4   | 23:DB:2695:U:H4'   | 2.21        | 0.41     |
| 23:BB:2350:C:H2'  | 23:BB:2351:G:O4'   | 2.20        | 0.41     |
| 48:BG:42:VAL:HA   | 48:BG:50:THR:O     | 2.21        | 0.41     |
| 10:AK:70:ALA:C    | 10:AK:72:ALA:N     | 2.74        | 0.41     |
| 48:BG:102:ILE:CD1 | 48:BG:116:LEU:HD11 | 2.51        | 0.41     |
| 48:BG:83:THR:C    | 48:BG:84:LYS:HD3   | 2.41        | 0.41     |
| 23:DB:948:C:H1'   | 23:DB:984:A:N3     | 2.35        | 0.41     |
| 48:DG:84:LYS:HG3  | 48:DG:131:VAL:HB   | 2.03        | 0.41     |
| 47:DF:91:ARG:HD3  | 47:DF:91:ARG:N     | 2.35        | 0.41     |
| 40:BH:82:SER:HB2  | 40:BH:146:VAL:CG1  | 2.51        | 0.41     |
| 41:DJ:6:ALA:HB3   | 41:DJ:45:THR:CG2   | 2.49        | 0.41     |
| 27:BK:47:ILE:HG23 | 27:BK:48:PRO:N     | 2.34        | 0.41     |
| 13:CN:68:ARG:HH12 | 13:CN:71:GLY:H     | 1.68        | 0.41     |
| 30:DY:51:SER:HA   | 30:DY:54:VAL:CG2   | 2.51        | 0.41     |
| 13:CN:9:GLU:HB2   | 13:CN:62:ARG:CZ    | 2.51        | 0.41     |
| 48:BG:17:LYS:CA   | 48:BG:17:LYS:HZ2   | 2.33        | 0.41     |
| 46:DU:85:ARG:N    | 46:DU:91:LYS:O     | 2.50        | 0.41     |
| 42:BN:96:ARG:HH11 | 42:BN:116:VAL:HA   | 1.85        | 0.41     |
| 37:BL:57:LEU:HD13 | 37:BL:60:ARG:NH2   | 2.36        | 0.41     |
| 1:AA:920:U:C2     | 1:AA:921:U:C5      | 3.08        | 0.41     |
| 4:AE:132:PRO:HG2  | 4:AE:133:ILE:H     | 1.85        | 0.41     |
| 47:DF:131:VAL:C   | 47:DF:133:GLU:N    | 2.74        | 0.41     |
| 24:BI:32:VAL:HG22 | 24:BI:60:VAL:HG21  | 2.02        | 0.41     |
| 12:AM:3:ILE:CA    | 12:AM:56:ARG:HG2   | 2.43        | 0.41     |
| 13:AN:32:ASP:CG   | 13:AN:33:VAL:H     | 2.23        | 0.41     |
| 29:BE:69:ARG:HH11 | 29:BE:69:ARG:HG2   | 1.85        | 0.41     |
| 23:DB:137:U:C5    | 23:DB:138:U:N3     | 2.88        | 0.41     |
| 50:DT:49:LYS:HB2  | 50:DT:50:LEU:HD22  | 2.02        | 0.41     |
| 38:DM:66:ARG:HB2  | 38:DM:101:VAL:HG13 | 2.02        | 0.41     |
| 23:BB:981:A:H2'   | 23:BB:982:C:C5'    | 2.50        | 0.41     |
| 1:CA:1324:A:H2'   | 1:CA:1325:C:C6     | 2.55        | 0.41     |
| 29:BE:171:ASP:CG  | 29:BE:172:ALA:N    | 2.74        | 0.41     |
| 29:BE:192:ALA:HA  | 29:BE:195:GLN:NE2  | 2.36        | 0.41     |
| 35:DV:83:LYS:HA   | 35:DV:84:PRO:HD3   | 1.92        | 0.41     |
| 9:CJ:5:ARG:N      | 9:CJ:76:ILE:O      | 2.54        | 0.41     |
| 45:BS:24:ILE:O    | 45:BS:25:ARG:C     | 2.59        | 0.41     |
| 25:BC:203:VAL:O   | 25:BC:204:LEU:HB2  | 2.20        | 0.41     |
| 29:DE:161:ALA:HB1 | 29:DE:167:VAL:HG13 | 2.02        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 29:DE:160:ALA:O   | 29:DE:161:ALA:HB3  | 2.20        | 0.41     |
| 32:D4:3:VAL:O     | 32:D4:4:ARG:O      | 2.38        | 0.41     |
| 26:DD:112:THR:O   | 26:DD:113:SER:HB2  | 2.20        | 0.41     |
| 27:DK:104:THR:C   | 27:DK:106:GLU:H    | 2.24        | 0.41     |
| 44:BQ:105:PHE:HA  | 44:BQ:108:LEU:HD12 | 2.01        | 0.41     |
| 37:DL:100:ILE:O   | 37:DL:100:ILE:HG12 | 2.20        | 0.41     |
| 23:DB:1439:A:N3   | 23:DB:1553:A:C6    | 2.88        | 0.41     |
| 36:B2:31:LEU:HD22 | 36:B2:42:LEU:HD12  | 2.01        | 0.41     |
| 23:DB:455:C:N3    | 23:DB:473:G:H5'    | 2.35        | 0.41     |
| 23:BB:1439:A:C5   | 23:BB:1552:A:N6    | 2.88        | 0.41     |
| 20:AB:120:SER:CA  | 20:AB:125:PHE:HB3  | 2.45        | 0.41     |
| 1:CA:271:C:O2'    | 1:CA:272:C:H5'     | 2.20        | 0.41     |
| 51:BZ:14:THR:HA   | 51:BZ:28:ARG:CB    | 2.50        | 0.41     |
| 3:AD:110:ARG:HH11 | 3:AD:110:ARG:HG3   | 1.84        | 0.41     |
| 46:DU:78:LYS:HE3  | 46:DU:79:ALA:N     | 2.35        | 0.41     |
| 46:DU:62:ALA:O    | 46:DU:63:ALA:HB3   | 2.20        | 0.41     |
| 1:CA:958:A:N6     | 1:CA:959:A:N1      | 2.69        | 0.41     |
| 23:BB:2747:G:O6   | 23:BB:2754:U:H2'   | 2.20        | 0.41     |
| 11:AL:107:LYS:H   | 11:AL:107:LYS:HZ2  | 1.66        | 0.41     |
| 23:DB:616:A:H4'   | 29:DE:101:TYR:CE2  | 2.55        | 0.41     |
| 23:BB:220:G:N1    | 23:BB:427:U:H2'    | 2.34        | 0.41     |
| 3:CD:100:VAL:HG21 | 3:CD:136:VAL:CG2   | 2.49        | 0.41     |
| 23:DB:2087:G:H2'  | 23:DB:2088:A:H8    | 1.84        | 0.41     |
| 1:CA:861:G:O2'    | 1:CA:862:C:H5'     | 2.19        | 0.41     |
| 23:BB:2846:G:OP1  | 28:BP:51:ASN:HB2   | 2.20        | 0.41     |
| 1:CA:734:G:H2'    | 1:CA:735:C:C6      | 2.56        | 0.41     |
| 23:DB:2137:U:O2'  | 23:DB:2138:G:H5'   | 2.20        | 0.41     |
| 40:DH:37:VAL:HG23 | 40:DH:38:PRO:HD2   | 2.03        | 0.41     |
| 1:CA:1099:G:H2'   | 1:CA:1100:C:O4'    | 2.21        | 0.41     |
| 1:CA:548:G:H2'    | 1:CA:549:C:C6      | 2.55        | 0.41     |
| 2:CC:114:LEU:O    | 2:CC:115:VAL:C     | 2.58        | 0.41     |
| 2:AC:104:GLU:HG2  | 2:AC:105:VAL:N     | 2.33        | 0.41     |
| 1:CA:1404:C:O4'   | 1:CA:1499:A:C2     | 2.73        | 0.41     |
| 1:CA:1053:G:H4'   | 1:CA:1054:C:H5'    | 2.01        | 0.41     |
| 38:BM:11:LYS:HD2  | 38:BM:86:LYS:HG2   | 2.02        | 0.41     |
| 23:DB:866:A:H61   | 23:DB:913:U:C4'    | 2.33        | 0.41     |
| 23:BB:1045:C:C2   | 23:BB:1047:G:C2    | 3.08        | 0.41     |
| 1:AA:547:A:H4'    | 1:AA:548:G:O5'     | 2.20        | 0.41     |
| 23:DB:377:G:O2'   | 23:DB:378:C:H5'    | 2.21        | 0.41     |
| 1:CA:1277:C:O2'   | 1:CA:1279:G:C8     | 2.73        | 0.41     |
| 8:CI:98:ARG:NE    | 8:CI:103:VAL:HG21  | 2.35        | 0.41     |
| 23:BB:1745:A:H2'  | 23:BB:1746:A:O4'   | 2.21        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:2785:C:H2'  | 23:BB:2786:U:C6    | 2.54        | 0.41     |
| 19:AT:31:ILE:O    | 19:AT:34:VAL:HG23  | 2.21        | 0.41     |
| 26:BD:67:HIS:ND1  | 26:BD:67:HIS:C     | 2.74        | 0.41     |
| 43:DO:106:LEU:CA  | 43:DO:109:ALA:HB3  | 2.50        | 0.41     |
| 38:BM:82:MET:HE3  | 38:BM:83:GLY:N     | 2.34        | 0.41     |
| 48:BG:87:GLN:H    | 48:BG:164:ALA:HB2  | 1.84        | 0.41     |
| 23:BB:2528:U:O2'  | 23:BB:2529:G:H3'   | 2.20        | 0.41     |
| 23:DB:2323:G:O2'  | 23:DB:2324:U:H5'   | 2.20        | 0.41     |
| 22:DA:83:G:H4'    | 30:DY:52:PHE:CD2   | 2.55        | 0.41     |
| 49:DR:58:VAL:HG22 | 49:DR:58:VAL:O     | 2.19        | 0.41     |
| 1:AA:28:A:C2      | 1:AA:296:U:H4'     | 2.55        | 0.41     |
| 1:AA:648:A:H2'    | 1:AA:649:A:C8      | 2.55        | 0.41     |
| 22:DA:91:C:O2'    | 22:DA:92:C:H5'     | 2.20        | 0.41     |
| 1:AA:614:C:C2'    | 1:AA:615:G:H5'     | 2.51        | 0.41     |
| 23:DB:1313:U:O2   | 23:DB:1313:U:C2'   | 2.68        | 0.41     |
| 23:BB:189:G:H2'   | 23:BB:205:G:N2     | 2.35        | 0.41     |
| 3:AD:145:ARG:HH21 | 3:AD:147:LYS:HE2   | 1.84        | 0.41     |
| 6:AG:45:ALA:HB2   | 6:AG:116:ALA:O     | 2.20        | 0.41     |
| 19:AT:68:LYS:HE2  | 19:AT:68:LYS:CA    | 2.50        | 0.41     |
| 1:CA:1422:G:O2'   | 1:CA:1423:G:H5'    | 2.21        | 0.41     |
| 1:AA:655:A:H2'    | 1:AA:656:G:O4'     | 2.20        | 0.41     |
| 23:DB:1385:A:HO2' | 23:DB:1396:U:H6    | 1.65        | 0.41     |
| 39:BX:45:GLN:O    | 39:BX:47:ARG:N     | 2.46        | 0.41     |
| 28:BP:44:GLY:HA3  | 28:BP:60:VAL:CG1   | 2.50        | 0.41     |
| 36:B2:12:ARG:HH21 | 36:B2:12:ARG:HG3   | 1.86        | 0.41     |
| 23:DB:1751:U:H2'  | 23:DB:1752:C:C6    | 2.56        | 0.41     |
| 6:AG:67:ASN:ND2   | 6:AG:127:ALA:HA    | 2.34        | 0.41     |
| 22:BA:19:C:O2'    | 22:BA:20:G:H5'     | 2.19        | 0.41     |
| 7:AH:62:LEU:HB3   | 7:AH:64:TYR:CE1    | 2.55        | 0.41     |
| 1:CA:1265:C:O2'   | 1:CA:1266:G:H5'    | 2.19        | 0.41     |
| 1:AA:757:U:O2'    | 1:AA:758:C:H5'     | 2.20        | 0.41     |
| 7:CH:91:LEU:HD12  | 7:CH:116:ARG:HB2   | 2.03        | 0.41     |
| 19:AT:72:ALA:HA   | 19:AT:75:LYS:HD3   | 2.02        | 0.41     |
| 23:DB:2013:A:C2'  | 23:DB:2014:A:H5'   | 2.50        | 0.41     |
| 2:AC:202:PHE:HZ   | 2:AC:205:GLU:HG2   | 1.84        | 0.41     |
| 23:BB:2083:G:H2'  | 23:BB:2084:C:H6    | 1.84        | 0.41     |
| 10:AK:70:ALA:HA   | 10:AK:73:VAL:CG2   | 2.50        | 0.41     |
| 48:BG:104:LEU:HB3 | 48:BG:106:LEU:HD21 | 2.02        | 0.41     |
| 44:DQ:24:TYR:CD1  | 44:DQ:25:GLY:N     | 2.86        | 0.41     |
| 22:BA:44:G:N2     | 22:BA:48:U:C2      | 2.89        | 0.41     |
| 48:DG:110:HIS:HA  | 48:DG:111:PRO:HD3  | 1.95        | 0.41     |
| 48:DG:93:TYR:CG   | 48:DG:106:LEU:HB3  | 2.55        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:BK:34:GLY:O    | 27:BK:36:GLY:N     | 2.53        | 0.41     |
| 53:D6:39:LEU:O    | 53:D6:53:ASN:N     | 2.54        | 0.41     |
| 47:DF:65:LEU:HD23 | 47:DF:87:LYS:CD    | 2.49        | 0.41     |
| 53:B6:52:LEU:HA   | 53:B6:55:ILE:HG23  | 2.01        | 0.41     |
| 53:B6:67:VAL:O    | 53:B6:67:VAL:HG23  | 2.20        | 0.41     |
| 41:DJ:45:THR:H    | 41:DJ:46:PRO:CD    | 2.33        | 0.41     |
| 44:DQ:63:ARG:HG3  | 44:DQ:63:ARG:H     | 1.63        | 0.41     |
| 5:AF:3:HIS:ND1    | 5:AF:95:ALA:N      | 2.66        | 0.41     |
| 35:DV:32:GLY:O    | 35:DV:93:ARG:NH1   | 2.53        | 0.41     |
| 26:DD:76:GLY:O    | 26:DD:77:ARG:C     | 2.58        | 0.41     |
| 7:AH:77:VAL:HG12  | 7:AH:78:SER:N      | 2.36        | 0.41     |
| 7:CH:86:LYS:CG    | 7:CH:124:ILE:HD11  | 2.50        | 0.41     |
| 3:CD:24:VAL:HG12  | 3:CD:160:LEU:HD12  | 2.02        | 0.41     |
| 46:BU:1:ALA:HB1   | 46:BU:84:PHE:CZ    | 2.56        | 0.41     |
| 25:BC:109:LEU:H   | 25:BC:109:LEU:HD23 | 1.84        | 0.41     |
| 43:BO:51:ALA:HB1  | 43:BO:77:ALA:CB    | 2.51        | 0.41     |
| 24:DI:72:THR:HG23 | 24:DI:112:LYS:HD2  | 2.02        | 0.41     |
| 37:BL:57:LEU:C    | 37:BL:59:ARG:N     | 2.74        | 0.41     |
| 47:DF:21:TYR:CD2  | 47:DF:27:VAL:HG12  | 2.56        | 0.41     |
| 18:CS:40:PHE:O    | 18:CS:43:MET:HG3   | 2.20        | 0.41     |
| 1:CA:1320:C:H1'   | 18:CS:72:GLU:HB3   | 2.02        | 0.41     |
| 1:AA:1271:A:H5'   | 1:AA:1314:C:C5'    | 2.47        | 0.41     |
| 23:BB:2848:G:N3   | 23:BB:2849:U:C5    | 2.88        | 0.41     |
| 23:DB:138:U:H2'   | 23:DB:140:C:C6     | 2.55        | 0.41     |
| 25:DC:14:HIS:O    | 25:DC:15:VAL:C     | 2.59        | 0.41     |
| 22:DA:97:C:C2'    | 22:DA:98:G:H5'     | 2.50        | 0.41     |
| 16:AQ:66:LEU:HD12 | 16:AQ:70:LYS:HG2   | 2.01        | 0.41     |
| 37:BL:13:LYS:O    | 37:BL:14:LYS:HG2   | 2.20        | 0.41     |
| 34:D3:30:HIS:HD2  | 34:D3:31:ILE:H     | 1.68        | 0.41     |
| 38:DM:64:TRP:C    | 38:DM:65:ILE:HG13  | 2.39        | 0.41     |
| 1:CA:972:C:O2'    | 9:CJ:57:VAL:HA     | 2.21        | 0.41     |
| 23:BB:2886:A:N7   | 31:B0:39:ARG:NH2   | 2.65        | 0.41     |
| 48:DG:148:ARG:HD3 | 48:DG:152:ARG:CD   | 2.51        | 0.41     |
| 26:DD:98:VAL:C    | 26:DD:100:LEU:N    | 2.74        | 0.41     |
| 48:BG:152:ARG:HA  | 48:BG:152:ARG:HD2  | 1.82        | 0.41     |
| 23:DB:2105:U:H2'  | 23:DB:2106:U:H6    | 1.85        | 0.41     |
| 23:DB:2106:U:H2'  | 23:DB:2107:G:OP1   | 2.20        | 0.41     |
| 23:DB:2151:U:O2'  | 23:DB:2152:G:H5'   | 2.20        | 0.41     |
| 44:BQ:8:ILE:HG23  | 44:BQ:9:ALA:N      | 2.35        | 0.41     |
| 42:DN:70:THR:OG1  | 42:DN:70:THR:O     | 2.39        | 0.41     |
| 49:DR:39:LEU:HB3  | 49:DR:53:PHE:HA    | 2.02        | 0.41     |
| 34:B3:23:HIS:O    | 34:B3:46:LYS:HB3   | 2.20        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 20:CB:68:PHE:CG   | 20:CB:83:ALA:HB2   | 2.55        | 0.41     |
| 25:BC:156:SER:HB3 | 25:BC:159:THR:CG2  | 2.51        | 0.41     |
| 34:D3:24:LYS:HB2  | 37:DL:64:PHE:CD2   | 2.56        | 0.41     |
| 38:DM:114:ARG:HB2 | 38:DM:114:ARG:NH2  | 2.28        | 0.41     |
| 45:DS:22:ASP:HA   | 45:DS:25:ARG:HH12  | 1.83        | 0.41     |
| 23:BB:62:U:HO2'   | 23:BB:63:A:H5'     | 1.84        | 0.41     |
| 2:CC:116:ALA:HB1  | 2:CC:186:SER:OG    | 2.21        | 0.41     |
| 14:CO:82:ILE:O    | 14:CO:86:GLY:N     | 2.53        | 0.41     |
| 26:BD:113:SER:CB  | 26:BD:168:GLU:H    | 2.32        | 0.41     |
| 23:BB:2746:U:O4'  | 48:BG:138:GLN:HA   | 2.20        | 0.41     |
| 23:BB:2795:C:H2'  | 23:BB:2796:U:C1'   | 2.50        | 0.41     |
| 10:CK:17:ASP:HB3  | 10:CK:80:ASN:HD21  | 1.85        | 0.41     |
| 4:CE:157:GLY:O    | 4:CE:158:LYS:HB2   | 2.20        | 0.41     |
| 23:DB:265:A:N6    | 23:DB:427:U:O2'    | 2.54        | 0.41     |
| 1:CA:1120:C:H2'   | 1:CA:1121:U:H6     | 1.85        | 0.41     |
| 1:AA:142:G:N3     | 1:AA:196:A:H2      | 2.18        | 0.41     |
| 12:CM:2:ARG:HG3   | 12:CM:5:GLY:HA2    | 2.01        | 0.41     |
| 12:CM:2:ARG:CG    | 12:CM:6:ILE:H      | 2.29        | 0.41     |
| 1:CA:835:U:O2'    | 1:CA:836:G:H5'     | 2.20        | 0.41     |
| 23:DB:1179:G:H2'  | 23:DB:1180:U:H5'   | 2.01        | 0.41     |
| 23:BB:1591:A:H2'  | 23:BB:1592:C:O4'   | 2.20        | 0.41     |
| 33:D1:3:GLY:O     | 33:D1:5:ARG:N      | 2.54        | 0.41     |
| 23:BB:2578:G:C6   | 26:BD:145:SER:HB2  | 2.55        | 0.41     |
| 23:BB:2099:U:H2'  | 23:BB:2100:G:C8    | 2.53        | 0.41     |
| 22:DA:114:C:H1'   | 43:DO:47:VAL:HG21  | 2.03        | 0.41     |
| 11:CL:107:LYS:HD2 | 11:CL:107:LYS:O    | 2.20        | 0.41     |
| 1:CA:374:A:H5''   | 1:CA:452:A:N1      | 2.36        | 0.41     |
| 1:AA:1178:G:H2'   | 1:AA:1180:A:OP2    | 2.20        | 0.41     |
| 1:CA:720:C:H5''   | 17:CR:40:PRO:HA    | 2.02        | 0.41     |
| 1:CA:284:C:O2'    | 1:CA:285:C:H5'     | 2.20        | 0.41     |
| 23:BB:2415:G:O2'  | 23:BB:2416:C:H5'   | 2.19        | 0.41     |
| 23:DB:2231:U:H2'  | 23:DB:2232:C:H6    | 1.85        | 0.41     |
| 33:B1:18:HIS:ND1  | 33:B1:19:PHE:N     | 2.69        | 0.41     |
| 1:AA:880:C:H2'    | 1:AA:881:G:C8      | 2.51        | 0.41     |
| 37:BL:132:ARG:C   | 37:BL:135:ILE:HG22 | 2.41        | 0.41     |
| 23:DB:2259:U:H2'  | 23:DB:2260:C:H6    | 1.86        | 0.41     |
| 23:DB:2708:G:H2'  | 23:DB:2709:G:C8    | 2.54        | 0.41     |
| 49:DR:15:SER:OG   | 49:DR:18:GLN:HG2   | 2.20        | 0.41     |
| 17:CR:22:TYR:HA   | 17:CR:57:ALA:HB1   | 2.01        | 0.41     |
| 1:AA:818:G:C2'    | 1:AA:819:A:H5''    | 2.51        | 0.41     |
| 23:DB:2543:G:H8   | 23:DB:2543:G:H5'   | 1.86        | 0.41     |
| 12:CM:22:TYR:HB2  | 12:CM:65:GLU:HA    | 2.03        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 46:BU:4:ILE:HG13   | 46:BU:66:VAL:HG23  | 2.02        | 0.41     |
| 5:CF:7:VAL:O       | 5:CF:7:VAL:HG13    | 2.20        | 0.41     |
| 23:DB:1230:A:H2'   | 23:DB:1231:U:H6    | 1.85        | 0.41     |
| 1:CA:614:C:C2'     | 1:CA:615:G:H5'     | 2.51        | 0.41     |
| 40:BH:59:ALA:HA    | 40:BH:62:LEU:CD2   | 2.51        | 0.41     |
| 23:BB:1368:G:O2'   | 23:BB:1369:G:H5'   | 2.20        | 0.41     |
| 33:B1:39:ASP:OD1   | 33:B1:41:VAL:HB    | 2.21        | 0.41     |
| 32:D4:27:CYS:CB    | 32:D4:33:HIS:HB2   | 2.50        | 0.41     |
| 44:BQ:42:GLY:HA3   | 49:BR:75:VAL:CG2   | 2.50        | 0.41     |
| 1:AA:177:G:N3      | 1:AA:177:G:O4'     | 2.52        | 0.41     |
| 1:AA:632:U:H5''    | 1:AA:633:G:C8      | 2.56        | 0.41     |
| 23:BB:1838:C:H4'   | 23:BB:1839:G:C8    | 2.54        | 0.41     |
| 28:BP:29:VAL:O     | 28:BP:40:GLN:N     | 2.54        | 0.41     |
| 20:CB:35:ASN:O     | 20:CB:37:VAL:N     | 2.53        | 0.41     |
| 23:BB:838:C:H2'    | 23:BB:839:U:C6     | 2.55        | 0.41     |
| 23:DB:1541:C:H2'   | 23:DB:1542:U:H6    | 1.85        | 0.41     |
| 1:CA:664:G:H22     | 1:CA:741:G:H22     | 1.69        | 0.41     |
| 1:CA:291:U:H2'     | 1:CA:292:G:C8      | 2.55        | 0.41     |
| 23:BB:1248:G:OP1   | 29:BE:44:ARG:NH1   | 2.54        | 0.41     |
| 8:CI:10:ARG:HA     | 8:CI:77:ALA:HB1    | 2.03        | 0.41     |
| 1:AA:916:U:H2'     | 1:AA:917:G:H8      | 1.85        | 0.41     |
| 23:DB:2089:C:H2'   | 23:DB:2090:A:C8    | 2.55        | 0.41     |
| 5:CF:74:LEU:HA     | 5:CF:77:THR:OG1    | 2.21        | 0.41     |
| 1:CA:753:A:OP1     | 14:CO:73:LYS:HE3   | 2.20        | 0.41     |
| 43:DO:69:ASP:O     | 43:DO:72:ALA:HB3   | 2.21        | 0.41     |
| 2:CC:32:LEU:O      | 2:CC:35:ASP:HB2    | 2.20        | 0.41     |
| 23:DB:388:G:N7     | 23:DB:390:U:H2'    | 2.35        | 0.41     |
| 25:DC:89:ASN:HA    | 25:DC:89:ASN:HD22  | 1.58        | 0.41     |
| 6:AG:146:ALA:CA    | 10:AK:55:ARG:HH12  | 2.33        | 0.41     |
| 1:AA:1526:G:OP2    | 21:AU:38:GLU:HB3   | 2.21        | 0.41     |
| 48:DG:7:PRO:O      | 48:DG:8:VAL:HB     | 2.20        | 0.41     |
| 37:BL:121:THR:HG22 | 37:BL:141:LYS:CB   | 2.50        | 0.41     |
| 48:DG:118:ALA:O    | 48:DG:120:ILE:N    | 2.52        | 0.41     |
| 48:DG:83:THR:O     | 48:DG:84:LYS:HD3   | 2.21        | 0.41     |
| 23:DB:2365:G:O6    | 34:D3:42:HIS:HE1   | 2.03        | 0.41     |
| 52:DW:24:ARG:HA    | 52:DW:66:VAL:N     | 2.16        | 0.41     |
| 41:BJ:59:ALA:O     | 41:BJ:62:VAL:HG12  | 2.19        | 0.41     |
| 44:DQ:94:LEU:HD12  | 49:DR:13:ARG:HB2   | 2.02        | 0.41     |
| 1:CA:1491:G:C5     | 55:CA:1662:PAR:H21 | 2.56        | 0.41     |
| 35:BV:62:THR:HG21  | 35:BV:71:LYS:NZ    | 2.35        | 0.41     |
| 37:DL:77:ILE:CG2   | 37:DL:78:ARG:N     | 2.83        | 0.41     |
| 23:BB:496:G:H4'    | 45:BS:61:ASN:ND2   | 2.35        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 30:DY:51:SER:C    | 30:DY:53:MET:N     | 2.74        | 0.41     |
| 44:BQ:63:ARG:H    | 44:BQ:63:ARG:HG3   | 1.64        | 0.41     |
| 43:BO:37:ALA:CB   | 43:BO:78:VAL:HG21  | 2.51        | 0.41     |
| 30:BY:12:ALA:HB2  | 30:BY:53:MET:CE    | 2.51        | 0.41     |
| 42:BN:83:LEU:HA   | 42:BN:86:ARG:CG    | 2.51        | 0.41     |
| 23:DB:1060:U:C1'  | 23:DB:1062:G:H5'   | 2.51        | 0.41     |
| 47:BF:76:PHE:HD2  | 47:BF:78:ILE:CD1   | 2.31        | 0.41     |
| 47:BF:169:LEU:HB3 | 47:BF:174:PHE:CD1  | 2.55        | 0.41     |
| 23:BB:322:A:H5'   | 23:BB:340:A:C1'    | 2.50        | 0.41     |
| 23:BB:1461:C:H2'  | 23:BB:1462:C:C5    | 2.56        | 0.41     |
| 4:AE:131:ASN:HD22 | 4:AE:134:ASN:H     | 1.69        | 0.41     |
| 47:DF:29:ARG:HB2  | 47:DF:29:ARG:HH11  | 1.85        | 0.41     |
| 1:CA:924:C:H5'    | 1:CA:1399:C:OP2    | 2.20        | 0.41     |
| 1:CA:923:A:H2'    | 1:CA:924:C:H6      | 1.85        | 0.41     |
| 1:AA:1315:U:H5    | 18:AS:5:LYS:CE     | 2.33        | 0.41     |
| 23:BB:2867:G:HO2' | 23:BB:2868:A:H8    | 1.66        | 0.41     |
| 11:CL:88:ASP:C    | 11:CL:89:LEU:HD22  | 2.40        | 0.41     |
| 13:CN:40:ARG:O    | 13:CN:41:TRP:HE3   | 2.02        | 0.41     |
| 1:AA:1249:C:H2'   | 1:AA:1250:A:H5'    | 2.03        | 0.41     |
| 35:DV:77:VAL:HG23 | 35:DV:89:ILE:CG2   | 2.51        | 0.41     |
| 27:BK:54:LYS:C    | 27:BK:56:ASP:H     | 2.23        | 0.41     |
| 5:CF:67:PRO:O     | 5:CF:71:ILE:HG22   | 2.20        | 0.41     |
| 38:BM:66:ARG:CZ   | 38:BM:101:VAL:HG11 | 2.50        | 0.41     |
| 1:AA:313:A:H2'    | 1:AA:314:C:H6      | 1.85        | 0.41     |
| 23:DB:2886:A:N7   | 31:D0:39:ARG:NH2   | 2.63        | 0.41     |
| 11:CL:20:VAL:HG12 | 11:CL:93:ARG:CB    | 2.45        | 0.41     |
| 27:DK:119:ALA:HB3 | 27:DK:120:PRO:HD3  | 2.03        | 0.41     |
| 26:BD:26:VAL:HG13 | 26:BD:188:LEU:CD2  | 2.50        | 0.41     |
| 23:BB:116:C:O2    | 23:BB:127:A:H2     | 2.03        | 0.41     |
| 23:BB:1439:A:N3   | 23:BB:1553:A:C6    | 2.89        | 0.41     |
| 13:CN:88:MET:C    | 13:CN:90:GLY:H     | 2.22        | 0.41     |
| 23:DB:2016:U:C4   | 23:DB:2017:U:C4    | 3.08        | 0.41     |
| 23:BB:2742:G:O2'  | 23:BB:2743:U:H5'   | 2.21        | 0.41     |
| 20:AB:122:ASP:C   | 20:AB:124:THR:H    | 2.23        | 0.41     |
| 1:AA:1343:G:H4'   | 8:AI:123:ARG:HB2   | 2.03        | 0.41     |
| 1:CA:1382:C:H4'   | 6:CG:78:ARG:HH21   | 1.86        | 0.41     |
| 2:AC:23:ALA:HB1   | 2:AC:27:GLU:OE2    | 2.20        | 0.41     |
| 5:AF:70:VAL:HG23  | 5:AF:71:ILE:N      | 2.35        | 0.41     |
| 14:CO:25:THR:CG2  | 14:CO:70:LEU:HD23  | 2.50        | 0.41     |
| 28:DP:50:ARG:HB2  | 28:DP:56:SER:CB    | 2.50        | 0.41     |
| 14:AO:82:ILE:O    | 14:AO:86:GLY:N     | 2.53        | 0.41     |
| 15:CP:40:ASN:HD21 | 15:CP:43:ALA:CA    | 2.33        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:142:G:H2'    | 1:CA:143:A:O4'    | 2.19        | 0.41     |
| 41:BJ:106:LYS:HD2 | 41:BJ:106:LYS:HA  | 1.85        | 0.41     |
| 26:BD:14:ILE:HA   | 28:BP:11:GLN:HE22 | 1.86        | 0.41     |
| 27:BK:88:ASN:C    | 27:BK:88:ASN:HD22 | 2.22        | 0.41     |
| 3:AD:197:HIS:O    | 3:AD:201:GLU:HG3  | 2.20        | 0.41     |
| 23:BB:648:G:O2'   | 23:BB:649:G:H5'   | 2.20        | 0.41     |
| 35:DV:78:GLN:N    | 35:DV:88:HIS:O    | 2.53        | 0.41     |
| 23:BB:150:U:O2'   | 23:BB:151:C:H5'   | 2.20        | 0.41     |
| 6:CG:37:THR:O     | 6:CG:41:ILE:HG13  | 2.21        | 0.41     |
| 1:AA:141:G:O2'    | 1:AA:142:G:H5'    | 2.21        | 0.41     |
| 20:AB:68:PHE:CG   | 20:AB:83:ALA:HB2  | 2.55        | 0.41     |
| 9:CJ:10:LEU:HD12  | 9:CJ:72:ARG:HB2   | 2.03        | 0.41     |
| 23:BB:633:A:H2'   | 23:BB:634:C:O4'   | 2.20        | 0.41     |
| 23:DB:2578:G:C6   | 26:DD:145:SER:HB2 | 2.55        | 0.41     |
| 10:CK:50:GLY:O    | 10:CK:51:PHE:C    | 2.59        | 0.41     |
| 23:BB:4:U:O2'     | 23:BB:5:A:H5'     | 2.21        | 0.41     |
| 23:BB:866:A:H61   | 23:BB:913:U:C4'   | 2.33        | 0.41     |
| 6:CG:77:ARG:HG3   | 6:CG:79:VAL:CG2   | 2.49        | 0.41     |
| 26:DD:159:LYS:HZ3 | 26:DD:159:LYS:HA  | 1.86        | 0.41     |
| 16:AQ:31:PRO:O    | 16:AQ:32:ILE:HB   | 2.20        | 0.41     |
| 23:BB:1572:A:O2'  | 23:BB:1573:G:H5'  | 2.19        | 0.41     |
| 3:CD:16:THR:CG2   | 3:CD:17:ASP:N     | 2.84        | 0.41     |
| 23:BB:1684:G:O2'  | 23:BB:1685:C:H5'  | 2.20        | 0.41     |
| 23:DB:528:A:C2    | 23:DB:2043:C:H4'  | 2.55        | 0.41     |
| 15:AP:20:VAL:HG21 | 15:AP:32:PHE:CG   | 2.56        | 0.41     |
| 1:CA:658:C:H2'    | 1:CA:659:U:H6     | 1.85        | 0.41     |
| 25:BC:255:LYS:C   | 25:BC:257:ARG:H   | 2.24        | 0.41     |
| 23:DB:1419:A:N6   | 23:DB:1494:A:N1   | 2.59        | 0.41     |
| 50:DT:72:GLN:HG2  | 50:DT:72:GLN:H    | 1.64        | 0.41     |
| 1:CA:1488:G:O2'   | 1:CA:1489:G:H5'   | 2.20        | 0.41     |
| 23:DB:1885:A:H3'  | 23:DB:1886:U:H6   | 1.83        | 0.41     |
| 23:BB:597:G:H21   | 37:BL:12:SER:HA   | 1.86        | 0.41     |
| 23:DB:1205:A:N1   | 29:DE:165:HIS:HB2 | 2.35        | 0.41     |
| 17:CR:21:ASP:OD2  | 17:CR:23:LYS:HD2  | 2.20        | 0.41     |
| 1:CA:1508:A:H2'   | 1:CA:1509:C:C6    | 2.55        | 0.41     |
| 23:DB:2651:C:O2'  | 23:DB:2652:C:H5'  | 2.21        | 0.41     |
| 29:BE:1:MET:HB2   | 29:BE:16:GLU:CA   | 2.50        | 0.41     |
| 10:AK:67:GLU:HG3  | 10:AK:68:ARG:N    | 2.34        | 0.41     |
| 24:DI:10:LEU:C    | 24:DI:10:LEU:HD12 | 2.40        | 0.41     |
| 23:BB:1370:C:H2'  | 23:BB:1371:G:O4'  | 2.20        | 0.41     |
| 23:BB:1396:U:O4'  | 23:BB:1396:U:O2   | 2.38        | 0.41     |
| 6:AG:121:ASN:N    | 6:AG:121:ASN:ND2  | 2.69        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:CI:35:GLU:HG3   | 8:CI:44:ARG:HD2   | 2.02        | 0.41     |
| 29:DE:3:LEU:O     | 29:DE:12:LEU:N    | 2.53        | 0.41     |
| 28:BP:54:LEU:HA   | 28:BP:76:HIS:CD2  | 2.56        | 0.41     |
| 1:CA:536:C:H2'    | 1:CA:537:G:C8     | 2.55        | 0.41     |
| 23:DB:1541:C:O2'  | 23:DB:1542:U:H5'  | 2.20        | 0.41     |
| 47:BF:56:LEU:O    | 47:BF:56:LEU:HD13 | 2.21        | 0.41     |
| 23:BB:1831:G:O2'  | 23:BB:1832:C:H5'  | 2.20        | 0.41     |
| 39:BX:38:GLN:H    | 39:BX:38:GLN:HG2  | 1.79        | 0.41     |
| 1:AA:537:G:H2'    | 1:AA:538:G:H8     | 1.86        | 0.41     |
| 20:AB:80:LYS:HG3  | 20:AB:81:ASP:N    | 2.35        | 0.41     |
| 22:BA:22:U:H2'    | 22:BA:23:G:C8     | 2.56        | 0.41     |
| 40:BH:119:ASN:HB2 | 40:BH:120:GLY:H   | 1.62        | 0.41     |
| 2:AC:10:ARG:HH11  | 2:AC:10:ARG:HG3   | 1.85        | 0.41     |
| 24:BI:35:MET:C    | 24:BI:35:MET:SD   | 2.98        | 0.41     |
| 23:BB:857:G:H5'   | 52:BW:68:PHE:CD1  | 2.56        | 0.41     |
| 25:BC:120:ASP:O   | 25:BC:121:ALA:C   | 2.59        | 0.41     |
| 48:BG:50:THR:HG22 | 48:BG:51:PHE:N    | 2.36        | 0.41     |
| 23:DB:569:U:H1'   | 23:DB:947:A:O4'   | 2.21        | 0.41     |
| 47:BF:33:ILE:HG22 | 47:BF:34:THR:N    | 2.35        | 0.41     |
| 10:CK:70:ALA:C    | 10:CK:72:ALA:N    | 2.73        | 0.41     |
| 48:DG:8:VAL:CG1   | 48:DG:49:LEU:HB2  | 2.40        | 0.41     |
| 37:BL:90:VAL:HG23 | 37:BL:120:VAL:CG1 | 2.50        | 0.41     |
| 53:D6:84:ARG:HD2  | 53:D6:92:PRO:HD3  | 2.01        | 0.41     |
| 47:DF:34:THR:CG2  | 47:DF:89:THR:HG22 | 2.48        | 0.41     |
| 53:B6:61:PRO:HD2  | 53:B6:65:THR:HG22 | 2.02        | 0.41     |
| 23:DB:2211:A:C2'  | 23:DB:2212:A:OP1  | 2.68        | 0.41     |
| 8:AI:46:VAL:HG23  | 8:AI:47:VAL:N     | 2.36        | 0.41     |
| 35:DV:4:ILE:HD11  | 35:DV:61:LEU:HB3  | 2.03        | 0.41     |
| 23:BB:141:G:C6    | 50:BT:2:ILE:HG21  | 2.55        | 0.41     |
| 38:DM:72:PRO:O    | 38:DM:73:ILE:HB   | 2.21        | 0.41     |
| 50:BT:54:GLU:HG2  | 50:BT:90:GLY:HA3  | 2.02        | 0.41     |
| 13:AN:68:ARG:HB2  | 13:AN:79:SER:HB3  | 2.02        | 0.41     |
| 3:AD:164:ARG:NH1  | 3:AD:164:ARG:HG2  | 2.35        | 0.41     |
| 42:BN:55:ALA:HA   | 42:BN:80:PHE:CD1  | 2.55        | 0.41     |
| 47:BF:43:ILE:O    | 47:BF:46:LYS:HE2  | 2.20        | 0.41     |
| 47:BF:8:LYS:HD3   | 47:BF:9:ASP:OD2   | 2.21        | 0.41     |
| 42:DN:96:ARG:HH11 | 42:DN:116:VAL:HA  | 1.85        | 0.41     |
| 4:AE:136:VAL:HG13 | 4:AE:137:ARG:H    | 1.86        | 0.41     |
| 47:DF:102:LEU:O   | 47:DF:103:ILE:CB  | 2.69        | 0.41     |
| 4:CE:132:PRO:HG2  | 4:CE:133:ILE:H    | 1.86        | 0.41     |
| 1:CA:765:G:C6     | 1:CA:812:G:C5     | 3.09        | 0.41     |
| 18:CS:66:VAL:C    | 18:CS:68:HIS:H    | 2.24        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 33:D1:26:LYS:HB2  | 33:D1:52:LYS:HZ3   | 1.84        | 0.41     |
| 40:BH:106:ALA:C   | 40:BH:108:VAL:N    | 2.73        | 0.41     |
| 34:D3:30:HIS:O    | 34:D3:31:ILE:C     | 2.59        | 0.41     |
| 46:BU:73:ASN:HD22 | 46:BU:73:ASN:N     | 2.18        | 0.41     |
| 29:BE:149:ILE:O   | 29:BE:188:MET:HA   | 2.20        | 0.41     |
| 35:DV:9:ARG:HG2   | 35:DV:40:ILE:C     | 2.41        | 0.41     |
| 22:DA:76:G:O2'    | 22:DA:77:U:H5'     | 2.21        | 0.41     |
| 48:BG:86:LEU:HD23 | 48:BG:163:TYR:HA   | 2.03        | 0.41     |
| 29:DE:171:ASP:CG  | 29:DE:172:ALA:N    | 2.74        | 0.41     |
| 1:CA:1236:A:C4'   | 1:CA:1304:G:H4'    | 2.44        | 0.41     |
| 38:BM:63:ILE:N    | 38:BM:63:ILE:HD12  | 2.35        | 0.41     |
| 2:CC:149:LYS:HE2  | 2:CC:200:TRP:CZ3   | 2.55        | 0.41     |
| 49:BR:39:LEU:HA   | 49:BR:49:ILE:HG21  | 2.03        | 0.41     |
| 27:BK:116:ILE:H   | 27:BK:116:ILE:HG13 | 1.74        | 0.41     |
| 10:CK:23:HIS:HB3  | 10:CK:30:ILE:HG12  | 2.02        | 0.41     |
| 35:BV:89:ILE:HD13 | 35:BV:91:PHE:CZ    | 2.56        | 0.41     |
| 4:CE:52:ALA:HB3   | 4:CE:58:ALA:N      | 2.36        | 0.41     |
| 23:DB:1441:G:H4'  | 23:DB:1628:G:OP1   | 2.20        | 0.41     |
| 53:B6:110:ARG:O   | 53:B6:114:LEU:HB2  | 2.21        | 0.41     |
| 23:BB:1723:G:C2'  | 23:BB:1724:G:H5'   | 2.51        | 0.41     |
| 23:BB:1729:U:C2'  | 23:BB:1730:C:H5'   | 2.51        | 0.41     |
| 9:AJ:6:ILE:HG23   | 9:AJ:101:SER:O     | 2.20        | 0.41     |
| 34:D3:21:PHE:O    | 34:D3:22:LYS:O     | 2.39        | 0.41     |
| 23:BB:2391:G:P    | 34:B3:34:LYS:HZ3   | 2.44        | 0.41     |
| 23:DB:362:A:H3'   | 23:DB:363:G:C8     | 2.55        | 0.41     |
| 51:DZ:14:THR:HA   | 51:DZ:28:ARG:CB    | 2.50        | 0.41     |
| 4:CE:104:ILE:HG23 | 4:CE:104:ILE:O     | 2.21        | 0.41     |
| 1:AA:1087:G:O2'   | 1:AA:1088:G:H5'    | 2.21        | 0.41     |
| 19:CT:67:HIS:CD2  | 19:CT:68:LYS:H     | 2.39        | 0.41     |
| 4:AE:111:ARG:O    | 4:AE:112:ALA:C     | 2.59        | 0.41     |
| 4:CE:156:ARG:HB3  | 7:CH:42:GLU:O      | 2.21        | 0.41     |
| 1:AA:1048:G:OP1   | 13:AN:3:GLN:HB2    | 2.20        | 0.41     |
| 23:BB:2419:U:O5'  | 34:B3:32:LEU:HD12  | 2.20        | 0.41     |
| 35:BV:21:ARG:HE   | 35:BV:87:GLN:HB3   | 1.86        | 0.41     |
| 1:CA:1122:U:H2'   | 1:CA:1123:U:C6     | 2.55        | 0.41     |
| 23:DB:1854:A:H62  | 23:DB:1888:G:H8    | 1.67        | 0.41     |
| 23:BB:947:A:O2'   | 23:BB:984:A:H2     | 2.00        | 0.41     |
| 1:AA:140:U:H2'    | 1:AA:141:G:H8      | 1.83        | 0.41     |
| 35:DV:53:LYS:HZ3  | 35:DV:53:LYS:HA    | 1.82        | 0.41     |
| 23:BB:1854:A:H62  | 23:BB:1888:G:H8    | 1.67        | 0.41     |
| 23:BB:1431:A:O2'  | 23:BB:1432:G:H5'   | 2.21        | 0.41     |
| 2:CC:9:ILE:O      | 2:CC:9:ILE:HG13    | 2.20        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:1085:U:H3'   | 1:CA:1086:U:C6    | 2.55        | 0.41     |
| 20:CB:94:ARG:NE   | 20:CB:94:ARG:N    | 2.69        | 0.41     |
| 26:BD:136:ASN:OD1 | 26:BD:139:SER:HB3 | 2.20        | 0.41     |
| 1:CA:502:A:C4'    | 1:CA:550:G:H4'    | 2.51        | 0.41     |
| 19:CT:78:LEU:HA   | 19:CT:78:LEU:HD23 | 1.93        | 0.41     |
| 23:BB:753:A:O2'   | 23:BB:754:U:H5'   | 2.20        | 0.41     |
| 2:CC:50:SER:O     | 2:CC:114:LEU:HD21 | 2.20        | 0.41     |
| 23:BB:634:C:O5'   | 23:BB:634:C:H6    | 2.04        | 0.41     |
| 1:AA:1142:G:H2'   | 1:AA:1143:G:O4'   | 2.21        | 0.41     |
| 50:BT:73:ARG:HH21 | 50:BT:73:ARG:HB3  | 1.86        | 0.41     |
| 1:CA:481:G:OP1    | 1:CA:481:G:H4'    | 2.21        | 0.41     |
| 1:CA:377:G:O2'    | 1:CA:378:G:H5'    | 2.20        | 0.41     |
| 29:BE:34:ALA:CB   | 29:BE:96:VAL:HG21 | 2.51        | 0.41     |
| 1:CA:1307:U:H2'   | 1:CA:1308:U:H6    | 1.84        | 0.41     |
| 23:DB:2349:G:OP2  | 34:D3:41:ARG:HD3  | 2.20        | 0.41     |
| 23:DB:710:U:O2'   | 23:DB:711:G:H5'   | 2.20        | 0.41     |
| 1:AA:1036:A:H2'   | 1:AA:1037:C:H6    | 1.83        | 0.41     |
| 23:BB:1341:G:O4'  | 50:BT:61:LEU:HD23 | 2.21        | 0.41     |
| 27:BK:107:LEU:C   | 27:BK:109:SER:N   | 2.73        | 0.41     |
| 23:BB:2020:A:O2'  | 23:BB:2021:C:H5'  | 2.21        | 0.41     |
| 4:CE:92:ARG:HB3   | 4:CE:92:ARG:HH11  | 1.85        | 0.41     |
| 9:CJ:65:TYR:OH    | 13:CN:84:ARG:HG3  | 2.21        | 0.41     |
| 23:DB:1275:A:H2'  | 23:DB:1276:A:O4'  | 2.21        | 0.41     |
| 23:DB:255:A:H2'   | 23:DB:256:A:O4'   | 2.21        | 0.41     |
| 48:DG:154:GLU:HB3 | 48:DG:158:GLY:H   | 1.84        | 0.41     |
| 1:AA:565:U:H3'    | 1:AA:566:G:H2'    | 2.03        | 0.41     |
| 6:CG:42:VAL:O     | 6:CG:46:LEU:HB2   | 2.21        | 0.41     |
| 22:DA:53:A:C2'    | 22:DA:54:G:H5'    | 2.51        | 0.41     |
| 6:CG:15:PRO:HG2   | 6:CG:16:LYS:H     | 1.85        | 0.41     |
| 2:CC:128:MET:N    | 2:CC:128:MET:SD   | 2.88        | 0.41     |
| 23:DB:1517:G:H2'  | 23:DB:1518:C:H6   | 1.86        | 0.41     |
| 1:CA:290:C:O2'    | 1:CA:291:U:H5'    | 2.20        | 0.41     |
| 1:AA:1172:C:O2'   | 1:AA:1173:U:H5'   | 2.21        | 0.41     |
| 22:BA:18:G:H2'    | 22:BA:19:C:C6     | 2.55        | 0.41     |
| 7:AH:91:LEU:HD12  | 7:AH:116:ARG:HB2  | 2.02        | 0.41     |
| 1:CA:260:G:O2'    | 1:CA:261:U:H5'    | 2.21        | 0.41     |
| 49:BR:32:THR:HA   | 49:BR:61:ALA:O    | 2.20        | 0.41     |
| 22:BA:67:G:O2'    | 22:BA:68:C:H5'    | 2.19        | 0.41     |
| 24:DI:68:PHE:N    | 24:DI:68:PHE:CD1  | 2.89        | 0.41     |
| 4:AE:78:GLY:O     | 4:AE:119:VAL:HA   | 2.20        | 0.41     |
| 23:BB:2352:A:H8   | 23:BB:2352:A:O5'  | 2.03        | 0.41     |
| 23:BB:1818:U:HO2' | 23:BB:1819:A:P    | 2.42        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DC:121:ALA:HB3  | 25:DC:129:LEU:HG   | 2.02        | 0.41     |
| 25:DC:153:LEU:HD13 | 25:DC:175:LEU:CD2  | 2.50        | 0.41     |
| 9:CJ:9:ARG:HB2     | 9:CJ:99:GLN:CB     | 2.30        | 0.41     |
| 6:AG:148:LYS:HG3   | 6:AG:151:ALA:HB3   | 2.03        | 0.41     |
| 48:DG:47:ASN:CG    | 48:DG:48:THR:H     | 2.24        | 0.41     |
| 37:BL:90:VAL:HG23  | 37:BL:120:VAL:HG11 | 2.03        | 0.41     |
| 8:AI:43:ALA:C      | 8:AI:45:MET:H      | 2.24        | 0.41     |
| 25:BC:140:VAL:CG2  | 25:BC:163:ILE:HG12 | 2.51        | 0.41     |
| 1:AA:1217:C:H2'    | 1:AA:1218:C:H6     | 1.86        | 0.41     |
| 47:DF:47:LYS:HA    | 47:DF:50:ASP:OD2   | 2.20        | 0.41     |
| 43:DO:53:THR:HG23  | 43:DO:74:VAL:HG21  | 2.02        | 0.41     |
| 37:DL:61:LEU:HA    | 37:DL:62:PRO:HD3   | 1.95        | 0.41     |
| 1:CA:598:U:H2'     | 1:CA:599:C:H6      | 1.86        | 0.41     |
| 44:BQ:89:ILE:HB    | 44:BQ:90:ASP:H     | 1.73        | 0.41     |
| 22:BA:28:C:C2'     | 22:BA:29:A:H5'     | 2.51        | 0.41     |
| 12:CM:38:ILE:HG13  | 12:CM:55:LEU:CD2   | 2.45        | 0.41     |
| 45:DS:8:ARG:HB3    | 45:DS:102:HIS:ND1  | 2.36        | 0.41     |
| 1:CA:1225:A:OP1    | 12:CM:100:ARG:HA   | 2.21        | 0.41     |
| 1:AA:1317:C:H2'    | 1:AA:1318:A:O4'    | 2.21        | 0.41     |
| 18:AS:23:GLU:HG3   | 18:AS:23:GLU:H     | 1.71        | 0.41     |
| 18:AS:40:PHE:HB2   | 18:AS:42:ASN:ND2   | 2.35        | 0.41     |
| 23:BB:2849:U:OP2   | 28:BP:92:ARG:HG3   | 2.21        | 0.41     |
| 25:DC:212:TRP:CD1  | 25:DC:212:TRP:C    | 2.94        | 0.41     |
| 16:AQ:45:VAL:HG11  | 16:AQ:60:ILE:CG2   | 2.48        | 0.41     |
| 37:BL:116:VAL:CG1  | 37:BL:117:THR:H    | 2.23        | 0.41     |
| 23:DB:816:C:O2'    | 23:DB:817:C:H5'    | 2.21        | 0.41     |
| 23:DB:162:U:OP1    | 23:DB:162:U:H6     | 2.04        | 0.41     |
| 23:BB:162:U:H6     | 23:BB:162:U:OP1    | 2.03        | 0.41     |
| 23:DB:2038:G:H2'   | 23:DB:2039:U:H6    | 1.86        | 0.41     |
| 1:AA:1250:A:H4'    | 8:AI:69:GLY:O      | 2.21        | 0.41     |
| 39:DX:27:ASN:HA    | 39:DX:30:MET:HG2   | 2.01        | 0.41     |
| 25:BC:212:TRP:CD1  | 25:BC:212:TRP:C    | 2.93        | 0.41     |
| 32:D4:2:LYS:CG     | 32:D4:4:ARG:HE     | 2.25        | 0.41     |
| 1:CA:1237:C:H4'    | 1:CA:1334:G:N2     | 2.35        | 0.41     |
| 38:BM:66:ARG:NE    | 38:BM:101:VAL:HG21 | 2.36        | 0.41     |
| 38:BM:23:GLY:HA3   | 38:BM:66:ARG:NH1   | 2.36        | 0.41     |
| 2:CC:149:LYS:HE3   | 2:CC:166:TRP:CH2   | 2.56        | 0.41     |
| 48:DG:30:GLY:HA3   | 48:DG:78:VAL:CA    | 2.41        | 0.41     |
| 6:CG:145:GLU:CA    | 6:CG:148:LYS:HB2   | 2.45        | 0.41     |
| 26:DD:91:THR:HG23  | 26:DD:92:VAL:N     | 2.27        | 0.41     |
| 23:DB:1444:G:H2'   | 23:DB:1445:G:H8    | 1.85        | 0.41     |
| 23:BB:1549:A:H2'   | 23:BB:1550:C:H6    | 1.86        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 11:AL:29:LYS:HB3   | 11:AL:56:LEU:HD22  | 2.01        | 0.41     |
| 1:AA:134:G:H1'     | 1:AA:325:A:C5      | 2.56        | 0.41     |
| 23:DB:280:U:H6     | 23:DB:280:U:O5'    | 2.04        | 0.41     |
| 20:CB:98:GLY:HA2   | 20:CB:101:THR:HG22 | 2.03        | 0.41     |
| 23:DB:2079:U:H2'   | 23:DB:2080:A:O4'   | 2.21        | 0.41     |
| 46:DU:26:ASN:H     | 46:DU:26:ASN:HD22  | 1.65        | 0.41     |
| 26:DD:146:ILE:HG13 | 26:DD:147:GLY:H    | 1.86        | 0.41     |
| 1:AA:302:G:N3      | 1:AA:556:C:H4'     | 2.35        | 0.41     |
| 25:DC:63:ILE:HD13  | 25:DC:63:ILE:HA    | 1.90        | 0.41     |
| 1:CA:142:G:N3      | 1:CA:196:A:H2      | 2.19        | 0.41     |
| 1:CA:957:U:H2'     | 1:CA:959:A:OP2     | 2.20        | 0.41     |
| 1:CA:9:G:OP1       | 4:CE:125:LYS:HD2   | 2.20        | 0.41     |
| 23:DB:1237:A:N3    | 23:DB:1237:A:H2'   | 2.35        | 0.41     |
| 29:DE:42:GLY:O     | 29:DE:43:THR:O     | 2.39        | 0.41     |
| 29:BE:83:VAL:HG12  | 29:BE:86:ALA:HA    | 2.03        | 0.41     |
| 6:AG:41:ILE:CG2    | 6:AG:115:MET:HG3   | 2.49        | 0.41     |
| 6:AG:37:THR:O      | 6:AG:41:ILE:HG13   | 2.19        | 0.41     |
| 23:DB:150:U:O2'    | 23:DB:151:C:H5'    | 2.21        | 0.41     |
| 1:AA:142:G:H2'     | 1:AA:143:A:O4'     | 2.20        | 0.41     |
| 29:DE:83:VAL:HG12  | 29:DE:86:ALA:HA    | 2.03        | 0.41     |
| 6:AG:19:SER:HB2    | 6:AG:21:LEU:CD2    | 2.51        | 0.41     |
| 23:DB:1873:G:O2'   | 23:DB:1874:C:H5'   | 2.20        | 0.41     |
| 1:CA:1028:C:H3'    | 1:CA:1029:U:C5     | 2.56        | 0.41     |
| 23:BB:1595:C:O2'   | 23:BB:1596:A:H5'   | 2.21        | 0.41     |
| 23:DB:2462:C:H2'   | 23:DB:2463:C:H6    | 1.85        | 0.41     |
| 23:DB:1400:U:H2'   | 23:DB:1401:G:H8    | 1.85        | 0.41     |
| 22:DA:113:C:H2'    | 22:DA:114:C:H6     | 1.84        | 0.41     |
| 23:DB:1635:A:C2'   | 23:DB:1636:U:H5'   | 2.50        | 0.41     |
| 1:CA:86:G:H1'      | 1:CA:87:C:C6       | 2.56        | 0.41     |
| 50:BT:68:LYS:O     | 50:BT:69:ARG:CB    | 2.68        | 0.41     |
| 23:BB:1904:G:N3    | 23:BB:1928:A:H2    | 2.19        | 0.41     |
| 42:BN:69:ARG:H     | 42:BN:69:ARG:HD3   | 1.86        | 0.41     |
| 23:BB:1064:C:O2'   | 23:BB:1065:U:H5'   | 2.21        | 0.41     |
| 27:DK:97:THR:C     | 27:DK:98:ARG:HE    | 2.24        | 0.41     |
| 23:BB:2368:C:H2'   | 23:BB:2369:A:C8    | 2.56        | 0.41     |
| 27:DK:76:VAL:HG12  | 27:DK:77:ILE:H     | 1.85        | 0.41     |
| 28:DP:59:THR:H     | 28:DP:72:VAL:HA    | 1.86        | 0.41     |
| 3:AD:80:ARG:NH1    | 3:AD:81:LEU:HD23   | 2.36        | 0.41     |
| 23:BB:2708:G:H2'   | 23:BB:2709:G:C8    | 2.52        | 0.41     |
| 50:BT:13:ALA:O     | 50:BT:32:LEU:HB2   | 2.20        | 0.41     |
| 23:BB:962:G:H21    | 23:BB:2250:G:N2    | 2.17        | 0.41     |
| 23:BB:528:A:C8     | 23:BB:528:A:H3'    | 2.56        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 35:BV:49:ASN:ND2   | 35:BV:49:ASN:N     | 2.68        | 0.41     |
| 28:BP:61:ARG:HD3   | 28:BP:70:GLU:HG3   | 2.02        | 0.41     |
| 1:CA:903:G:H2'     | 1:CA:904:U:C6      | 2.56        | 0.41     |
| 6:AG:70:PRO:HA     | 6:AG:141:HIS:NE2   | 2.36        | 0.41     |
| 31:B0:33:SER:C     | 31:B0:35:GLU:N     | 2.74        | 0.41     |
| 37:DL:132:ARG:C    | 37:DL:135:ILE:HG22 | 2.41        | 0.41     |
| 1:CA:1458:G:O3'    | 19:CT:22:SER:HA    | 2.20        | 0.41     |
| 6:CG:72:VAL:HG12   | 6:CG:89:GLU:HA     | 2.03        | 0.41     |
| 1:AA:903:G:H2'     | 1:AA:904:U:H6      | 1.86        | 0.41     |
| 23:BB:247:G:H4'    | 23:BB:386:G:C4     | 2.55        | 0.41     |
| 53:B6:4:LYS:HE2    | 53:B6:4:LYS:HB3    | 1.89        | 0.41     |
| 24:BI:48:ILE:O     | 24:BI:49:GLU:HB3   | 2.21        | 0.41     |
| 23:DB:346:A:H5'    | 23:DB:346:A:N3     | 2.36        | 0.41     |
| 23:DB:348:A:H2'    | 23:DB:349:U:C1'    | 2.51        | 0.41     |
| 1:AA:993:G:H21     | 1:AA:996:A:H62     | 1.69        | 0.41     |
| 23:BB:2104:C:C3'   | 23:BB:2104:C:C6    | 3.04        | 0.41     |
| 23:DB:2320:U:O2'   | 23:DB:2322:A:N7    | 2.48        | 0.41     |
| 23:DB:1704:C:H2'   | 23:DB:1705:A:H8    | 1.85        | 0.41     |
| 1:CA:986:U:H2'     | 1:CA:987:G:C8      | 2.55        | 0.41     |
| 27:BK:18:ARG:HB2   | 27:BK:45:GLU:CG    | 2.51        | 0.41     |
| 23:DB:1843:C:O2'   | 23:DB:1844:C:H5'   | 2.20        | 0.41     |
| 25:DC:6:LYS:HA     | 25:DC:7:PRO:HD3    | 1.91        | 0.41     |
| 23:DB:1670:C:H3'   | 23:DB:1671:U:H6    | 1.86        | 0.41     |
| 1:AA:1132:C:H2'    | 1:AA:1133:G:H8     | 1.85        | 0.41     |
| 28:BP:80:VAL:CG1   | 28:BP:81:ASP:N     | 2.83        | 0.41     |
| 23:DB:1517:G:H2'   | 23:DB:1518:C:C6    | 2.56        | 0.41     |
| 1:AA:1222:G:O2'    | 1:AA:1223:C:H5'    | 2.21        | 0.41     |
| 23:DB:584:C:O2'    | 23:DB:585:G:H5'    | 2.21        | 0.41     |
| 23:DB:2207:C:H2'   | 23:DB:2208:C:C6    | 2.56        | 0.41     |
| 23:BB:1653:G:O6    | 42:BN:11:ASN:ND2   | 2.54        | 0.41     |
| 40:DH:110:VAL:HG13 | 40:DH:110:VAL:O    | 2.21        | 0.41     |
| 24:DI:46:ASP:HA    | 24:DI:50:LYS:HE2   | 2.03        | 0.41     |
| 1:AA:230:G:O2'     | 1:AA:231:U:H5'     | 2.20        | 0.41     |
| 24:DI:91:LYS:HD2   | 24:DI:91:LYS:N     | 2.35        | 0.41     |
| 20:AB:127:LYS:HB3  | 20:AB:127:LYS:NZ   | 2.36        | 0.41     |
| 23:BB:1951:U:H2'   | 23:BB:1952:A:H3'   | 2.03        | 0.41     |
| 50:DT:5:GLU:HA     | 50:DT:8:LEU:HD12   | 2.02        | 0.41     |
| 52:BW:28:GLU:O     | 52:BW:30:VAL:N     | 2.54        | 0.41     |
| 52:BW:43:LYS:HD2   | 52:BW:79:ILE:CD1   | 2.42        | 0.41     |
| 52:DW:18:LYS:O     | 52:DW:34:SER:HA    | 2.20        | 0.41     |
| 6:AG:148:LYS:N     | 10:AK:55:ARG:NH2   | 2.69        | 0.41     |
| 48:DG:10:VAL:CG1   | 48:DG:14:VAL:HG21  | 2.51        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2751:G:H4'   | 48:DG:3:VAL:CG1    | 2.51        | 0.41     |
| 37:DL:90:VAL:HG23  | 37:DL:120:VAL:HG11 | 2.03        | 0.41     |
| 16:AQ:61:ARG:C     | 16:AQ:61:ARG:HD2   | 2.40        | 0.41     |
| 40:BH:68:ARG:H     | 40:BH:68:ARG:HG2   | 1.60        | 0.41     |
| 16:CQ:62:GLU:HB2   | 16:CQ:72:TRP:CE2   | 2.56        | 0.41     |
| 53:D6:43:VAL:HG22  | 53:D6:82:ALA:HB3   | 2.02        | 0.41     |
| 53:B6:64:ARG:HD3   | 53:B6:104:PRO:HA   | 2.03        | 0.41     |
| 53:B6:30:THR:C     | 53:B6:32:ARG:N     | 2.73        | 0.41     |
| 53:B6:57:THR:HG22  | 53:B6:58:VAL:N     | 2.35        | 0.41     |
| 40:BH:81:ALA:HB1   | 40:BH:147:VAL:HG23 | 2.03        | 0.41     |
| 40:BH:80:ILE:O     | 40:BH:146:VAL:HG22 | 2.21        | 0.41     |
| 23:BB:1141:U:H5'   | 41:BJ:27:ARG:HH21  | 1.85        | 0.41     |
| 44:DQ:94:LEU:HG    | 49:DR:11:GLN:HE21  | 1.86        | 0.41     |
| 27:DK:47:ILE:HG23  | 27:DK:48:PRO:N     | 2.34        | 0.41     |
| 8:AI:35:GLU:C      | 8:AI:37:TYR:H      | 2.24        | 0.41     |
| 35:DV:50:MET:O     | 35:DV:56:PHE:HB2   | 2.21        | 0.41     |
| 25:BC:76:VAL:O     | 25:BC:93:VAL:O     | 2.38        | 0.41     |
| 26:DD:4:LEU:N      | 26:DD:4:LEU:HD22   | 2.35        | 0.41     |
| 37:DL:77:ILE:HG22  | 37:DL:78:ARG:N     | 2.34        | 0.41     |
| 38:DM:71:LYS:HA    | 38:DM:72:PRO:HD3   | 1.90        | 0.41     |
| 47:DF:48:LEU:N     | 47:DF:48:LEU:HD23  | 2.36        | 0.41     |
| 13:CN:79:SER:HG    | 13:CN:82:LYS:HG2   | 1.85        | 0.41     |
| 45:BS:61:ASN:HB3   | 45:BS:62:ASP:H     | 1.45        | 0.41     |
| 23:DB:825:A:O2'    | 37:DL:54:GLN:HB3   | 2.21        | 0.41     |
| 23:DB:2444:G:P     | 29:DE:63:LYS:HD2   | 2.60        | 0.41     |
| 1:CA:599:C:O2'     | 1:CA:600:A:H5'     | 2.20        | 0.41     |
| 23:DB:2673:G:H2'   | 23:DB:2674:G:H8    | 1.85        | 0.41     |
| 44:BQ:56:PHE:O     | 44:BQ:59:LEU:HB3   | 2.21        | 0.41     |
| 44:BQ:63:ARG:NH2   | 44:BQ:96:ASP:CA    | 2.82        | 0.41     |
| 48:BG:26:LYS:HA    | 48:BG:32:LEU:N     | 2.34        | 0.41     |
| 46:DU:5:ARG:HH22   | 46:DU:93:ARG:HD3   | 1.86        | 0.41     |
| 23:BB:337:C:H2'    | 23:BB:338:G:O4'    | 2.20        | 0.41     |
| 25:BC:109:LEU:O    | 25:BC:110:LYS:C    | 2.59        | 0.41     |
| 33:B1:8:ILE:HA     | 33:B1:8:ILE:HD13   | 1.87        | 0.41     |
| 47:BF:38:GLY:HA2   | 47:BF:85:GLY:HA3   | 2.03        | 0.41     |
| 46:DU:71:ILE:HD11  | 46:DU:81:ARG:O     | 2.21        | 0.41     |
| 37:BL:77:ILE:HG22  | 37:BL:78:ARG:N     | 2.36        | 0.41     |
| 1:AA:1082:A:O2'    | 1:AA:1083:U:H5'    | 2.21        | 0.41     |
| 47:DF:135:ILE:CD1  | 47:DF:137:PHE:HB3  | 2.51        | 0.41     |
| 47:DF:134:GLN:HE21 | 47:DF:134:GLN:HB3  | 1.53        | 0.41     |
| 47:DF:168:LEU:O    | 47:DF:169:LEU:CB   | 2.66        | 0.41     |
| 10:AK:90:PRO:C     | 10:AK:92:ARG:N     | 2.73        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 21:AU:19:LYS:CD   | 21:AU:20:ARG:HH21  | 2.34        | 0.41     |
| 24:BI:37:PHE:HZ   | 24:BI:56:VAL:HG11  | 1.86        | 0.41     |
| 4:CE:33:THR:HB    | 4:CE:49:TYR:CZ     | 2.56        | 0.41     |
| 1:CA:1077:G:N1    | 1:CA:1081:A:C6     | 2.89        | 0.41     |
| 12:CM:79:LEU:HA   | 12:CM:82:LEU:HB2   | 2.02        | 0.41     |
| 18:AS:18:VAL:O    | 18:AS:22:VAL:HG23  | 2.20        | 0.41     |
| 18:AS:48:ILE:HG22 | 18:AS:49:ALA:N     | 2.29        | 0.41     |
| 18:AS:40:PHE:O    | 18:AS:43:MET:HG3   | 2.21        | 0.41     |
| 33:D1:37:LYS:HB2  | 33:D1:48:TYR:CD2   | 2.55        | 0.41     |
| 23:BB:2848:G:N3   | 23:BB:2849:U:H5    | 2.19        | 0.41     |
| 23:BB:674:G:H4'   | 29:BE:69:ARG:HB3   | 2.03        | 0.41     |
| 23:BB:372:G:O2'   | 23:BB:373:U:P      | 2.78        | 0.41     |
| 50:DT:50:LEU:O    | 50:DT:52:GLU:N     | 2.45        | 0.41     |
| 16:AQ:60:ILE:CG2  | 16:AQ:74:LEU:HA    | 2.42        | 0.41     |
| 23:DB:2468:A:H2'  | 23:DB:2476:A:C5    | 2.56        | 0.41     |
| 38:DM:124:LEU:HA  | 38:DM:125:PRO:HD3  | 1.89        | 0.41     |
| 37:DL:57:LEU:C    | 37:DL:59:ARG:N     | 2.74        | 0.41     |
| 23:BB:1027:A:N3   | 23:BB:2488:G:H5''  | 2.36        | 0.41     |
| 21:CU:3:ILE:CD1   | 21:CU:19:LYS:HA    | 2.46        | 0.41     |
| 23:DB:850:U:O2    | 30:DY:46:MET:HE3   | 2.21        | 0.41     |
| 32:D4:8:LYS:O     | 32:D4:35:GLN:NE2   | 2.51        | 0.41     |
| 23:BB:1056:G:H4'  | 23:BB:1086:A:H8    | 1.85        | 0.41     |
| 18:CS:5:LYS:HB2   | 18:CS:6:LYS:H      | 1.61        | 0.41     |
| 23:BB:971:G:H2'   | 23:BB:972:A:O4'    | 2.20        | 0.41     |
| 35:DV:24:ASN:O    | 35:DV:44:HIS:HB2   | 2.21        | 0.41     |
| 23:DB:1459:G:P    | 23:DB:1459:G:H8    | 2.44        | 0.41     |
| 23:BB:2674:G:H2'  | 23:BB:2675:A:C8    | 2.56        | 0.41     |
| 3:AD:138:PRO:C    | 3:AD:140:ASP:H     | 2.24        | 0.41     |
| 45:BS:25:ARG:CZ   | 45:BS:74:ILE:HG23  | 2.51        | 0.41     |
| 27:DK:54:LYS:C    | 27:DK:56:ASP:H     | 2.24        | 0.41     |
| 20:AB:16:GLY:HA2  | 20:AB:40:ILE:CD1   | 2.51        | 0.41     |
| 23:BB:30:G:H4'    | 23:BB:1215:G:H5'   | 2.02        | 0.41     |
| 20:AB:65:LYS:O    | 20:AB:157:PRO:HB2  | 2.20        | 0.41     |
| 20:AB:53:LEU:CD1  | 20:AB:216:VAL:HG12 | 2.41        | 0.41     |
| 23:DB:591:U:H1'   | 34:D3:1:PRO:H3     | 1.84        | 0.41     |
| 44:DQ:107:ALA:HB1 | 49:DR:48:LYS:CE    | 2.48        | 0.41     |
| 49:DR:4:VAL:CG2   | 49:DR:39:LEU:HG    | 2.51        | 0.41     |
| 23:DB:10:A:N6     | 23:DB:2895:G:H1'   | 2.35        | 0.41     |
| 3:AD:123:MET:HG3  | 3:AD:127:ARG:C     | 2.42        | 0.41     |
| 23:DB:1795:C:O2'  | 23:DB:1796:U:H5'   | 2.21        | 0.41     |
| 35:BV:30:ILE:HG13 | 35:BV:40:ILE:HD11  | 2.03        | 0.41     |
| 1:AA:846:G:H2'    | 1:AA:847:G:C8      | 2.56        | 0.41     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:AA:716:A:N3      | 10:AK:118:ASN:O   | 2.54        | 0.41     |
| 26:DD:149:ASN:C    | 26:DD:152:PRO:HD2 | 2.41        | 0.41     |
| 28:DP:5:LYS:O      | 28:DP:9:GLN:HG2   | 2.21        | 0.41     |
| 36:B2:31:LEU:O     | 36:B2:34:ARG:N    | 2.54        | 0.41     |
| 48:BG:71:LEU:HD13  | 48:BG:74:MET:SD   | 2.61        | 0.41     |
| 13:CN:88:MET:HE2   | 13:CN:88:MET:HA   | 2.03        | 0.41     |
| 34:D3:16:THR:HG21  | 34:D3:48:MET:CE   | 2.51        | 0.41     |
| 1:AA:1073:U:H2'    | 1:AA:1074:G:O4'   | 2.20        | 0.41     |
| 33:B1:22:THR:OG1   | 33:B1:23:THR:N    | 2.53        | 0.41     |
| 1:AA:93:U:H3'      | 1:AA:94:G:C5'     | 2.48        | 0.41     |
| 23:DB:279:A:N6     | 23:DB:361:G:O2'   | 2.44        | 0.41     |
| 23:DB:2146:C:H4'   | 23:DB:2148:G:H1'  | 2.01        | 0.41     |
| 23:DB:98:G:C3'     | 23:DB:99:U:H5''   | 2.51        | 0.41     |
| 15:AP:23:ASP:CG    | 15:AP:25:ARG:HE   | 2.23        | 0.41     |
| 39:DX:20:ASN:HA    | 39:DX:24:GLU:OE1  | 2.21        | 0.41     |
| 23:BB:783:A:H4'    | 23:BB:1779:U:O2   | 2.21        | 0.41     |
| 23:DB:1365:A:O3'   | 51:DZ:11:ARG:NH1  | 2.54        | 0.41     |
| 1:CA:927:G:OP2     | 1:CA:1503:A:C4    | 2.74        | 0.41     |
| 41:BJ:72:LYS:CG    | 41:BJ:89:PHE:HB2  | 2.51        | 0.41     |
| 1:AA:1099:G:H2'    | 1:AA:1100:C:O4'   | 2.21        | 0.41     |
| 4:AE:104:ILE:O     | 4:AE:104:ILE:HG23 | 2.20        | 0.41     |
| 27:BK:88:ASN:ND2   | 27:BK:89:ASN:N    | 2.69        | 0.41     |
| 23:BB:720:U:HO2'   | 23:BB:721:A:H5'   | 1.85        | 0.41     |
| 23:BB:2317:A:H2'   | 23:BB:2318:G:O4'  | 2.20        | 0.41     |
| 19:AT:66:ILE:HG23  | 19:AT:70:LYS:CB   | 2.45        | 0.41     |
| 19:AT:70:LYS:HA    | 19:AT:73:ARG:CZ   | 2.51        | 0.41     |
| 16:CQ:67:SER:O     | 16:CQ:68:LYS:C    | 2.58        | 0.41     |
| 10:CK:17:ASP:HB3   | 10:CK:80:ASN:CG   | 2.41        | 0.41     |
| 13:AN:1:ALA:HB1    | 13:AN:6:LYS:CE    | 2.51        | 0.41     |
| 23:BB:2346:A:O4'   | 23:BB:2383:G:O4'  | 2.38        | 0.41     |
| 47:BF:19:PHE:CZ    | 47:BF:164:GLU:HG2 | 2.55        | 0.41     |
| 23:BB:122:G:O2'    | 23:BB:123:G:H5'   | 2.21        | 0.41     |
| 34:B3:6:VAL:HG23   | 34:B3:60:CYS:O    | 2.20        | 0.41     |
| 25:DC:86:ARG:HH11  | 25:DC:86:ARG:HB3  | 1.85        | 0.41     |
| 39:DX:59:GLU:CD    | 39:DX:60:LYS:H    | 2.24        | 0.41     |
| 25:BC:123:ILE:HD13 | 25:BC:135:PRO:HD2 | 2.03        | 0.41     |
| 6:AG:22:LEU:O      | 6:AG:25:PHE:HB3   | 2.21        | 0.41     |
| 28:BP:33:GLU:OE1   | 28:BP:33:GLU:HA   | 2.20        | 0.41     |
| 28:BP:23:ASP:O     | 28:BP:46:VAL:HG22 | 2.21        | 0.41     |
| 1:CA:1459:G:O2'    | 1:CA:1460:C:H5'   | 2.21        | 0.41     |
| 23:DB:20:C:O2'     | 23:DB:21:A:H5'    | 2.21        | 0.41     |
| 23:DB:2028:U:H2'   | 23:DB:2029:G:O4'  | 2.20        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 15:CP:1:MET:HA    | 15:CP:1:MET:HE3   | 2.03        | 0.41     |
| 45:DS:95:ARG:O    | 45:DS:96:ILE:HG22 | 2.20        | 0.41     |
| 1:CA:1099:G:OP1   | 20:CB:94:ARG:HD3  | 2.21        | 0.41     |
| 15:CP:61:VAL:HA   | 15:CP:65:ALA:HB3  | 2.03        | 0.41     |
| 23:BB:1739:A:H2'  | 23:BB:1740:G:C8   | 2.55        | 0.41     |
| 3:AD:19:PHE:HB3   | 3:AD:22:SER:OG    | 2.20        | 0.41     |
| 39:BX:5:GLU:HA    | 39:BX:5:GLU:OE2   | 2.21        | 0.41     |
| 1:AA:734:G:H2'    | 1:AA:735:C:C6     | 2.56        | 0.41     |
| 1:AA:66:A:H5'     | 1:AA:173:U:O4     | 2.21        | 0.41     |
| 1:CA:1009:U:H1'   | 1:CA:1021:A:N1    | 2.35        | 0.41     |
| 52:DW:77:LYS:N    | 52:DW:77:LYS:NZ   | 2.62        | 0.41     |
| 14:AO:11:ILE:HG13 | 14:AO:15:PHE:CE1  | 2.56        | 0.41     |
| 42:BN:13:ASN:C    | 42:BN:15:SER:H    | 2.24        | 0.41     |
| 23:DB:1924:C:H2'  | 23:DB:1925:C:C6   | 2.55        | 0.41     |
| 1:AA:377:G:H2'    | 1:AA:378:G:C8     | 2.53        | 0.41     |
| 23:BB:510:C:H2'   | 23:BB:511:U:O4'   | 2.20        | 0.41     |
| 50:BT:69:ARG:HH11 | 50:BT:69:ARG:CB   | 2.34        | 0.41     |
| 23:BB:1904:G:O2'  | 23:BB:1905:C:H5'  | 2.21        | 0.41     |
| 23:DB:1317:G:H2'  | 23:DB:1318:U:C6   | 2.56        | 0.41     |
| 23:DB:2020:A:C2   | 23:DB:2022:U:O4'  | 2.74        | 0.41     |
| 23:BB:2603:G:O2'  | 23:BB:2604:U:H5'  | 2.21        | 0.41     |
| 1:AA:499:A:H1'    | 1:AA:500:G:O4'    | 2.20        | 0.41     |
| 23:DB:2228:G:H2'  | 23:DB:2229:U:C6   | 2.56        | 0.41     |
| 23:BB:2292:U:O2'  | 23:BB:2293:G:H5'  | 2.21        | 0.41     |
| 23:DB:2568:U:H6   | 23:DB:2568:U:O5'  | 2.04        | 0.41     |
| 51:BZ:63:GLY:HA3  | 51:BZ:66:THR:OG1  | 2.21        | 0.41     |
| 51:DZ:68:LEU:O    | 51:DZ:72:ARG:HG2  | 2.20        | 0.41     |
| 23:DB:4:U:O2'     | 23:DB:5:A:H5'     | 2.21        | 0.41     |
| 23:BB:1400:U:H2'  | 23:BB:1401:G:H8   | 1.85        | 0.41     |
| 28:DP:48:ALA:HB3  | 28:DP:59:THR:CB   | 2.50        | 0.41     |
| 14:AO:45:GLU:HB3  | 14:AO:46:HIS:HD1  | 1.85        | 0.41     |
| 22:BA:46:A:H2'    | 22:BA:47:C:C6     | 2.56        | 0.41     |
| 23:DB:958:U:H3    | 38:DM:16:ARG:HB3  | 1.86        | 0.41     |
| 23:DB:814:C:H2'   | 23:DB:815:C:H6    | 1.85        | 0.41     |
| 23:DB:1883:U:H2'  | 23:DB:1884:G:C1'  | 2.51        | 0.41     |
| 23:BB:832:U:P     | 37:BL:38:GLN:H    | 2.43        | 0.41     |
| 19:AT:27:MET:HE2  | 19:AT:28:ARG:HG2  | 2.03        | 0.41     |
| 1:AA:692:U:O4     | 10:AK:53:GLY:HA2  | 2.20        | 0.41     |
| 23:BB:1930:G:H2'  | 23:BB:1968:G:N1   | 2.35        | 0.41     |
| 23:DB:1013:C:H2'  | 23:DB:1014:A:H8   | 1.86        | 0.41     |
| 51:BZ:20:HIS:O    | 51:BZ:21:ALA:HB3  | 2.21        | 0.41     |
| 23:DB:2552:U:C2   | 23:DB:2554:U:H5'  | 2.56        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:BB:2730:C:O2'   | 23:BB:2731:G:H5'   | 2.21        | 0.41     |
| 37:DL:136:GLU:HA   | 37:DL:140:GLY:N    | 2.35        | 0.41     |
| 23:BB:779:U:O2'    | 23:BB:780:G:H5'    | 2.20        | 0.41     |
| 1:CA:384:G:H2'     | 1:CA:385:C:H6      | 1.85        | 0.41     |
| 26:DD:172:VAL:HG11 | 26:DD:175:LEU:HD11 | 2.03        | 0.41     |
| 23:BB:1885:A:H3'   | 23:BB:1886:U:H6    | 1.84        | 0.41     |
| 2:CC:10:ARG:NH2    | 2:CC:181:ILE:HD13  | 2.35        | 0.41     |
| 47:DF:119:LYS:HD2  | 47:DF:119:LYS:N    | 2.36        | 0.41     |
| 34:B3:57:VAL:C     | 34:B3:59:ALA:H     | 2.23        | 0.41     |
| 23:BB:1670:C:H3'   | 23:BB:1671:U:H6    | 1.86        | 0.41     |
| 23:BB:1676:A:C2    | 23:BB:1677:A:H1'   | 2.55        | 0.41     |
| 23:DB:1426:G:H8    | 23:DB:1426:G:OP2   | 2.04        | 0.41     |
| 14:AO:58:ARG:HH21  | 14:AO:62:GLN:HE22  | 1.67        | 0.41     |
| 23:BB:1843:C:O2'   | 23:BB:1844:C:H5'   | 2.20        | 0.41     |
| 23:DB:963:U:H2'    | 23:DB:964:C:C6     | 2.56        | 0.41     |
| 23:DB:2301:C:H2'   | 23:DB:2302:U:H6    | 1.86        | 0.41     |
| 10:AK:115:ILE:O    | 10:AK:115:ILE:HD12 | 2.21        | 0.41     |
| 23:BB:428:A:H2'    | 23:BB:429:A:O4'    | 2.21        | 0.41     |
| 2:AC:40:GLN:HG3    | 2:AC:41:TYR:N      | 2.36        | 0.41     |
| 23:DB:1435:G:H2'   | 23:DB:1436:G:C8    | 2.56        | 0.41     |
| 49:DR:81:LYS:HA    | 49:DR:81:LYS:HD3   | 1.84        | 0.41     |
| 37:BL:81:ASP:HA    | 37:BL:84:LYS:CE    | 2.51        | 0.41     |
| 26:DD:35:THR:OG1   | 26:DD:49:GLN:HG2   | 2.20        | 0.41     |
| 14:CO:45:GLU:O     | 14:CO:47:LYS:N     | 2.52        | 0.41     |
| 1:CA:1065:U:H1'    | 1:CA:1066:C:OP2    | 2.20        | 0.41     |
| 23:BB:1009:A:P     | 41:BJ:39:LYS:HZ2   | 2.44        | 0.41     |
| 1:AA:51:A:C2       | 1:AA:353:A:N7      | 2.89        | 0.41     |
| 24:DI:14:ALA:HB3   | 24:DI:51:GLY:H     | 1.86        | 0.41     |
| 23:DB:146:A:H2'    | 23:DB:147:C:C6     | 2.56        | 0.41     |
| 51:DZ:36:HIS:CG    | 51:DZ:37:ARG:N     | 2.89        | 0.41     |
| 23:BB:2582:G:O2'   | 23:BB:2583:G:H5'   | 2.20        | 0.41     |
| 43:DO:30:ARG:HG3   | 43:DO:30:ARG:HH11  | 1.85        | 0.41     |
| 23:BB:268:C:H2'    | 23:BB:268:C:O2     | 2.21        | 0.41     |
| 47:DF:51:ASN:HD22  | 47:DF:51:ASN:HA    | 1.66        | 0.41     |
| 23:BB:1806:C:C2'   | 23:BB:1807:G:H5'   | 2.51        | 0.41     |
| 23:DB:1068:G:C6    | 23:DB:1069:A:N6    | 2.89        | 0.41     |
| 25:BC:29:PHE:CE2   | 25:BC:31:PRO:HG2   | 2.55        | 0.41     |
| 23:DB:1904:G:O2'   | 23:DB:1905:C:H5'   | 2.20        | 0.41     |
| 40:DH:117:LEU:HA   | 40:DH:118:PRO:HD3  | 1.96        | 0.41     |
| 31:B0:56:LYS:O     | 31:B0:56:LYS:HD3   | 2.20        | 0.41     |
| 1:AA:355:C:O2'     | 1:AA:356:A:H5'     | 2.21        | 0.41     |
| 23:DB:490:C:H3'    | 23:DB:491:G:H5''   | 2.03        | 0.41     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:DB:1099:G:C4'  | 24:DI:4:VAL:HB     | 2.51        | 0.41     |
| 10:AK:124:LYS:CA  | 21:AU:34:ARG:HB3   | 2.26        | 0.41     |
| 23:BB:852:U:H2'   | 23:BB:853:C:H6     | 1.86        | 0.41     |
| 52:BW:42:THR:O    | 52:BW:43:LYS:HE3   | 2.21        | 0.41     |
| 52:BW:49:ASN:HB2  | 52:BW:60:ALA:CA    | 2.45        | 0.41     |
| 52:BW:64:GLY:HA2  | 52:BW:84:GLU:HG2   | 2.02        | 0.41     |
| 48:BG:8:VAL:CG1   | 48:BG:49:LEU:HB2   | 2.45        | 0.41     |
| 48:BG:7:PRO:O     | 48:BG:8:VAL:HB     | 2.20        | 0.41     |
| 23:DB:1819:A:OP1  | 25:DC:154:ALA:HA   | 2.20        | 0.41     |
| 25:DC:109:LEU:O   | 25:DC:110:LYS:C    | 2.59        | 0.41     |
| 25:DC:251:THR:O   | 25:DC:252:LYS:HD2  | 2.20        | 0.41     |
| 23:DB:1824:G:OP2  | 25:DC:52:HIS:CE1   | 2.74        | 0.41     |
| 48:BG:91:VAL:HG23 | 48:BG:92:GLY:N     | 2.35        | 0.41     |
| 21:AU:36:PHE:O    | 21:AU:39:LYS:HE3   | 2.21        | 0.41     |
| 27:DK:34:GLY:O    | 27:DK:36:GLY:N     | 2.53        | 0.41     |
| 40:BH:116:ARG:HD3 | 40:BH:133:GLN:HB2  | 2.03        | 0.41     |
| 40:BH:84:ALA:HB3  | 40:BH:148:ALA:HB2  | 2.02        | 0.41     |
| 51:DZ:31:PRO:HB2  | 51:DZ:33:LEU:CD1   | 2.44        | 0.41     |
| 23:DB:988:A:P     | 30:DY:11:SER:HB3   | 2.60        | 0.41     |
| 1:AA:1422:G:H5'   | 27:BK:48:PRO:HB3   | 2.03        | 0.41     |
| 25:BC:117:SER:HA  | 25:BC:128:THR:O    | 2.20        | 0.41     |
| 25:BC:93:VAL:CG2  | 25:BC:115:ILE:HD11 | 2.50        | 0.41     |
| 23:DB:1005:C:H1'  | 23:DB:1012:U:C4    | 2.55        | 0.41     |
| 25:DC:94:LEU:CD1  | 25:DC:100:ARG:HD3  | 2.46        | 0.41     |
| 48:BG:15:ASP:HA   | 48:BG:26:LYS:NZ    | 2.36        | 0.41     |
| 51:BZ:36:HIS:CG   | 51:BZ:37:ARG:N     | 2.89        | 0.41     |
| 53:B6:130:ARG:HG3 | 53:B6:130:ARG:HH11 | 1.86        | 0.41     |
| 22:BA:24:G:C2     | 22:BA:28:C:C5      | 3.09        | 0.41     |
| 30:BY:16:LEU:N    | 30:BY:16:LEU:HD22  | 2.17        | 0.41     |
| 42:BN:79:LEU:HA   | 42:BN:83:LEU:HD12  | 2.02        | 0.41     |
| 24:DI:73:PRO:CG   | 24:DI:78:LEU:HD21  | 2.47        | 0.41     |
| 47:BF:42:ALA:O    | 47:BF:45:ASP:N     | 2.53        | 0.41     |
| 47:BF:48:LEU:N    | 47:BF:48:LEU:HD23  | 2.36        | 0.41     |
| 47:BF:27:VAL:O    | 47:BF:27:VAL:HG23  | 2.21        | 0.41     |
| 42:BN:100:CYS:SG  | 42:BN:101:GLY:N    | 2.94        | 0.41     |
| 7:AH:35:ILE:HG13  | 7:AH:35:ILE:H      | 1.70        | 0.41     |
| 1:CA:954:G:H2'    | 1:CA:955:U:C6      | 2.55        | 0.41     |
| 1:CA:865:A:H2     | 1:CA:918:A:H4'     | 1.85        | 0.41     |
| 1:AA:1271:A:O2'   | 1:AA:1272:G:H5'    | 2.21        | 0.41     |
| 18:AS:20:LYS:HD2  | 18:AS:20:LYS:O     | 2.21        | 0.41     |
| 11:AL:49:ARG:HH12 | 11:AL:88:ASP:CB    | 2.33        | 0.41     |
| 23:BB:804:A:H5"   | 23:BB:805:G:OP1    | 2.21        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 37:DL:29:LYS:CG    | 37:DL:30:THR:HG23  | 2.42        | 0.41     |
| 9:CJ:52:LEU:CA     | 9:CJ:62:ARG:HA     | 2.44        | 0.41     |
| 48:BG:148:ARG:HD3  | 48:BG:152:ARG:CD   | 2.51        | 0.41     |
| 20:CB:27:LYS:C     | 20:CB:27:LYS:HD2   | 2.40        | 0.41     |
| 1:AA:123:U:H5''    | 1:AA:311:C:O2'     | 2.21        | 0.41     |
| 23:DB:2886:A:N6    | 31:D0:39:ARG:CZ    | 2.84        | 0.41     |
| 29:DE:69:ARG:HG2   | 29:DE:69:ARG:HH11  | 1.86        | 0.41     |
| 26:DD:186:LEU:HD11 | 28:DP:3:ILE:CG1    | 2.45        | 0.41     |
| 20:CB:161:PHE:CZ   | 20:CB:216:VAL:HG11 | 2.56        | 0.41     |
| 23:BB:125:A:C6     | 36:B2:10:LEU:HD23  | 2.56        | 0.41     |
| 23:BB:1104:C:O2'   | 23:BB:1105:U:H5'   | 2.20        | 0.41     |
| 11:AL:21:PRO:HG2   | 11:AL:94:TYR:OH    | 2.20        | 0.41     |
| 37:BL:101:ILE:HG22 | 37:BL:102:GLY:N    | 2.35        | 0.41     |
| 20:CB:119:GLN:CD   | 20:CB:136:ARG:HH11 | 2.25        | 0.41     |
| 23:DB:360:U:H2'    | 23:DB:361:G:N9     | 2.35        | 0.41     |
| 7:CH:45:ILE:HD13   | 7:CH:60:LEU:HD11   | 2.03        | 0.41     |
| 1:AA:1003:G:H21    | 1:AA:1005:A:H5'    | 1.86        | 0.41     |
| 3:CD:90:LEU:H      | 3:CD:90:LEU:HD22   | 1.86        | 0.41     |
| 2:CC:155:ARG:HD2   | 2:CC:155:ARG:HA    | 1.88        | 0.41     |
| 23:BB:580:U:O2'    | 23:BB:581:C:H5'    | 2.21        | 0.41     |
| 23:BB:1785:A:H2'   | 23:BB:1787:A:N7    | 2.36        | 0.41     |
| 1:CA:1342:C:O2'    | 1:CA:1343:G:H5'    | 2.22        | 0.41     |
| 4:CE:148:SER:OG    | 4:CE:151:MET:HB2   | 2.21        | 0.41     |
| 11:AL:107:LYS:C    | 11:AL:109:ARG:H    | 2.23        | 0.41     |
| 29:BE:191:ASP:O    | 29:BE:194:LYS:HB3  | 2.21        | 0.41     |
| 49:BR:63:VAL:HA    | 49:BR:95:ASP:O     | 2.21        | 0.41     |
| 35:BV:31:TYR:CB    | 35:BV:37:PRO:HG3   | 2.50        | 0.41     |
| 23:DB:1729:U:H2'   | 23:DB:1730:C:H5'   | 2.03        | 0.41     |
| 23:DB:1430:G:O2'   | 23:DB:1431:A:H5'   | 2.21        | 0.41     |
| 53:B6:137:LEU:HD11 | 53:B6:158:GLU:CD   | 2.42        | 0.41     |
| 1:AA:167:A:O2'     | 1:AA:168:G:H5'     | 2.21        | 0.41     |
| 1:AA:103:U:H1'     | 1:AA:171:A:N1      | 2.36        | 0.41     |
| 1:AA:173:U:H5      | 1:AA:198:G:N3      | 2.19        | 0.41     |
| 27:DK:2:ILE:HA     | 27:DK:33:ALA:H     | 1.86        | 0.41     |
| 45:BS:95:ARG:O     | 45:BS:96:ILE:HG22  | 2.21        | 0.41     |
| 23:DB:543:G:H2'    | 23:DB:545:U:OP1    | 2.21        | 0.41     |
| 23:BB:636:G:H4'    | 23:BB:638:G:O3'    | 2.21        | 0.41     |
| 1:CA:373:A:H1'     | 1:CA:481:G:H1'     | 2.03        | 0.41     |
| 23:BB:228:C:O2     | 23:BB:418:C:H4'    | 2.21        | 0.41     |
| 23:DB:121:G:H2'    | 23:DB:122:G:H8     | 1.86        | 0.41     |
| 23:DB:510:C:H2'    | 23:DB:511:U:O4'    | 2.21        | 0.41     |
| 1:CA:1118:U:H1'    | 1:CA:1179:A:C4     | 2.56        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:DB:747:U:OP2   | 45:DS:90:LYS:NZ   | 2.54        | 0.41     |
| 23:DB:862:G:H2'   | 23:DB:863:A:C8    | 2.56        | 0.41     |
| 23:DB:440:C:H2'   | 23:DB:441:U:H6    | 1.86        | 0.41     |
| 27:BK:70:ARG:HB3  | 27:BK:70:ARG:HH11 | 1.85        | 0.41     |
| 26:DD:127:PHE:HB3 | 26:DD:128:ARG:H   | 1.70        | 0.41     |
| 1:AA:1030:U:O2    | 1:AA:1030:U:C2'   | 2.69        | 0.41     |
| 23:BB:1880:U:H2'  | 23:BB:1881:C:C6   | 2.56        | 0.41     |
| 46:DU:25:LYS:CE   | 46:DU:36:GLU:HG3  | 2.49        | 0.41     |
| 1:CA:628:G:H2'    | 1:CA:629:A:H8     | 1.86        | 0.41     |
| 23:DB:599:A:O2'   | 23:DB:600:G:H5'   | 2.20        | 0.41     |
| 9:CJ:65:TYR:C     | 13:CN:98:ALA:HB2  | 2.41        | 0.41     |
| 23:DB:2544:G:O2'  | 23:DB:2545:G:H5'  | 2.21        | 0.41     |
| 42:BN:6:SER:OG    | 42:BN:7:GLY:N     | 2.54        | 0.41     |
| 26:DD:40:LEU:HA   | 26:DD:45:TYR:N    | 2.36        | 0.41     |
| 53:D6:150:SER:HB3 | 53:D6:153:GLU:OE1 | 2.20        | 0.41     |
| 23:DB:346:A:H3'   | 23:DB:347:A:H8    | 1.86        | 0.41     |
| 37:BL:40:SER:OG   | 37:BL:41:ARG:HG3  | 2.21        | 0.41     |
| 23:DB:1053:C:C2'  | 23:DB:1054:A:H5'  | 2.50        | 0.41     |
| 23:BB:2595:G:N1   | 23:BB:2599:G:C6   | 2.89        | 0.41     |
| 1:AA:884:U:H4'    | 1:AA:885:G:H5''   | 2.03        | 0.41     |
| 23:BB:437:U:H2'   | 23:BB:438:G:H8    | 1.85        | 0.41     |
| 28:DP:44:GLY:HA3  | 28:DP:60:VAL:CG1  | 2.51        | 0.41     |
| 1:AA:1367:C:O2'   | 1:AA:1368:A:H5'   | 2.20        | 0.41     |
| 1:CA:1222:G:O2'   | 1:CA:1223:C:H5'   | 2.20        | 0.41     |
| 5:CF:10:VAL:HG12  | 5:CF:11:HIS:H     | 1.86        | 0.41     |
| 23:BB:2010:G:O2'  | 23:BB:2011:U:H5'  | 2.20        | 0.41     |
| 23:DB:1228:G:H2'  | 23:DB:1229:C:C6   | 2.56        | 0.41     |
| 23:DB:1360:G:H2'  | 23:DB:1361:G:C5'  | 2.51        | 0.41     |
| 43:BO:14:ALA:C    | 43:BO:16:ARG:N    | 2.74        | 0.41     |
| 24:DI:53:PRO:HG2  | 24:DI:77:VAL:HG11 | 2.01        | 0.41     |
| 47:DF:61:GLY:HA3  | 47:DF:94:ARG:HD2  | 2.03        | 0.41     |
| 23:BB:388:G:N7    | 23:BB:390:U:H2'   | 2.36        | 0.41     |
| 2:AC:89:VAL:HG12  | 2:AC:93:ILE:HD11  | 2.03        | 0.41     |
| 1:AA:51:A:H4'     | 1:AA:52:C:H5'     | 2.03        | 0.41     |
| 1:AA:1204:A:H2'   | 1:AA:1205:U:O4'   | 2.21        | 0.41     |
| 23:BB:2696:U:O2'  | 23:BB:2697:G:H5'  | 2.21        | 0.41     |
| 1:CA:1023:U:O2'   | 1:CA:1024:G:H5'   | 2.21        | 0.41     |
| 41:BJ:121:LYS:HB2 | 41:BJ:121:LYS:HE3 | 1.97        | 0.41     |
| 11:CL:65:TYR:HB3  | 11:CL:95:HIS:CD2  | 2.56        | 0.41     |
| 23:BB:93:G:O2'    | 23:BB:94:A:H5'    | 2.21        | 0.41     |
| 23:BB:2366:A:H4'  | 52:BW:61:LYS:HE2  | 2.02        | 0.40     |
| 52:DW:17:ALA:HA   | 52:DW:35:ILE:CG2  | 2.26        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 52:DW:32:ALA:C    | 52:DW:34:SER:N     | 2.74        | 0.40     |
| 25:DC:145:MET:CE  | 25:DC:153:LEU:HD11 | 2.51        | 0.40     |
| 23:DB:1818:U:C4   | 25:DC:152:GLN:HB3  | 2.56        | 0.40     |
| 37:DL:108:ALA:HB3 | 37:DL:125:LEU:HD21 | 2.03        | 0.40     |
| 37:DL:121:THR:HB  | 37:DL:141:LYS:HD2  | 2.03        | 0.40     |
| 53:D6:43:VAL:CG2  | 53:D6:52:LEU:HD12  | 2.47        | 0.40     |
| 53:B6:66:LEU:O    | 53:B6:101:ILE:N    | 2.45        | 0.40     |
| 23:DB:2210:U:C4   | 23:DB:2212:A:N7    | 2.89        | 0.40     |
| 1:AA:1346:A:N1    | 1:AA:1374:A:H5'    | 2.36        | 0.40     |
| 1:AA:1014:A:H2'   | 1:AA:1015:G:O4'    | 2.21        | 0.40     |
| 35:BV:1:MET:CE    | 35:BV:2:PHE:H      | 2.35        | 0.40     |
| 23:DB:637:A:OP2   | 37:DL:128:THR:HG21 | 2.21        | 0.40     |
| 23:BB:996:A:O2'   | 23:BB:997:G:H5'    | 2.20        | 0.40     |
| 44:BQ:79:ILE:HG23 | 44:BQ:80:ASN:N     | 2.36        | 0.40     |
| 23:BB:338:G:N2    | 23:BB:339:U:H1'    | 2.36        | 0.40     |
| 30:BY:51:SER:C    | 30:BY:53:MET:N     | 2.74        | 0.40     |
| 33:B1:51:ALA:O    | 33:B1:52:LYS:C     | 2.60        | 0.40     |
| 23:BB:2306:C:H6   | 23:BB:2306:C:O5'   | 2.04        | 0.40     |
| 47:BF:137:PHE:O   | 47:BF:138:PRO:C    | 2.58        | 0.40     |
| 40:DH:126:GLY:C   | 40:DH:146:VAL:H    | 2.20        | 0.40     |
| 45:DS:13:SER:HB3  | 45:DS:16:LYS:HE3   | 2.03        | 0.40     |
| 47:DF:141:ASP:O   | 47:DF:142:TYR:C    | 2.58        | 0.40     |
| 47:DF:116:LEU:HB3 | 47:DF:176:PHE:CA   | 2.51        | 0.40     |
| 47:DF:27:VAL:O    | 47:DF:27:VAL:HG23  | 2.21        | 0.40     |
| 18:CS:50:VAL:HG22 | 18:CS:70:LEU:HD23  | 2.03        | 0.40     |
| 12:AM:38:ILE:HG13 | 12:AM:55:LEU:CD2   | 2.47        | 0.40     |
| 50:DT:1:MET:HG3   | 50:DT:2:ILE:N      | 2.33        | 0.40     |
| 1:AA:333:U:H2'    | 1:AA:334:C:C6      | 2.56        | 0.40     |
| 48:DG:152:ARG:HG3 | 48:DG:153:PRO:HD2  | 2.03        | 0.40     |
| 35:DV:24:ASN:HB3  | 35:DV:44:HIS:HB3   | 2.02        | 0.40     |
| 35:DV:89:ILE:HD13 | 35:DV:91:PHE:CZ    | 2.57        | 0.40     |
| 28:BP:105:LYS:HA  | 28:BP:108:ARG:NE   | 2.35        | 0.40     |
| 23:DB:2621:G:OP1  | 26:DD:124:ARG:NH2  | 2.54        | 0.40     |
| 42:BN:33:ILE:CG2  | 42:BN:114:GLU:HB2  | 2.45        | 0.40     |
| 42:BN:28:LEU:C    | 42:BN:28:LEU:HD13  | 2.42        | 0.40     |
| 23:DB:2884:U:H4'  | 31:D0:49:ARG:NH2   | 2.36        | 0.40     |
| 23:DB:9:G:H21     | 23:DB:10:A:N6      | 2.07        | 0.40     |
| 9:CJ:7:ARG:CZ     | 9:CJ:101:SER:HB2   | 2.51        | 0.40     |
| 20:CB:65:LYS:O    | 20:CB:157:PRO:HB2  | 2.20        | 0.40     |
| 9:CJ:12:ALA:HB2   | 9:CJ:96:VAL:HG12   | 2.03        | 0.40     |
| 5:CF:39:LEU:HD13  | 5:CF:40:GLU:N      | 2.35        | 0.40     |
| 2:CC:153:SER:OG   | 2:CC:196:GLY:N     | 2.54        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 14:CO:26:GLU:OE2  | 14:CO:77:ARG:HD2   | 2.22        | 0.40     |
| 14:AO:89:ARG:HH22 | 23:BB:716:A:P      | 2.44        | 0.40     |
| 42:BN:3:HIS:O     | 42:BN:4:ARG:HB2    | 2.22        | 0.40     |
| 1:AA:309:A:H2'    | 1:AA:310:G:H8      | 1.87        | 0.40     |
| 1:CA:926:G:H3'    | 1:CA:1505:G:N2     | 2.36        | 0.40     |
| 23:DB:1309:G:H4'  | 36:D2:7:PRO:HB2    | 2.03        | 0.40     |
| 1:CA:1120:C:H2'   | 1:CA:1121:U:C6     | 2.56        | 0.40     |
| 34:B3:60:CYS:C    | 34:B3:61:LEU:HD23  | 2.41        | 0.40     |
| 48:DG:155:PRO:C   | 48:DG:170:THR:HB   | 2.41        | 0.40     |
| 23:DB:1243:C:O2'  | 37:DL:4:ASN:O      | 2.37        | 0.40     |
| 1:CA:781:A:H2'    | 1:CA:782:A:C5'     | 2.48        | 0.40     |
| 8:AI:9:GLY:HA3    | 8:AI:81:GLY:H      | 1.84        | 0.40     |
| 27:BK:73:ASP:OD2  | 27:BK:75:SER:HB3   | 2.21        | 0.40     |
| 23:BB:2001:C:H4'  | 23:BB:2689:U:C2'   | 2.51        | 0.40     |
| 11:CL:14:LYS:HG2  | 11:CL:16:ALA:H     | 1.86        | 0.40     |
| 23:BB:1993:U:H4'  | 26:BD:133:THR:HG21 | 2.01        | 0.40     |
| 10:CK:16:SER:HB3  | 10:CK:79:LYS:CG    | 2.52        | 0.40     |
| 25:BC:166:ARG:HA  | 25:BC:171:VAL:HA   | 2.03        | 0.40     |
| 38:BM:69:PRO:HA   | 38:BM:94:ALA:HA    | 2.02        | 0.40     |
| 23:BB:1040:A:C2   | 23:BB:1116:G:N1    | 2.90        | 0.40     |
| 1:CA:1418:A:H2    | 23:DB:1948:G:N3    | 2.19        | 0.40     |
| 52:BW:77:LYS:N    | 52:BW:77:LYS:NZ    | 2.67        | 0.40     |
| 23:DB:1506:U:H2'  | 23:DB:1507:C:C6    | 2.55        | 0.40     |
| 23:BB:1454:C:O2   | 23:BB:1454:C:O4'   | 2.39        | 0.40     |
| 23:BB:1914:C:H2'  | 23:BB:1915:U:O4'   | 2.21        | 0.40     |
| 23:BB:1508:A:H5'  | 23:BB:1509:A:N6    | 2.36        | 0.40     |
| 23:BB:2277:G:O3'  | 38:BM:11:LYS:HE3   | 2.21        | 0.40     |
| 22:BA:49:C:OP1    | 43:BO:102:ARG:N    | 2.45        | 0.40     |
| 29:DE:1:MET:HB2   | 29:DE:16:GLU:CA    | 2.50        | 0.40     |
| 53:B6:2:THR:H     | 53:B6:5:GLU:CD     | 2.23        | 0.40     |
| 23:DB:509:C:H5''  | 23:DB:510:C:OP2    | 2.20        | 0.40     |
| 1:CA:1258:G:C2    | 1:CA:1278:G:N2     | 2.90        | 0.40     |
| 23:BB:871:U:H2'   | 23:BB:872:U:C6     | 2.54        | 0.40     |
| 23:DB:1292:G:O2'  | 23:DB:1293:C:H5'   | 2.21        | 0.40     |
| 23:DB:1027:A:N3   | 23:DB:2488:G:H5''  | 2.36        | 0.40     |
| 23:DB:1112:G:H2'  | 23:DB:1113:U:O4'   | 2.21        | 0.40     |
| 27:DK:111:LYS:HD3 | 27:DK:111:LYS:N    | 2.36        | 0.40     |
| 23:BB:1292:G:H2'  | 23:BB:1293:C:H6    | 1.83        | 0.40     |
| 23:BB:2320:U:O2'  | 23:BB:2322:A:N7    | 2.48        | 0.40     |
| 28:BP:61:ARG:NH1  | 28:BP:100:ARG:HA   | 2.35        | 0.40     |
| 15:CP:20:VAL:HG21 | 15:CP:32:PHE:CG    | 2.56        | 0.40     |
| 47:BF:120:SER:O   | 47:BF:127:TYR:HA   | 2.21        | 0.40     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:2727:A:O2'   | 23:DB:2728:U:H5'   | 2.21        | 0.40     |
| 23:BB:237:C:O2'    | 23:BB:238:C:H5'    | 2.21        | 0.40     |
| 23:DB:2494:G:O2'   | 38:DM:79:ALA:HA    | 2.20        | 0.40     |
| 25:DC:259:ASN:OD1  | 25:DC:262:THR:HG23 | 2.21        | 0.40     |
| 47:DF:13:LYS:C     | 47:DF:13:LYS:HZ2   | 2.25        | 0.40     |
| 6:AG:120:ALA:HA    | 6:AG:123:LEU:HD12  | 2.02        | 0.40     |
| 1:AA:1491:G:C5     | 55:AA:1661:PAR:H21 | 2.56        | 0.40     |
| 46:BU:60:LYS:HA    | 46:BU:60:LYS:HE2   | 2.02        | 0.40     |
| 23:DB:2298:A:H2'   | 23:DB:2299:U:O4'   | 2.20        | 0.40     |
| 23:DB:2301:C:O2'   | 23:DB:2302:U:H5'   | 2.21        | 0.40     |
| 23:BB:2818:U:H4'   | 23:BB:2837:A:H4'   | 2.02        | 0.40     |
| 18:AS:11:ASP:N     | 18:AS:14:LEU:HD21  | 2.35        | 0.40     |
| 3:CD:106:PHE:CG    | 3:CD:144:ILE:HD11  | 2.56        | 0.40     |
| 1:CA:1434:A:H2'    | 1:CA:1435:G:C8     | 2.56        | 0.40     |
| 23:BB:839:U:H1'    | 23:BB:1191:G:H1'   | 2.04        | 0.40     |
| 23:DB:2515:C:H2'   | 23:DB:2516:A:H8    | 1.86        | 0.40     |
| 23:DB:1396:U:O2    | 23:DB:1396:U:O4'   | 2.39        | 0.40     |
| 20:AB:35:ASN:HD22  | 20:AB:35:ASN:HA    | 1.53        | 0.40     |
| 53:B6:164:ILE:O    | 53:B6:167:GLU:HB2  | 2.21        | 0.40     |
| 1:CA:815:A:OP2     | 1:CA:816:A:H5''    | 2.21        | 0.40     |
| 23:BB:282:A:O2'    | 23:BB:283:G:H5'    | 2.21        | 0.40     |
| 23:BB:1360:G:H2'   | 23:BB:1361:G:H5'   | 2.03        | 0.40     |
| 1:CA:704:A:C2      | 1:CA:705:G:H1'     | 2.56        | 0.40     |
| 23:DB:2856:A:H2'   | 23:DB:2857:G:H8    | 1.87        | 0.40     |
| 24:DI:56:VAL:CG2   | 24:DI:68:PHE:HB2   | 2.51        | 0.40     |
| 23:BB:329:G:H1     | 46:BU:16:LYS:HZ3   | 1.69        | 0.40     |
| 6:CG:67:ASN:ND2    | 6:CG:127:ALA:HA    | 2.36        | 0.40     |
| 38:DM:131:VAL:HG12 | 38:DM:132:THR:N    | 2.36        | 0.40     |
| 1:AA:1394:A:C5     | 1:AA:1501:C:H4'    | 2.55        | 0.40     |
| 38:DM:20:LEU:N     | 38:DM:20:LEU:HD22  | 2.36        | 0.40     |
| 15:AP:51:ARG:NH1   | 15:AP:51:ARG:HG2   | 2.36        | 0.40     |
| 9:AJ:31:ARG:HE     | 9:AJ:31:ARG:HB2    | 1.63        | 0.40     |
| 24:DI:2:LYS:N      | 24:DI:2:LYS:HD2    | 2.36        | 0.40     |
| 10:CK:125:LYS:O    | 21:CU:33:ARG:CZ    | 2.69        | 0.40     |
| 10:AK:125:LYS:O    | 10:AK:126:ARG:C    | 2.59        | 0.40     |
| 52:BW:37:VAL:C     | 52:BW:39:GLN:H     | 2.24        | 0.40     |
| 25:DC:51:ARG:O     | 25:DC:52:HIS:C     | 2.60        | 0.40     |
| 6:AG:87:PRO:HG2    | 6:AG:151:ALA:HB2   | 2.03        | 0.40     |
| 16:CQ:75:VAL:HG23  | 16:CQ:76:ARG:N     | 2.36        | 0.40     |
| 53:B6:69:GLN:CD    | 53:B6:98:ALA:HB2   | 2.41        | 0.40     |
| 23:DB:633:A:H2'    | 23:DB:634:C:O4'    | 2.21        | 0.40     |
| 29:BE:105:LEU:HD21 | 29:BE:177:PRO:CA   | 2.51        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:2199:A:H5'' | 23:BB:2200:C:H5    | 1.86        | 0.40     |
| 40:DH:128:HIS:N   | 40:DH:144:VAL:O    | 2.49        | 0.40     |
| 43:BO:35:ILE:O    | 43:BO:35:ILE:HG22  | 2.20        | 0.40     |
| 51:BZ:40:VAL:O    | 51:BZ:42:SER:N     | 2.51        | 0.40     |
| 23:DB:1059:G:H2'  | 23:DB:1060:U:C6    | 2.56        | 0.40     |
| 23:DB:1060:U:O4   | 24:DI:131:THR:HG22 | 2.21        | 0.40     |
| 47:BF:107:VAL:HA  | 47:BF:111:ARG:HH12 | 1.87        | 0.40     |
| 24:BI:91:LYS:O    | 24:BI:91:LYS:HG3   | 2.21        | 0.40     |
| 23:BB:299:A:N6    | 23:BB:322:A:O2'    | 2.50        | 0.40     |
| 23:BB:322:A:P     | 29:BE:163:ASN:ND2  | 2.94        | 0.40     |
| 23:BB:1461:C:H2'  | 23:BB:1462:C:C6    | 2.56        | 0.40     |
| 45:DS:15:GLN:HA   | 45:DS:18:ARG:HG2   | 2.02        | 0.40     |
| 18:CS:20:LYS:O    | 18:CS:23:GLU:HG3   | 2.21        | 0.40     |
| 23:DB:483:A:H8    | 46:DU:44:HIS:HB3   | 1.86        | 0.40     |
| 29:BE:33:VAL:O    | 29:BE:36:ALA:HB3   | 2.21        | 0.40     |
| 41:BJ:83:GLY:O    | 41:BJ:84:ILE:C     | 2.60        | 0.40     |
| 39:DX:7:ARG:HB2   | 39:DX:7:ARG:CZ     | 2.51        | 0.40     |
| 10:CK:59:PRO:N    | 10:CK:90:PRO:HB2   | 2.36        | 0.40     |
| 2:AC:120:THR:HA   | 2:AC:123:LEU:HD12  | 2.03        | 0.40     |
| 1:AA:1350:A:H2'   | 1:AA:1351:U:H6     | 1.86        | 0.40     |
| 15:CP:66:THR:HG22 | 15:CP:67:ILE:N     | 2.36        | 0.40     |
| 29:DE:147:LEU:O   | 29:DE:168:ASP:O    | 2.39        | 0.40     |
| 23:BB:27:G:O2'    | 23:BB:28:A:H8      | 2.02        | 0.40     |
| 44:BQ:71:ASN:HB3  | 44:BQ:72:GLY:H     | 1.70        | 0.40     |
| 49:BR:4:VAL:H     | 49:BR:38:VAL:HG23  | 1.85        | 0.40     |
| 49:BR:49:ILE:CG2  | 49:BR:54:VAL:HB    | 2.51        | 0.40     |
| 27:DK:112:PHE:O   | 27:DK:113:MET:C    | 2.58        | 0.40     |
| 27:BK:112:PHE:O   | 27:BK:113:MET:C    | 2.60        | 0.40     |
| 27:BK:119:ALA:HB3 | 27:BK:120:PRO:HD3  | 2.03        | 0.40     |
| 29:BE:176:ASP:O   | 29:BE:180:LEU:HG   | 2.22        | 0.40     |
| 23:DB:1444:G:H2'  | 23:DB:1445:G:C8    | 2.56        | 0.40     |
| 9:AJ:12:ALA:HB2   | 9:AJ:96:VAL:HG12   | 2.03        | 0.40     |
| 5:CF:96:VAL:HG12  | 5:CF:97:THR:H      | 1.86        | 0.40     |
| 1:CA:1057:G:H5''  | 2:CC:153:SER:CB    | 2.51        | 0.40     |
| 1:AA:92:U:OP2     | 1:AA:92:U:H6       | 2.04        | 0.40     |
| 23:DB:182:A:H2'   | 23:DB:183:C:H6     | 1.87        | 0.40     |
| 28:DP:50:ARG:HB2  | 28:DP:56:SER:OG    | 2.20        | 0.40     |
| 28:DP:57:ALA:HA   | 28:DP:73:PHE:O     | 2.21        | 0.40     |
| 23:BB:2774:C:H2'  | 23:BB:2775:G:O4'   | 2.22        | 0.40     |
| 29:DE:191:ASP:O   | 29:DE:194:LYS:HB3  | 2.21        | 0.40     |
| 12:AM:89:ARG:HH22 | 12:AM:94:LEU:HD12  | 1.83        | 0.40     |
| 23:DB:320:A:C2    | 29:DE:163:ASN:HB3  | 2.57        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:BB:1139:G:OP1  | 41:BJ:103:ILE:HD12 | 2.21        | 0.40     |
| 16:AQ:67:SER:O    | 16:AQ:68:LYS:C     | 2.58        | 0.40     |
| 11:CL:23:LEU:C    | 11:CL:25:ALA:N     | 2.75        | 0.40     |
| 23:DB:419:U:H2'   | 23:DB:420:C:H6     | 1.84        | 0.40     |
| 23:DB:2592:G:O2'  | 23:DB:2593:U:H5'   | 2.22        | 0.40     |
| 1:AA:237:G:H5''   | 16:AQ:26:ARG:NH2   | 2.36        | 0.40     |
| 1:AA:16:A:C2'     | 1:AA:17:U:H5'      | 2.51        | 0.40     |
| 39:DX:44:LYS:HZ1  | 39:DX:48:ARG:CZ    | 2.34        | 0.40     |
| 39:DX:9:LYS:HZ2   | 39:DX:60:LYS:HE3   | 1.86        | 0.40     |
| 28:BP:51:ASN:O    | 28:BP:52:ARG:HD3   | 2.22        | 0.40     |
| 28:BP:57:ALA:HA   | 28:BP:73:PHE:O     | 2.20        | 0.40     |
| 23:BB:2847:U:OP1  | 28:BP:95:LYS:HD3   | 2.21        | 0.40     |
| 42:DN:92:GLY:HA2  | 42:DN:94:TYR:CZ    | 2.56        | 0.40     |
| 1:AA:66:A:C2'     | 1:AA:67:C:H5'      | 2.51        | 0.40     |
| 19:AT:78:LEU:HA   | 19:AT:78:LEU:HD23  | 1.93        | 0.40     |
| 23:DB:1635:A:H2'  | 23:DB:1636:U:C5'   | 2.51        | 0.40     |
| 9:CJ:83:THR:O     | 9:CJ:87:LEU:HD22   | 2.22        | 0.40     |
| 16:CQ:30:HIS:CB   | 16:CQ:33:TYR:HB2   | 2.51        | 0.40     |
| 23:BB:1948:G:O2'  | 23:BB:1949:G:H5'   | 2.21        | 0.40     |
| 50:DT:13:ALA:O    | 50:DT:33:LYS:N     | 2.54        | 0.40     |
| 6:CG:20:GLU:O     | 6:CG:23:ALA:HB3    | 2.21        | 0.40     |
| 23:DB:1967:C:C2'  | 23:DB:1968:G:H5'   | 2.52        | 0.40     |
| 1:CA:1179:A:H2'   | 1:CA:1180:A:C8     | 2.56        | 0.40     |
| 41:BJ:64:VAL:HG11 | 41:BJ:69:ARG:HD2   | 2.03        | 0.40     |
| 1:AA:1037:C:H2'   | 1:AA:1038:C:H6     | 1.86        | 0.40     |
| 50:BT:13:ALA:O    | 50:BT:33:LYS:N     | 2.54        | 0.40     |
| 22:DA:87:U:C2'    | 22:DA:88:C:O5'     | 2.69        | 0.40     |
| 23:BB:2259:U:H2'  | 23:BB:2260:C:C6    | 2.56        | 0.40     |
| 41:DJ:96:ARG:NE   | 41:DJ:99:ARG:HD2   | 2.35        | 0.40     |
| 23:DB:1900:A:N1   | 23:DB:1970:A:C5    | 2.88        | 0.40     |
| 11:AL:122:LYS:HG3 | 11:AL:123:ALA:N    | 2.35        | 0.40     |
| 23:DB:2691:C:C4   | 23:DB:2719:G:N2    | 2.89        | 0.40     |
| 35:DV:16:ALA:O    | 35:DV:19:ARG:HB2   | 2.22        | 0.40     |
| 23:BB:409:G:H2'   | 23:BB:410:G:C8     | 2.57        | 0.40     |
| 19:AT:19:HIS:CE1  | 19:AT:23:ARG:HG3   | 2.56        | 0.40     |
| 23:BB:247:G:H5''  | 23:BB:386:G:H2'    | 2.03        | 0.40     |
| 1:AA:1289:A:H61   | 8:AI:71:ILE:CD1    | 2.34        | 0.40     |
| 1:AA:1489:G:OP2   | 55:AA:1661:PAR:H54 | 2.19        | 0.40     |
| 23:BB:499:U:H5''  | 46:BU:42:LYS:HG2   | 2.03        | 0.40     |
| 28:DP:60:VAL:O    | 28:DP:70:GLU:HA    | 2.21        | 0.40     |
| 27:DK:18:ARG:HB2  | 27:DK:45:GLU:CG    | 2.51        | 0.40     |
| 23:BB:1693:U:O2'  | 25:BC:13:ARG:NH2   | 2.54        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 28:BP:29:VAL:HG12 | 28:BP:80:VAL:HA    | 2.02        | 0.40     |
| 6:CG:94:ARG:HH12  | 6:CG:98:LEU:HD21   | 1.86        | 0.40     |
| 23:DB:437:U:H2'   | 23:DB:438:G:H8     | 1.86        | 0.40     |
| 1:AA:1121:U:O2'   | 1:AA:1122:U:H5'    | 2.22        | 0.40     |
| 23:BB:2643:G:O2'  | 23:BB:2644:G:H5'   | 2.21        | 0.40     |
| 23:BB:2771:C:H1'  | 26:BD:208:LYS:NZ   | 2.37        | 0.40     |
| 23:BB:103:A:H2'   | 23:BB:104:A:H8     | 1.86        | 0.40     |
| 1:CA:1157:A:H5'   | 1:CA:1158:C:C5     | 2.56        | 0.40     |
| 23:BB:35:G:H1'    | 23:BB:454:A:O4'    | 2.21        | 0.40     |
| 25:BC:24:HIS:CE1  | 25:BC:26:GLY:H     | 2.39        | 0.40     |
| 26:BD:12:THR:HG22 | 26:BD:13:ARG:N     | 2.36        | 0.40     |
| 13:AN:64:ARG:HB2  | 13:AN:77:GLY:O     | 2.21        | 0.40     |
| 1:AA:682:G:O2'    | 1:AA:683:G:H5'     | 2.21        | 0.40     |
| 13:AN:47:LEU:O    | 13:AN:49:THR:N     | 2.54        | 0.40     |
| 14:CO:17:ARG:NH1  | 14:CO:17:ARG:HA    | 2.37        | 0.40     |
| 18:CS:33:TRP:CE3  | 18:CS:33:TRP:N     | 2.90        | 0.40     |
| 23:DB:757:G:H2'   | 23:DB:758:C:H5'    | 2.03        | 0.40     |
| 14:CO:31:LEU:O    | 14:CO:34:ALA:HB3   | 2.20        | 0.40     |
| 23:DB:2417:C:H2'  | 23:DB:2418:A:H8    | 1.87        | 0.40     |
| 23:DB:1099:G:H3'  | 24:DI:2:LYS:HA     | 2.03        | 0.40     |
| 50:BT:4:GLU:O     | 50:BT:8:LEU:HG     | 2.21        | 0.40     |
| 23:DB:2331:G:C4'  | 52:DW:39:GLN:HA    | 2.50        | 0.40     |
| 48:BG:10:VAL:HG13 | 48:BG:14:VAL:HB    | 2.03        | 0.40     |
| 23:DB:2751:G:O4'  | 48:DG:2:ARG:HD3    | 2.21        | 0.40     |
| 53:D6:30:THR:C    | 53:D6:32:ARG:N     | 2.75        | 0.40     |
| 53:D6:68:VAL:CG2  | 53:D6:99:LEU:HD12  | 2.50        | 0.40     |
| 41:BJ:59:ALA:C    | 41:BJ:61:LYS:N     | 2.75        | 0.40     |
| 44:DQ:79:ILE:HG23 | 44:DQ:80:ASN:N     | 2.36        | 0.40     |
| 44:DQ:93:ILE:HG23 | 44:DQ:94:LEU:N     | 2.36        | 0.40     |
| 44:DQ:63:ARG:CZ   | 44:DQ:96:ASP:HA    | 2.51        | 0.40     |
| 1:AA:958:A:N1     | 18:AS:53:GLY:C     | 2.75        | 0.40     |
| 13:CN:68:ARG:CB   | 13:CN:68:ARG:HH11  | 2.17        | 0.40     |
| 1:AA:600:A:O2'    | 1:AA:601:G:H5'     | 2.21        | 0.40     |
| 42:DN:38:LEU:CD1  | 42:DN:42:LYS:HD2   | 2.51        | 0.40     |
| 50:BT:28:ASN:ND2  | 50:BT:29:THR:HG23  | 2.36        | 0.40     |
| 25:DC:76:VAL:O    | 25:DC:78:GLU:N     | 2.54        | 0.40     |
| 1:CA:1328:C:H5''  | 12:CM:27:THR:CG2   | 2.37        | 0.40     |
| 51:BZ:30:LEU:HA   | 51:BZ:31:PRO:HD3   | 1.95        | 0.40     |
| 22:BA:29:A:C4     | 22:BA:56:G:N2      | 2.89        | 0.40     |
| 47:BF:134:GLN:H   | 47:BF:150:GLY:N    | 2.16        | 0.40     |
| 1:AA:1396:A:O4'   | 1:AA:1398:A:H1'    | 2.21        | 0.40     |
| 47:DF:140:ILE:H   | 47:DF:140:ILE:HG13 | 1.58        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 47:DF:8:LYS:HD3   | 47:DF:9:ASP:OD2    | 2.21        | 0.40     |
| 1:CA:1077:G:N2    | 1:CA:1080:A:OP2    | 2.53        | 0.40     |
| 18:CS:18:VAL:O    | 18:CS:22:VAL:HG23  | 2.22        | 0.40     |
| 18:CS:49:ALA:HB1  | 18:CS:56:HIS:HB3   | 2.03        | 0.40     |
| 20:AB:46:VAL:N    | 20:AB:47:PRO:CD    | 2.83        | 0.40     |
| 23:BB:2468:A:H2'  | 23:BB:2476:A:C5    | 2.56        | 0.40     |
| 50:DT:41:ALA:C    | 50:DT:43:ILE:N     | 2.75        | 0.40     |
| 3:AD:172:VAL:HG23 | 3:AD:178:GLU:O     | 2.22        | 0.40     |
| 13:AN:80:ARG:HG2  | 13:AN:80:ARG:HH11  | 1.86        | 0.40     |
| 16:AQ:45:VAL:HG12 | 16:AQ:46:HIS:H     | 1.85        | 0.40     |
| 29:BE:28:VAL:HG23 | 29:BE:29:HIS:N     | 2.36        | 0.40     |
| 23:BB:2893:A:H5'' | 23:BB:2894:G:H5'   | 2.04        | 0.40     |
| 23:DB:819:A:OP2   | 23:DB:1187:G:N2    | 2.54        | 0.40     |
| 23:BB:979:A:H2'   | 23:BB:982:C:N4     | 2.36        | 0.40     |
| 13:AN:88:MET:HE2  | 13:AN:88:MET:HA    | 2.02        | 0.40     |
| 23:DB:2869:G:H2'  | 23:DB:2870:C:O4'   | 2.21        | 0.40     |
| 1:CA:1324:A:H2'   | 1:CA:1325:C:H6     | 1.86        | 0.40     |
| 32:D4:36:ARG:O    | 32:D4:37:GLN:C     | 2.59        | 0.40     |
| 1:AA:1237:C:H3'   | 1:AA:1336:C:N4     | 2.30        | 0.40     |
| 9:CJ:76:ILE:HG13  | 9:CJ:76:ILE:H      | 1.70        | 0.40     |
| 45:BS:55:ILE:CG2  | 45:BS:56:ALA:N     | 2.85        | 0.40     |
| 29:DE:161:ALA:HA  | 29:DE:164:LEU:HD12 | 2.02        | 0.40     |
| 27:DK:19:VAL:HB   | 27:DK:41:ILE:CG1   | 2.51        | 0.40     |
| 19:CT:2:ASN:ND2   | 19:CT:3:ILE:N      | 2.62        | 0.40     |
| 42:DN:51:LEU:HD21 | 42:DN:70:THR:HG21  | 2.03        | 0.40     |
| 23:BB:2144:G:N2   | 23:BB:2146:C:C2    | 2.89        | 0.40     |
| 1:CA:279:A:H5'    | 1:CA:281:G:O4'     | 2.21        | 0.40     |
| 1:AA:715:A:O2'    | 1:AA:716:A:H5'     | 2.21        | 0.40     |
| 36:B2:43:THR:O    | 36:B2:44:VAL:C     | 2.59        | 0.40     |
| 20:CB:67:LEU:HD23 | 20:CB:67:LEU:HA    | 1.91        | 0.40     |
| 25:DC:43:ASN:CG   | 25:DC:44:ASN:H     | 2.22        | 0.40     |
| 45:DS:46:LEU:O    | 45:DS:50:VAL:HG23  | 2.21        | 0.40     |
| 23:BB:37:C:H4'    | 23:BB:451:U:OP1    | 2.21        | 0.40     |
| 23:DB:360:U:H2'   | 23:DB:361:G:O4'    | 2.21        | 0.40     |
| 1:CA:1103:C:C4    | 1:CA:1104:G:N7     | 2.90        | 0.40     |
| 28:DP:50:ARG:HB3  | 28:DP:57:ALA:H     | 1.86        | 0.40     |
| 26:BD:114:LYS:HE3 | 26:BD:116:LYS:CE   | 2.52        | 0.40     |
| 4:CE:39:GLY:CA    | 4:CE:116:VAL:HB    | 2.48        | 0.40     |
| 28:BP:112:ARG:HB2 | 28:BP:112:ARG:NH1  | 2.36        | 0.40     |
| 46:BU:10:VAL:HA   | 46:BU:70:ALA:O     | 2.21        | 0.40     |
| 4:AE:104:ILE:HD11 | 4:AE:111:ARG:HA    | 2.03        | 0.40     |
| 40:BH:18:GLN:HE22 | 40:BH:44:ILE:HD13  | 1.87        | 0.40     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 40:BH:44:ILE:O    | 40:BH:46:PHE:N    | 2.54        | 0.40     |
| 38:DM:41:LEU:O    | 38:DM:94:ALA:N    | 2.53        | 0.40     |
| 1:AA:191:G:H2'    | 1:AA:192:A:C8     | 2.55        | 0.40     |
| 28:BP:32:VAL:HG12 | 28:BP:33:GLU:O    | 2.21        | 0.40     |
| 23:BB:705:A:H61   | 23:BB:726:G:H1'   | 1.86        | 0.40     |
| 1:CA:547:A:H4'    | 1:CA:548:G:O5'    | 2.21        | 0.40     |
| 1:AA:1229:A:H2'   | 1:AA:1230:C:H6    | 1.86        | 0.40     |
| 19:AT:65:LEU:HA   | 19:AT:65:LEU:HD12 | 1.92        | 0.40     |
| 20:CB:26:MET:HE2  | 20:CB:26:MET:HB3  | 1.89        | 0.40     |
| 23:DB:2219:U:H2'  | 23:DB:2220:U:C6   | 2.56        | 0.40     |
| 42:BN:60:VAL:O    | 42:BN:63:ARG:HB3  | 2.21        | 0.40     |
| 1:AA:448:A:O2'    | 1:AA:449:G:H5'    | 2.22        | 0.40     |
| 1:CA:375:U:C2     | 1:CA:376:G:C8     | 3.10        | 0.40     |
| 1:CA:376:G:OP1    | 15:CP:5:ARG:HB2   | 2.21        | 0.40     |
| 43:BO:106:LEU:HA  | 43:BO:109:ALA:HB3 | 2.03        | 0.40     |
| 23:DB:962:G:H21   | 23:DB:2250:G:N2   | 2.18        | 0.40     |
| 6:AG:77:ARG:HG3   | 6:AG:79:VAL:CG2   | 2.50        | 0.40     |
| 23:DB:228:C:O2    | 23:DB:418:C:H4'   | 2.21        | 0.40     |
| 16:AQ:30:HIS:CB   | 16:AQ:33:TYR:HB2  | 2.51        | 0.40     |
| 23:DB:1562:U:O2'  | 23:DB:1563:U:H5'  | 2.22        | 0.40     |
| 23:DB:679:C:H2'   | 23:DB:680:C:C6    | 2.56        | 0.40     |
| 37:BL:132:ARG:HA  | 37:BL:135:ILE:CG2 | 2.52        | 0.40     |
| 25:BC:254:LYS:HB3 | 25:BC:255:LYS:H   | 1.68        | 0.40     |
| 23:BB:2262:U:H2'  | 23:BB:2263:C:H6   | 1.86        | 0.40     |
| 7:CH:29:SER:O     | 7:CH:30:LYS:C     | 2.59        | 0.40     |
| 3:CD:146:GLU:CD   | 3:CD:146:GLU:N    | 2.74        | 0.40     |
| 29:DE:31:VAL:HG21 | 29:DE:104:ALA:CB  | 2.51        | 0.40     |
| 43:DO:106:LEU:HA  | 43:DO:109:ALA:HB3 | 2.03        | 0.40     |
| 1:CA:152:A:H2'    | 1:CA:153:C:O4'    | 2.22        | 0.40     |
| 23:DB:2889:C:H2'  | 23:DB:2890:G:C8   | 2.56        | 0.40     |
| 1:CA:648:A:H2'    | 1:CA:649:A:H8     | 1.86        | 0.40     |
| 1:CA:691:G:H1'    | 1:CA:696:A:N6     | 2.35        | 0.40     |
| 22:BA:77:U:O2'    | 22:BA:78:A:H5'    | 2.21        | 0.40     |
| 24:DI:63:ASP:O    | 24:DI:63:ASP:OD1  | 2.39        | 0.40     |
| 1:AA:158:G:H2'    | 1:AA:159:G:O4'    | 2.21        | 0.40     |
| 47:DF:56:LEU:HD13 | 47:DF:56:LEU:O    | 2.20        | 0.40     |
| 23:DB:1054:A:H2'  | 23:DB:1055:G:O4'  | 2.22        | 0.40     |
| 23:BB:2757:A:H2'  | 23:BB:2757:A:N3   | 2.36        | 0.40     |
| 1:AA:177:G:C5     | 1:AA:178:C:C5     | 3.09        | 0.40     |
| 23:DB:2300:C:O2'  | 23:DB:2301:C:H5'  | 2.22        | 0.40     |
| 23:BB:2830:C:H1'  | 23:BB:2836:U:O4'  | 2.21        | 0.40     |
| 23:DB:1798:U:OP1  | 25:DC:255:LYS:HG2 | 2.21        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 29:DE:6:LYS:HB2   | 29:DE:120:VAL:O    | 2.21        | 0.40     |
| 23:BB:2408:U:H2'  | 23:BB:2409:G:H8    | 1.87        | 0.40     |
| 23:BB:1304:A:H2'  | 23:BB:1305:C:H6    | 1.86        | 0.40     |
| 43:DO:14:ALA:C    | 43:DO:16:ARG:N     | 2.75        | 0.40     |
| 1:CA:1112:C:O2    | 2:CC:178:ARG:HB3   | 2.21        | 0.40     |
| 23:BB:34:U:H4'    | 23:BB:35:G:OP2     | 2.22        | 0.40     |
| 23:BB:1068:G:C6   | 23:BB:1069:A:N6    | 2.89        | 0.40     |
| 23:BB:2295:C:O2'  | 23:BB:2296:U:H5'   | 2.21        | 0.40     |
| 23:DB:1058:U:H1'  | 24:DI:117:THR:HG22 | 2.03        | 0.40     |
| 1:CA:952:U:H2'    | 1:CA:953:G:C8      | 2.56        | 0.40     |
| 33:B1:38:PHE:HB2  | 33:B1:45:HIS:CE1   | 2.55        | 0.40     |
| 1:CA:750:C:H4'    | 14:CO:21:ASP:HA    | 2.03        | 0.40     |
| 27:DK:64:ARG:O    | 27:DK:82:ASN:HA    | 2.21        | 0.40     |
| 1:CA:792:A:C4     | 1:CA:794:A:C6      | 3.09        | 0.40     |
| 40:DH:26:ALA:O    | 40:DH:27:ARG:C     | 2.60        | 0.40     |
| 52:BW:49:ASN:ND2  | 52:BW:50:VAL:N     | 2.70        | 0.40     |
| 48:BG:84:LYS:HG3  | 48:BG:131:VAL:HB   | 2.03        | 0.40     |
| 22:BA:40:U:H1'    | 22:BA:43:C:C5      | 2.55        | 0.40     |
| 6:AG:148:LYS:O    | 6:AG:151:ALA:HB3   | 2.22        | 0.40     |
| 37:DL:90:VAL:HG23 | 37:DL:120:VAL:CG1  | 2.51        | 0.40     |
| 48:DG:108:PHE:HD1 | 48:DG:108:PHE:H    | 1.70        | 0.40     |
| 22:DA:42:C:C6     | 47:DF:65:LEU:HD22  | 2.57        | 0.40     |
| 41:DJ:40:HIS:ND1  | 41:DJ:41:LYS:HG3   | 2.36        | 0.40     |
| 41:DJ:41:LYS:HB3  | 41:DJ:42:ALA:H     | 1.65        | 0.40     |
| 41:DJ:4:PHE:O     | 41:DJ:44:TYR:CZ    | 2.74        | 0.40     |
| 23:BB:138:U:O2'   | 50:BT:1:MET:HA     | 2.22        | 0.40     |
| 23:DB:635:C:O2'   | 23:DB:636:G:H5'    | 2.20        | 0.40     |
| 37:DL:127:VAL:CG2 | 37:DL:128:THR:N    | 2.83        | 0.40     |
| 22:DA:24:G:C2     | 22:DA:28:C:C5      | 3.10        | 0.40     |
| 23:DB:2768:U:H2'  | 23:DB:2769:U:O4'   | 2.21        | 0.40     |
| 13:CN:60:ARG:HD3  | 13:CN:62:ARG:CZ    | 2.52        | 0.40     |
| 39:BX:27:ASN:HA   | 39:BX:30:MET:HG2   | 2.02        | 0.40     |
| 25:DC:92:LEU:HD12 | 25:DC:101:ARG:O    | 2.21        | 0.40     |
| 44:BQ:91:ARG:CB   | 44:BQ:94:LEU:HD23  | 2.50        | 0.40     |
| 12:CM:39:ALA:HB3  | 12:CM:42:VAL:HG13  | 2.02        | 0.40     |
| 1:AA:1259:C:O2    | 1:AA:1283:U:H1'    | 2.21        | 0.40     |
| 37:BL:79:LEU:HD23 | 37:BL:79:LEU:HA    | 1.95        | 0.40     |
| 43:DO:88:LYS:CE   | 43:DO:116:GLN:HB2  | 2.39        | 0.40     |
| 9:AJ:53:ILE:CG2   | 9:AJ:61:ALA:HB1    | 2.51        | 0.40     |
| 35:BV:24:ASN:O    | 35:BV:26:PHE:N     | 2.53        | 0.40     |
| 29:BE:58:LYS:HZ3  | 29:BE:58:LYS:N     | 2.13        | 0.40     |
| 23:BB:2806:C:H2'  | 23:BB:2807:U:O4'   | 2.21        | 0.40     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:DB:1190:G:P     | 37:DL:32:GLY:HA2   | 2.60        | 0.40     |
| 23:BB:1028:A:H1'   | 23:BB:2487:G:O5'   | 2.22        | 0.40     |
| 32:D4:36:ARG:HE    | 32:D4:37:GLN:H     | 1.70        | 0.40     |
| 48:DG:86:LEU:HD23  | 48:DG:163:TYR:HA   | 2.04        | 0.40     |
| 23:BB:971:G:OP2    | 23:BB:974:G:N2     | 2.55        | 0.40     |
| 35:DV:24:ASN:O     | 35:DV:26:PHE:N     | 2.55        | 0.40     |
| 29:DE:192:ALA:HA   | 29:DE:195:GLN:NE2  | 2.36        | 0.40     |
| 38:DM:46:ILE:CG1   | 38:DM:47:GLU:N     | 2.84        | 0.40     |
| 23:DB:591:U:H1'    | 34:D3:1:PRO:H2     | 1.84        | 0.40     |
| 2:CC:166:TRP:O     | 2:CC:167:TYR:CB    | 2.69        | 0.40     |
| 1:AA:20:U:O2'      | 1:AA:21:G:H5'      | 2.22        | 0.40     |
| 1:CA:723:U:H5'     | 21:CU:48:LYS:HG2   | 2.03        | 0.40     |
| 23:DB:2896:C:H2'   | 23:DB:2897:U:H6    | 1.86        | 0.40     |
| 23:BB:2896:C:H2'   | 23:BB:2897:U:H6    | 1.86        | 0.40     |
| 28:DP:4:ILE:HG22   | 28:DP:5:LYS:N      | 2.29        | 0.40     |
| 1:AA:279:A:H5'     | 1:AA:281:G:C5'     | 2.51        | 0.40     |
| 48:BG:71:LEU:HD13  | 48:BG:74:MET:HE1   | 2.04        | 0.40     |
| 1:CA:998:C:H2'     | 1:CA:999:C:H6      | 1.85        | 0.40     |
| 29:DE:126:VAL:HG22 | 29:DE:127:GLU:N    | 2.35        | 0.40     |
| 1:CA:1101:A:N6     | 20:CB:101:THR:HG21 | 2.37        | 0.40     |
| 44:DQ:51:GLN:O     | 44:DQ:54:ARG:HB2   | 2.21        | 0.40     |
| 1:CA:263:A:OP1     | 19:CT:73:ARG:NH1   | 2.55        | 0.40     |
| 35:BV:29:ILE:O     | 35:BV:29:ILE:HD12  | 2.21        | 0.40     |
| 23:BB:150:U:H2'    | 23:BB:151:C:O4'    | 2.20        | 0.40     |
| 25:BC:251:THR:O    | 25:BC:252:LYS:HD2  | 2.22        | 0.40     |
| 6:AG:19:SER:HB2    | 6:AG:21:LEU:HD21   | 2.03        | 0.40     |
| 11:CL:35:ARG:HH21  | 11:CL:36:VAL:HG22  | 1.86        | 0.40     |
| 6:AG:134:VAL:HG23  | 6:AG:135:LYS:N     | 2.36        | 0.40     |
| 25:BC:239:PHE:HD1  | 25:BC:241:LYS:H    | 1.68        | 0.40     |
| 23:BB:1374:G:H2'   | 23:BB:1375:U:H6    | 1.84        | 0.40     |
| 20:CB:191:ASP:OD2  | 20:CB:193:ASP:HB2  | 2.21        | 0.40     |
| 23:BB:1184:U:H2'   | 23:BB:1185:G:H8    | 1.87        | 0.40     |
| 1:CA:481:G:O2'     | 1:CA:482:A:H8      | 2.03        | 0.40     |
| 8:AI:98:ARG:NE     | 8:AI:103:VAL:HG21  | 2.37        | 0.40     |
| 1:AA:1483:A:H1'    | 23:BB:1948:G:H1'   | 2.04        | 0.40     |
| 1:AA:503:C:O2'     | 1:AA:504:C:H5'     | 2.22        | 0.40     |
| 23:DB:2250:G:H8    | 23:DB:2250:G:O5'   | 2.05        | 0.40     |
| 23:DB:2603:G:O2'   | 23:DB:2604:U:H5'   | 2.21        | 0.40     |
| 23:BB:1401:G:H2'   | 23:BB:1402:U:H6    | 1.85        | 0.40     |
| 23:BB:1745:A:H2'   | 23:BB:1746:A:C8    | 2.57        | 0.40     |
| 23:BB:493:G:H2'    | 23:BB:494:G:O4'    | 2.22        | 0.40     |
| 23:DB:1537:G:H3'   | 23:DB:1538:G:O4'   | 2.22        | 0.40     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:692:U:O2     | 1:CA:694:A:C8      | 2.74        | 0.40     |
| 14:AO:36:ILE:HD13 | 14:AO:59:MET:HE2   | 2.03        | 0.40     |
| 41:DJ:72:LYS:CG   | 41:DJ:89:PHE:HB2   | 2.52        | 0.40     |
| 1:AA:426:U:H2'    | 1:AA:427:U:C6      | 2.56        | 0.40     |
| 25:DC:221:GLY:C   | 25:DC:223:ALA:N    | 2.73        | 0.40     |
| 23:DB:1926:U:H3'  | 23:DB:1928:A:OP2   | 2.21        | 0.40     |
| 31:B0:10:SER:O    | 31:B0:11:LYS:C     | 2.60        | 0.40     |
| 25:BC:221:GLY:C   | 25:BC:223:ALA:N    | 2.75        | 0.40     |
| 23:BB:408:G:H2'   | 23:BB:409:G:H8     | 1.85        | 0.40     |
| 1:AA:761:G:H2'    | 1:AA:762:U:H6      | 1.82        | 0.40     |
| 23:DB:2730:C:H2'  | 23:DB:2731:G:C8    | 2.57        | 0.40     |
| 23:BB:1300:G:N2   | 23:BB:1634:A:C2    | 2.89        | 0.40     |
| 23:DB:1499:C:H2'  | 23:DB:1500:G:C8    | 2.54        | 0.40     |
| 23:BB:247:G:C2    | 23:BB:252:G:C6     | 3.09        | 0.40     |
| 24:BI:52:LEU:O    | 24:BI:54:ILE:HG13  | 2.22        | 0.40     |
| 24:DI:102:ARG:O   | 24:DI:106:GLN:HG3  | 2.22        | 0.40     |
| 1:CA:884:U:H4'    | 1:CA:885:G:H5''    | 2.03        | 0.40     |
| 7:CH:79:ARG:HH11  | 7:CH:79:ARG:HG2    | 1.87        | 0.40     |
| 6:AG:31:VAL:HG22  | 6:AG:32:ASP:N      | 2.36        | 0.40     |
| 1:CA:1423:G:H2'   | 1:CA:1424:U:C6     | 2.56        | 0.40     |
| 23:DB:1344:U:H5'  | 23:DB:1384:A:N1    | 2.36        | 0.40     |
| 23:DB:247:G:H4'   | 23:DB:386:G:C4     | 2.57        | 0.40     |
| 23:DB:1692:U:O2'  | 23:DB:1693:U:H2'   | 2.22        | 0.40     |
| 23:BB:963:U:H2'   | 23:BB:964:C:C6     | 2.55        | 0.40     |
| 48:DG:125:PRO:HB2 | 48:DG:129:GLU:CD   | 2.42        | 0.40     |
| 29:BE:196:VAL:O   | 29:BE:200:LEU:HD23 | 2.21        | 0.40     |
| 1:AA:1119:C:O2'   | 1:AA:1120:C:H5'    | 2.21        | 0.40     |
| 23:BB:2515:C:H2'  | 23:BB:2516:A:H8    | 1.87        | 0.40     |
| 9:CJ:31:ARG:HG3   | 9:CJ:31:ARG:H      | 1.64        | 0.40     |
| 1:AA:1485:U:O2'   | 1:AA:1486:G:H5'    | 2.22        | 0.40     |
| 9:CJ:49:PHE:O     | 9:CJ:64:GLN:HA     | 2.21        | 0.40     |
| 20:CB:80:LYS:HG3  | 20:CB:81:ASP:H     | 1.86        | 0.40     |
| 10:CK:108:ASN:ND2 | 21:CU:6:ARG:HG3    | 2.36        | 0.40     |
| 26:BD:2:ILE:CG2   | 26:BD:84:LEU:HB3   | 2.51        | 0.40     |
| 23:BB:531:C:O2'   | 23:BB:563:A:H5''   | 2.21        | 0.40     |
| 33:B1:25:ASN:OD1  | 33:B1:27:ARG:HB2   | 2.22        | 0.40     |
| 2:AC:55:VAL:HG12  | 2:AC:56:ILE:N      | 2.37        | 0.40     |
| 26:BD:191:GLY:O   | 26:BD:192:ALA:HB3  | 2.22        | 0.40     |
| 7:CH:83:ARG:C     | 7:CH:84:ILE:HG13   | 2.41        | 0.40     |
| 26:DD:12:THR:HG22 | 26:DD:13:ARG:N     | 2.37        | 0.40     |
| 26:DD:18:ASP:OD1  | 26:DD:19:GLY:N     | 2.54        | 0.40     |
| 23:DB:1614:A:H8   | 23:DB:1614:A:O5'   | 2.04        | 0.40     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 41:DJ:65:THR:HG23  | 41:DJ:66:GLY:N     | 2.36        | 0.40     |
| 1:AA:260:G:O2'     | 1:AA:261:U:H5'     | 2.21        | 0.40     |
| 1:AA:24:U:O2'      | 1:AA:25:C:H5'      | 2.21        | 0.40     |
| 23:DB:199:A:C6     | 23:DB:2434:A:C6    | 3.09        | 0.40     |
| 23:BB:2354:C:H2'   | 23:BB:2355:G:H8    | 1.87        | 0.40     |
| 52:BW:28:GLU:HB2   | 52:BW:31:LEU:HD21  | 2.03        | 0.40     |
| 25:DC:134:ILE:HD11 | 25:DC:163:ILE:HG13 | 2.04        | 0.40     |
| 25:DC:90:ILE:HA    | 25:DC:90:ILE:HD13  | 1.92        | 0.40     |
| 10:AK:42:GLY:HA3   | 10:AK:73:VAL:HG13  | 2.03        | 0.40     |
| 48:BG:106:LEU:N    | 48:BG:106:LEU:HD23 | 2.37        | 0.40     |
| 44:DQ:33:VAL:CG2   | 44:DQ:34:ALA:N     | 2.84        | 0.40     |
| 40:BH:116:ARG:HH11 | 40:BH:133:GLN:HB2  | 1.85        | 0.40     |
| 26:BD:105:LYS:HE3  | 26:BD:176:ASP:HB3  | 2.04        | 0.40     |
| 26:BD:51:THR:HG21  | 26:BD:75:ALA:O     | 2.21        | 0.40     |
| 26:BD:76:GLY:O     | 26:BD:77:ARG:C     | 2.60        | 0.40     |
| 53:D6:84:ARG:C     | 53:D6:86:SER:N     | 2.74        | 0.40     |
| 23:DB:2313:C:O3'   | 47:DF:87:LYS:HE2   | 2.22        | 0.40     |
| 47:DF:31:GLU:O     | 47:DF:32:LYS:O     | 2.38        | 0.40     |
| 47:DF:32:LYS:O     | 47:DF:32:LYS:HE2   | 2.21        | 0.40     |
| 52:DW:49:ASN:CB    | 52:DW:60:ALA:HA    | 2.46        | 0.40     |
| 53:B6:65:THR:HG22  | 53:B6:66:LEU:N     | 2.36        | 0.40     |
| 40:BH:144:VAL:HG12 | 40:BH:146:VAL:HG23 | 2.03        | 0.40     |
| 40:BH:90:LEU:HD11  | 40:BH:146:VAL:HG11 | 2.00        | 0.40     |
| 8:CI:56:MET:O      | 8:CI:58:GLU:N      | 2.45        | 0.40     |
| 41:DJ:3:THR:CB     | 41:DJ:44:TYR:OH    | 2.70        | 0.40     |
| 51:DZ:51:VAL:HG12  | 51:DZ:52:SER:N     | 2.36        | 0.40     |
| 13:AN:60:ARG:HD3   | 13:AN:62:ARG:CZ    | 2.52        | 0.40     |
| 35:BV:61:LEU:HD11  | 35:BV:74:ALA:HB2   | 2.03        | 0.40     |
| 23:DB:2307:G:O6    | 47:DF:40:GLY:HA3   | 2.21        | 0.40     |
| 47:DF:66:ILE:HD11  | 47:DF:83:PRO:CB    | 2.46        | 0.40     |
| 12:AM:15:VAL:CG2   | 12:AM:40:GLU:HB3   | 2.51        | 0.40     |
| 23:DB:1255:U:H5''  | 23:DB:1256:G:H5''  | 2.04        | 0.40     |
| 1:AA:598:U:H2'     | 1:AA:599:C:H6      | 1.87        | 0.40     |
| 50:BT:40:LYS:O     | 50:BT:43:ILE:HB    | 2.21        | 0.40     |
| 46:DU:85:ARG:NH1   | 46:DU:86:PHE:O     | 2.53        | 0.40     |
| 12:AM:106:ARG:HH12 | 12:AM:109:LYS:CD   | 2.20        | 0.40     |
| 25:BC:83:ASP:HA    | 25:BC:84:PRO:HD3   | 1.84        | 0.40     |
| 42:BN:87:PHE:CE1   | 42:BN:116:VAL:HG12 | 2.56        | 0.40     |
| 24:BI:73:PRO:HA    | 24:BI:74:PRO:HD3   | 1.99        | 0.40     |
| 47:BF:42:ALA:O     | 47:BF:44:ALA:N     | 2.54        | 0.40     |
| 29:BE:160:ALA:C    | 29:BE:162:ARG:H    | 2.24        | 0.40     |
| 40:DH:83:LYS:HG3   | 40:DH:149:GLU:CG   | 2.51        | 0.40     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:411:A:O2'     | 1:CA:412:A:O4'    | 2.39        | 0.40     |
| 1:CA:411:A:O3'     | 1:CA:412:A:H4'    | 2.20        | 0.40     |
| 10:AK:59:PRO:N     | 10:AK:90:PRO:HB2  | 2.36        | 0.40     |
| 4:CE:89:THR:HG21   | 4:CE:134:ASN:HD21 | 1.85        | 0.40     |
| 1:CA:1318:A:H5''   | 1:CA:1319:A:OP2   | 2.21        | 0.40     |
| 18:CS:10:ILE:HD13  | 18:CS:40:PHE:CE1  | 2.56        | 0.40     |
| 42:DN:100:CYS:SG   | 42:DN:101:GLY:N   | 2.95        | 0.40     |
| 13:AN:29:ILE:HB    | 13:AN:30:ILE:H    | 1.73        | 0.40     |
| 38:DM:126:ILE:H    | 38:DM:126:ILE:CD1 | 2.18        | 0.40     |
| 50:DT:55:VAL:HG13  | 50:DT:85:VAL:CG1  | 2.52        | 0.40     |
| 25:DC:208:GLY:O    | 25:DC:209:ALA:C   | 2.59        | 0.40     |
| 45:DS:26:GLY:CA    | 45:DS:71:VAL:HG13 | 2.51        | 0.40     |
| 45:DS:24:ILE:CG1   | 45:DS:36:LEU:HD21 | 2.49        | 0.40     |
| 23:BB:2883:A:OP1   | 31:B0:48:TYR:CE1  | 2.74        | 0.40     |
| 23:DB:2282:G:H5''  | 23:DB:2283:C:O4'  | 2.21        | 0.40     |
| 2:AC:166:TRP:O     | 2:AC:167:TYR:CB   | 2.69        | 0.40     |
| 49:BR:78:ARG:NH2   | 49:BR:78:ARG:HG3  | 2.36        | 0.40     |
| 1:AA:1336:C:H4'    | 1:AA:1337:G:O5'   | 2.20        | 0.40     |
| 48:BG:162:ARG:O    | 48:BG:162:ARG:HG2 | 2.22        | 0.40     |
| 23:DB:2772:C:H2'   | 23:DB:2773:C:C6   | 2.57        | 0.40     |
| 3:CD:105:GLY:HA3   | 3:CD:158:LEU:HG   | 2.03        | 0.40     |
| 22:DA:32:U:H2'     | 22:DA:33:G:C8     | 2.57        | 0.40     |
| 49:BR:39:LEU:HB3   | 49:BR:53:PHE:HA   | 2.03        | 0.40     |
| 40:BH:69:ALA:O     | 40:BH:141:LYS:NZ  | 2.51        | 0.40     |
| 23:BB:170:U:O2'    | 23:BB:171:U:H5'   | 2.21        | 0.40     |
| 23:DB:1778:U:N3    | 23:DB:1784:A:C8   | 2.89        | 0.40     |
| 26:DD:9:VAL:HA     | 26:DD:197:THR:CG2 | 2.52        | 0.40     |
| 23:BB:115:C:H2'    | 23:BB:116:C:H6    | 1.87        | 0.40     |
| 26:BD:186:LEU:HD11 | 28:BP:3:ILE:CG1   | 2.47        | 0.40     |
| 28:BP:1:SER:H1     | 28:BP:4:ILE:HD12  | 1.86        | 0.40     |
| 11:AL:85:ARG:HE    | 11:AL:85:ARG:HB2  | 1.72        | 0.40     |
| 4:AE:156:ARG:HB3   | 7:AH:42:GLU:O     | 2.21        | 0.40     |
| 4:AE:83:PRO:HA     | 4:AE:95:MET:O     | 2.22        | 0.40     |
| 20:CB:125:PHE:HE1  | 20:CB:136:ARG:HD2 | 1.87        | 0.40     |
| 1:AA:92:U:H2'      | 1:AA:93:U:C6      | 2.56        | 0.40     |
| 29:BE:41:GLN:O     | 29:BE:42:GLY:C    | 2.58        | 0.40     |
| 5:AF:60:VAL:HG12   | 5:AF:61:LEU:N     | 2.35        | 0.40     |
| 5:AF:98:GLU:O      | 5:AF:99:ALA:HB3   | 2.22        | 0.40     |
| 49:BR:23:GLU:O     | 49:BR:24:LYS:C    | 2.60        | 0.40     |
| 4:CE:111:ARG:O     | 4:CE:112:ALA:C    | 2.59        | 0.40     |
| 1:AA:1098:C:O2'    | 1:AA:1099:G:H5'   | 2.22        | 0.40     |
| 16:AQ:17:GLU:C     | 16:AQ:19:SER:H    | 2.25        | 0.40     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 28:DP:32:VAL:HG12 | 28:DP:33:GLU:O    | 2.21        | 0.40     |
| 23:DB:1724:G:O2'  | 23:DB:1725:U:H5'  | 2.21        | 0.40     |
| 1:AA:14:U:O2      | 1:AA:17:U:H5      | 2.05        | 0.40     |
| 23:BB:1131:G:H22  | 23:BB:2024:G:H21  | 1.68        | 0.40     |
| 23:BB:2344:U:H2'  | 33:B1:35:LEU:O    | 2.21        | 0.40     |
| 2:AC:6:PRO:HA     | 2:AC:9:ILE:CG2    | 2.49        | 0.40     |
| 34:D3:60:CYS:C    | 34:D3:61:LEU:HD23 | 2.41        | 0.40     |
| 23:DB:2139:U:H2'  | 23:DB:2140:G:H8   | 1.87        | 0.40     |
| 23:BB:1589:U:H2'  | 23:BB:1590:A:C8   | 2.56        | 0.40     |
| 2:AC:42:LEU:HD21  | 2:AC:90:VAL:HG22  | 2.02        | 0.40     |
| 1:CA:370:C:H2'    | 1:CA:371:A:C8     | 2.56        | 0.40     |
| 23:BB:692:C:H2'   | 23:BB:693:A:H8    | 1.87        | 0.40     |
| 24:BI:7:TYR:CD1   | 24:BI:7:TYR:C     | 2.95        | 0.40     |
| 3:AD:10:LEU:HD12  | 3:AD:20:LEU:HD13  | 2.03        | 0.40     |
| 1:CA:1142:G:H2'   | 1:CA:1143:G:O4'   | 2.21        | 0.40     |
| 23:BB:1405:U:H2'  | 23:BB:1406:U:H6   | 1.86        | 0.40     |
| 9:CJ:86:ALA:C     | 9:CJ:87:LEU:HD13  | 2.42        | 0.40     |
| 23:BB:1454:C:H5'  | 42:BN:63:ARG:NE   | 2.36        | 0.40     |
| 1:CA:283:U:O2'    | 1:CA:284:C:H5'    | 2.22        | 0.40     |
| 43:BO:106:LEU:CA  | 43:BO:109:ALA:HB3 | 2.51        | 0.40     |
| 1:AA:613:C:P      | 3:AD:80:ARG:HH21  | 2.44        | 0.40     |
| 23:BB:2785:C:H2'  | 23:BB:2786:U:H6   | 1.87        | 0.40     |
| 22:BA:87:U:C2'    | 22:BA:88:C:O5'    | 2.69        | 0.40     |
| 53:B6:16:LYS:N    | 53:B6:16:LYS:HE3  | 2.36        | 0.40     |
| 23:DB:1013:C:H2'  | 23:DB:1014:A:C8   | 2.57        | 0.40     |
| 23:BB:484:C:H2'   | 23:BB:485:C:H6    | 1.86        | 0.40     |
| 23:BB:1476:U:O2'  | 23:BB:1477:A:P    | 2.80        | 0.40     |
| 22:DA:109:A:H2'   | 22:DA:110:C:O4'   | 2.21        | 0.40     |
| 23:DB:1885:A:H3'  | 23:DB:1886:U:C5   | 2.56        | 0.40     |
| 49:DR:14:VAL:HG22 | 49:DR:15:SER:H    | 1.86        | 0.40     |
| 29:DE:97:ASN:OD1  | 29:DE:97:ASN:N    | 2.54        | 0.40     |
| 23:BB:2298:A:H2'  | 23:BB:2299:U:O4'  | 2.22        | 0.40     |
| 9:CJ:65:TYR:HA    | 13:CN:96:LYS:O    | 2.22        | 0.40     |
| 5:CF:86:ARG:CZ    | 17:CR:63:TYR:HB3  | 2.51        | 0.40     |
| 1:AA:1103:C:C4    | 1:AA:1104:G:N7    | 2.90        | 0.40     |
| 7:AH:79:ARG:HG2   | 7:AH:79:ARG:HH11  | 1.87        | 0.40     |
| 23:DB:1051:G:H2'  | 23:DB:1052:C:C6   | 2.56        | 0.40     |
| 1:AA:266:G:O2'    | 1:AA:267:C:H3'    | 2.21        | 0.40     |
| 44:BQ:2:ARG:HG3   | 44:BQ:3:VAL:N     | 2.36        | 0.40     |
| 46:DU:13:LEU:HD12 | 46:DU:68:ASN:C    | 2.42        | 0.40     |
| 10:CK:68:ARG:HH11 | 10:CK:68:ARG:HG3  | 1.86        | 0.40     |
| 41:BJ:133:ALA:O   | 41:BJ:135:GLN:N   | 2.55        | 0.40     |

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| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:DB:2299:U:H2'   | 23:DB:2300:C:C6   | 2.57        | 0.40     |
| 23:BB:619:G:H3'    | 23:BB:620:G:H21   | 1.86        | 0.40     |
| 23:BB:2047:C:O2'   | 23:BB:2048:G:H5'  | 2.22        | 0.40     |
| 23:DB:1733:G:H2'   | 23:DB:1734:G:H8   | 1.86        | 0.40     |
| 10:AK:108:ASN:HD21 | 21:AU:6:ARG:HG3   | 1.86        | 0.40     |
| 20:AB:117:GLU:O    | 20:AB:121:GLN:HB2 | 2.21        | 0.40     |
| 3:CD:35:GLN:HB2    | 3:CD:35:GLN:HE21  | 1.73        | 0.40     |
| 2:AC:111:ASP:OD2   | 2:AC:114:LEU:HG   | 2.22        | 0.40     |
| 23:BB:1423:G:H2'   | 23:BB:1424:G:H8   | 1.86        | 0.40     |
| 23:DB:311:A:H3'    | 23:DB:312:G:C8    | 2.57        | 0.40     |
| 25:BC:161:VAL:HG13 | 25:BC:174:ARG:O   | 2.22        | 0.40     |
| 23:DB:2083:G:H2'   | 23:DB:2084:C:H6   | 1.87        | 0.40     |
| 1:AA:528:C:H41     | 11:AL:45:ASN:CG   | 2.24        | 0.40     |
| 40:BH:75:LEU:HD21  | 40:BH:104:THR:O   | 2.22        | 0.40     |
| 1:AA:1210:C:H4'    | 1:AA:1214:C:C5    | 2.57        | 0.40     |
| 3:AD:47:LEU:HD11   | 3:AD:51:GLY:HA3   | 2.04        | 0.40     |
| 1:AA:687:A:C2      | 1:AA:704:A:C5     | 3.09        | 0.40     |
| 23:DB:2657:A:H2'   | 23:DB:2658:C:O4'  | 2.22        | 0.40     |
| 23:BB:765:C:H2'    | 23:BB:766:U:C6    | 2.57        | 0.40     |
| 1:AA:258:G:H2'     | 1:AA:258:G:N3     | 2.35        | 0.40     |
| 51:BZ:27:ARG:HG3   | 51:BZ:27:ARG:H    | 1.66        | 0.40     |
| 18:AS:33:TRP:CE3   | 18:AS:33:TRP:N    | 2.89        | 0.40     |
| 23:DB:2317:A:H2'   | 23:DB:2318:G:O4'  | 2.22        | 0.40     |
| 1:CA:1401:G:H2'    | 1:CA:1402:C:O4'   | 2.22        | 0.40     |
| 1:CA:787:A:O2'     | 1:CA:788:U:H5'    | 2.20        | 0.40     |
| 26:DD:191:GLY:O    | 26:DD:192:ALA:HB3 | 2.22        | 0.40     |

All (1) 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                  | Distance(Å) | Clash(Å) |
|----------------|-------------------------|-------------|----------|
| 22:DA:53:A:OP1 | 23:DB:1592:C:O2'[1.655] | 2.08        | 0.12     |

## 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   | AC    | 204/232 (88%) | 150 (74%) | 41 (20%) | 13 (6%)  | 2           | 36  |
| 2   | CC    | 204/232 (88%) | 154 (76%) | 36 (18%) | 14 (7%)  | 2           | 33  |
| 3   | AD    | 203/205 (99%) | 151 (74%) | 41 (20%) | 11 (5%)  | 3           | 41  |
| 3   | CD    | 203/205 (99%) | 150 (74%) | 41 (20%) | 12 (6%)  | 2           | 38  |
| 4   | AE    | 148/166 (89%) | 113 (76%) | 32 (22%) | 3 (2%)   | 11          | 67  |
| 4   | CE    | 148/166 (89%) | 116 (78%) | 28 (19%) | 4 (3%)   | 8           | 60  |
| 5   | AF    | 98/135 (73%)  | 66 (67%)  | 25 (26%) | 7 (7%)   | 2           | 32  |
| 5   | CF    | 98/135 (73%)  | 67 (68%)  | 24 (24%) | 7 (7%)   | 2           | 32  |
| 6   | AG    | 148/178 (83%) | 121 (82%) | 23 (16%) | 4 (3%)   | 8           | 60  |
| 6   | CG    | 150/178 (84%) | 123 (82%) | 23 (15%) | 4 (3%)   | 8           | 60  |
| 7   | AH    | 127/129 (98%) | 96 (76%)  | 27 (21%) | 4 (3%)   | 7           | 57  |
| 7   | CH    | 127/129 (98%) | 96 (76%)  | 28 (22%) | 3 (2%)   | 9           | 63  |
| 8   | AI    | 125/129 (97%) | 96 (77%)  | 23 (18%) | 6 (5%)   | 4           | 44  |
| 8   | CI    | 125/129 (97%) | 96 (77%)  | 22 (18%) | 7 (6%)   | 3           | 40  |
| 9   | AJ    | 96/103 (93%)  | 72 (75%)  | 16 (17%) | 8 (8%)   | 1           | 27  |
| 9   | CJ    | 96/103 (93%)  | 71 (74%)  | 17 (18%) | 8 (8%)   | 1           | 27  |
| 10  | AK    | 115/128 (90%) | 86 (75%)  | 22 (19%) | 7 (6%)   | 2           | 37  |
| 10  | CK    | 115/128 (90%) | 85 (74%)  | 23 (20%) | 7 (6%)   | 2           | 37  |
| 11  | AL    | 121/123 (98%) | 76 (63%)  | 34 (28%) | 11 (9%)  | 1           | 24  |
| 11  | CL    | 121/123 (98%) | 74 (61%)  | 36 (30%) | 11 (9%)  | 1           | 24  |
| 12  | AM    | 112/117 (96%) | 77 (69%)  | 28 (25%) | 7 (6%)   | 2           | 36  |
| 12  | CM    | 111/117 (95%) | 79 (71%)  | 25 (22%) | 7 (6%)   | 2           | 36  |
| 13  | AN    | 92/100 (92%)  | 58 (63%)  | 21 (23%) | 13 (14%) | 0           | 10  |
| 13  | CN    | 92/100 (92%)  | 59 (64%)  | 21 (23%) | 12 (13%) | 0           | 13  |
| 14  | AO    | 86/89 (97%)   | 66 (77%)  | 17 (20%) | 3 (4%)   | 6           | 54  |
| 14  | CO    | 86/89 (97%)   | 67 (78%)  | 16 (19%) | 3 (4%)   | 6           | 54  |
| 15  | AP    | 80/82 (98%)   | 58 (72%)  | 18 (22%) | 4 (5%)   | 3           | 43  |
| 15  | CP    | 78/82 (95%)   | 56 (72%)  | 17 (22%) | 5 (6%)   | 2           | 36  |
| 16  | AQ    | 78/83 (94%)   | 58 (74%)  | 16 (20%) | 4 (5%)   | 3           | 42  |
| 16  | CQ    | 79/83 (95%)   | 59 (75%)  | 15 (19%) | 5 (6%)   | 2           | 36  |
| 17  | AR    | 53/74 (72%)   | 45 (85%)  | 8 (15%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 17  | CR    | 53/74 (72%)   | 44 (83%)  | 9 (17%)  | 0        | 100         | 100 |
| 18  | AS    | 77/91 (85%)   | 52 (68%)  | 24 (31%) | 1 (1%)   | 18          | 75  |
| 18  | CS    | 78/91 (86%)   | 53 (68%)  | 23 (30%) | 2 (3%)   | 8           | 61  |
| 19  | AT    | 83/86 (96%)   | 67 (81%)  | 13 (16%) | 3 (4%)   | 5           | 53  |
| 19  | CT    | 83/86 (96%)   | 67 (81%)  | 13 (16%) | 3 (4%)   | 5           | 53  |
| 20  | AB    | 216/240 (90%) | 159 (74%) | 36 (17%) | 21 (10%) | 1           | 21  |
| 20  | CB    | 216/240 (90%) | 156 (72%) | 37 (17%) | 23 (11%) | 1           | 18  |
| 21  | AU    | 49/70 (70%)   | 27 (55%)  | 14 (29%) | 8 (16%)  | 0           | 7   |
| 21  | CU    | 49/70 (70%)   | 26 (53%)  | 14 (29%) | 9 (18%)  | 0           | 5   |
| 24  | BI    | 139/141 (99%) | 119 (86%) | 15 (11%) | 5 (4%)   | 5           | 53  |
| 24  | DI    | 139/141 (99%) | 114 (82%) | 21 (15%) | 4 (3%)   | 7           | 58  |
| 25  | BC    | 269/272 (99%) | 164 (61%) | 63 (23%) | 42 (16%) | 0           | 8   |
| 25  | DC    | 269/272 (99%) | 161 (60%) | 68 (25%) | 40 (15%) | 0           | 9   |
| 26  | BD    | 207/209 (99%) | 118 (57%) | 55 (27%) | 34 (16%) | 0           | 7   |
| 26  | DD    | 207/209 (99%) | 115 (56%) | 59 (28%) | 33 (16%) | 0           | 7   |
| 27  | BK    | 119/123 (97%) | 72 (60%)  | 30 (25%) | 17 (14%) | 0           | 10  |
| 27  | DK    | 119/123 (97%) | 71 (60%)  | 30 (25%) | 18 (15%) | 0           | 8   |
| 28  | BP    | 112/114 (98%) | 62 (55%)  | 37 (33%) | 13 (12%) | 1           | 15  |
| 28  | DP    | 112/114 (98%) | 63 (56%)  | 35 (31%) | 14 (12%) | 1           | 14  |
| 29  | BE    | 199/201 (99%) | 124 (62%) | 56 (28%) | 19 (10%) | 1           | 22  |
| 29  | DE    | 199/201 (99%) | 121 (61%) | 58 (29%) | 20 (10%) | 1           | 20  |
| 30  | BY    | 56/58 (97%)   | 36 (64%)  | 15 (27%) | 5 (9%)   | 1           | 24  |
| 30  | DY    | 56/58 (97%)   | 37 (66%)  | 14 (25%) | 5 (9%)   | 1           | 24  |
| 31  | B0    | 54/56 (96%)   | 35 (65%)  | 13 (24%) | 6 (11%)  | 1           | 17  |
| 31  | D0    | 54/56 (96%)   | 36 (67%)  | 11 (20%) | 7 (13%)  | 0           | 13  |
| 32  | B4    | 36/38 (95%)   | 18 (50%)  | 11 (31%) | 7 (19%)  | 0           | 4   |
| 32  | D4    | 36/38 (95%)   | 18 (50%)  | 11 (31%) | 7 (19%)  | 0           | 4   |
| 33  | B1    | 48/54 (89%)   | 36 (75%)  | 7 (15%)  | 5 (10%)  | 1           | 18  |
| 33  | D1    | 48/54 (89%)   | 36 (75%)  | 7 (15%)  | 5 (10%)  | 1           | 18  |
| 34  | B3    | 62/64 (97%)   | 40 (64%)  | 16 (26%) | 6 (10%)  | 1           | 21  |
| 34  | D3    | 62/64 (97%)   | 41 (66%)  | 14 (23%) | 7 (11%)  | 1           | 16  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 35  | BV    | 92/94 (98%)   | 70 (76%)  | 16 (17%) | 6 (6%)   | 2           | 35 |
| 35  | DV    | 92/94 (98%)   | 69 (75%)  | 18 (20%) | 5 (5%)   | 3           | 41 |
| 36  | B2    | 44/46 (96%)   | 26 (59%)  | 15 (34%) | 3 (7%)   | 2           | 33 |
| 36  | D2    | 44/46 (96%)   | 26 (59%)  | 15 (34%) | 3 (7%)   | 2           | 33 |
| 37  | BL    | 141/144 (98%) | 76 (54%)  | 42 (30%) | 23 (16%) | 0           | 7  |
| 37  | DL    | 141/144 (98%) | 76 (54%)  | 40 (28%) | 25 (18%) | 0           | 5  |
| 38  | BM    | 134/136 (98%) | 88 (66%)  | 31 (23%) | 15 (11%) | 1           | 16 |
| 38  | DM    | 134/136 (98%) | 89 (66%)  | 29 (22%) | 16 (12%) | 1           | 14 |
| 39  | BX    | 61/63 (97%)   | 36 (59%)  | 18 (30%) | 7 (12%)  | 1           | 15 |
| 39  | DX    | 61/63 (97%)   | 37 (61%)  | 17 (28%) | 7 (12%)  | 1           | 15 |
| 40  | BH    | 147/149 (99%) | 71 (48%)  | 49 (33%) | 27 (18%) | 0           | 5  |
| 40  | DH    | 147/149 (99%) | 96 (65%)  | 28 (19%) | 23 (16%) | 0           | 8  |
| 41  | BJ    | 140/142 (99%) | 89 (64%)  | 34 (24%) | 17 (12%) | 1           | 14 |
| 41  | DJ    | 140/142 (99%) | 88 (63%)  | 36 (26%) | 16 (11%) | 1           | 16 |
| 42  | BN    | 118/127 (93%) | 73 (62%)  | 34 (29%) | 11 (9%)  | 1           | 23 |
| 42  | DN    | 118/127 (93%) | 71 (60%)  | 35 (30%) | 12 (10%) | 1           | 19 |
| 43  | BO    | 114/117 (97%) | 80 (70%)  | 25 (22%) | 9 (8%)   | 1           | 28 |
| 43  | DO    | 114/117 (97%) | 79 (69%)  | 26 (23%) | 9 (8%)   | 1           | 28 |
| 44  | BQ    | 115/117 (98%) | 70 (61%)  | 34 (30%) | 11 (10%) | 1           | 21 |
| 44  | DQ    | 115/117 (98%) | 69 (60%)  | 35 (30%) | 11 (10%) | 1           | 21 |
| 45  | BS    | 108/110 (98%) | 72 (67%)  | 22 (20%) | 14 (13%) | 0           | 13 |
| 45  | DS    | 108/110 (98%) | 70 (65%)  | 24 (22%) | 14 (13%) | 0           | 13 |
| 46  | BU    | 100/103 (97%) | 52 (52%)  | 28 (28%) | 20 (20%) | 0           | 4  |
| 46  | DU    | 100/103 (97%) | 50 (50%)  | 29 (29%) | 21 (21%) | 0           | 4  |
| 47  | BF    | 176/178 (99%) | 106 (60%) | 43 (24%) | 27 (15%) | 0           | 8  |
| 47  | DF    | 176/178 (99%) | 107 (61%) | 42 (24%) | 27 (15%) | 0           | 8  |
| 48  | BG    | 174/176 (99%) | 100 (58%) | 49 (28%) | 25 (14%) | 0           | 10 |
| 48  | DG    | 174/176 (99%) | 99 (57%)  | 49 (28%) | 26 (15%) | 0           | 9  |
| 49  | BR    | 101/103 (98%) | 67 (66%)  | 21 (21%) | 13 (13%) | 0           | 13 |
| 49  | DR    | 101/103 (98%) | 68 (67%)  | 20 (20%) | 13 (13%) | 0           | 13 |
| 50  | BT    | 91/100 (91%)  | 51 (56%)  | 26 (29%) | 14 (15%) | 0           | 8  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 50  | DT    | 91/100 (91%)      | 50 (55%)   | 27 (30%)   | 14 (15%)   | 0           | 8  |
| 51  | BZ    | 75/78 (96%)       | 51 (68%)   | 18 (24%)   | 6 (8%)     | 1           | 28 |
| 51  | DZ    | 75/78 (96%)       | 51 (68%)   | 18 (24%)   | 6 (8%)     | 1           | 28 |
| 52  | BW    | 77/84 (92%)       | 31 (40%)   | 21 (27%)   | 25 (32%)   | 0           | 0  |
| 52  | DW    | 77/84 (92%)       | 31 (40%)   | 21 (27%)   | 25 (32%)   | 0           | 0  |
| 53  | B6    | 183/185 (99%)     | 151 (82%)  | 25 (14%)   | 7 (4%)     | 5           | 51 |
| 53  | D6    | 183/185 (99%)     | 132 (72%)  | 40 (22%)   | 11 (6%)    | 2           | 37 |
| All | All   | 11607/12284 (94%) | 7747 (67%) | 2693 (23%) | 1167 (10%) | 1           | 20 |

All (1167) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 54  | ILE  |
| 2   | AC    | 205 | GLU  |
| 6   | AG    | 6   | ILE  |
| 8   | AI    | 8   | THR  |
| 9   | AJ    | 36  | VAL  |
| 9   | AJ    | 57  | VAL  |
| 12  | AM    | 22  | TYR  |
| 12  | AM    | 105 | ALA  |
| 13  | AN    | 50  | LEU  |
| 13  | AN    | 61  | ASN  |
| 14  | AO    | 18  | ASP  |
| 14  | AO    | 34  | ALA  |
| 15  | AP    | 28  | ARG  |
| 15  | AP    | 44  | SER  |
| 15  | AP    | 67  | ILE  |
| 16  | AQ    | 32  | ILE  |
| 20  | AB    | 9   | LEU  |
| 20  | AB    | 15  | PHE  |
| 20  | AB    | 19  | THR  |
| 20  | AB    | 22  | TRP  |
| 21  | AU    | 12  | ASP  |
| 21  | AU    | 34  | ARG  |
| 24  | BI    | 18  | ASN  |
| 25  | BC    | 65  | ASP  |
| 25  | BC    | 77  | VAL  |
| 25  | BC    | 141 | HIS  |
| 26  | BD    | 9   | VAL  |
| 26  | BD    | 14  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | BD    | 74  | GLU  |
| 26  | BD    | 91  | THR  |
| 26  | BD    | 122 | VAL  |
| 26  | BD    | 169 | ARG  |
| 26  | BD    | 170 | VAL  |
| 27  | BK    | 17  | ARG  |
| 27  | BK    | 18  | ARG  |
| 27  | BK    | 31  | ARG  |
| 27  | BK    | 35  | VAL  |
| 27  | BK    | 72  | PRO  |
| 27  | BK    | 120 | PRO  |
| 28  | BP    | 25  | VAL  |
| 28  | BP    | 38  | ARG  |
| 28  | BP    | 50  | ARG  |
| 28  | BP    | 64  | SER  |
| 28  | BP    | 65  | ASN  |
| 28  | BP    | 75  | THR  |
| 28  | BP    | 100 | ARG  |
| 29  | BE    | 43  | THR  |
| 29  | BE    | 60  | TRP  |
| 29  | BE    | 165 | HIS  |
| 29  | BE    | 167 | VAL  |
| 30  | BY    | 2   | LYS  |
| 31  | B0    | 42  | ILE  |
| 31  | B0    | 48  | TYR  |
| 31  | B0    | 51  | ARG  |
| 34  | B3    | 29  | ARG  |
| 37  | BL    | 89  | VAL  |
| 37  | BL    | 100 | ILE  |
| 37  | BL    | 111 | ILE  |
| 37  | BL    | 116 | VAL  |
| 38  | BM    | 13  | HIS  |
| 38  | BM    | 36  | VAL  |
| 38  | BM    | 78  | LEU  |
| 39  | BX    | 2   | LYS  |
| 40  | BH    | 3   | VAL  |
| 40  | BH    | 10  | ALA  |
| 40  | BH    | 12  | LEU  |
| 40  | BH    | 31  | VAL  |
| 40  | BH    | 32  | PRO  |
| 40  | BH    | 33  | GLN  |
| 40  | BH    | 147 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BJ    | 4   | PHE  |
| 41  | BJ    | 41  | LYS  |
| 41  | BJ    | 44  | TYR  |
| 41  | BJ    | 45  | THR  |
| 41  | BJ    | 81  | ILE  |
| 44  | BQ    | 30  | VAL  |
| 44  | BQ    | 31  | TYR  |
| 45  | BS    | 13  | SER  |
| 45  | BS    | 27  | LYS  |
| 45  | BS    | 61  | ASN  |
| 46  | BU    | 6   | ARG  |
| 46  | BU    | 18  | LYS  |
| 46  | BU    | 42  | LYS  |
| 46  | BU    | 85  | ARG  |
| 47  | BF    | 32  | LYS  |
| 47  | BF    | 41  | GLU  |
| 47  | BF    | 43  | ILE  |
| 47  | BF    | 77  | LYS  |
| 47  | BF    | 92  | GLY  |
| 47  | BF    | 112 | ASP  |
| 47  | BF    | 135 | ILE  |
| 47  | BF    | 138 | PRO  |
| 47  | BF    | 148 | VAL  |
| 47  | BF    | 149 | ARG  |
| 48  | BG    | 9   | VAL  |
| 48  | BG    | 11  | PRO  |
| 48  | BG    | 84  | LYS  |
| 48  | BG    | 85  | LYS  |
| 48  | BG    | 91  | VAL  |
| 48  | BG    | 94  | ARG  |
| 48  | BG    | 117 | PRO  |
| 48  | BG    | 172 | GLU  |
| 50  | BT    | 38  | ALA  |
| 50  | BT    | 39  | THR  |
| 50  | BT    | 58  | VAL  |
| 50  | BT    | 88  | LYS  |
| 51  | BZ    | 33  | LEU  |
| 51  | BZ    | 77  | LYS  |
| 52  | BW    | 9   | THR  |
| 52  | BW    | 14  | ASP  |
| 52  | BW    | 30  | VAL  |
| 52  | BW    | 36  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | BW    | 50  | VAL  |
| 52  | BW    | 59  | PHE  |
| 52  | BW    | 60  | ALA  |
| 2   | CC    | 54  | ILE  |
| 2   | CC    | 205 | GLU  |
| 8   | CI    | 8   | THR  |
| 9   | CJ    | 36  | VAL  |
| 9   | CJ    | 57  | VAL  |
| 12  | CM    | 22  | TYR  |
| 12  | CM    | 105 | ALA  |
| 13  | CN    | 50  | LEU  |
| 13  | CN    | 61  | ASN  |
| 14  | CO    | 18  | ASP  |
| 14  | CO    | 34  | ALA  |
| 15  | CP    | 28  | ARG  |
| 15  | CP    | 44  | SER  |
| 15  | CP    | 67  | ILE  |
| 16  | CQ    | 32  | ILE  |
| 20  | CB    | 15  | PHE  |
| 20  | CB    | 19  | THR  |
| 20  | CB    | 22  | TRP  |
| 20  | CB    | 94  | ARG  |
| 20  | CB    | 119 | GLN  |
| 21  | CU    | 12  | ASP  |
| 21  | CU    | 34  | ARG  |
| 24  | DI    | 5   | GLN  |
| 24  | DI    | 18  | ASN  |
| 25  | DC    | 51  | ARG  |
| 25  | DC    | 65  | ASP  |
| 25  | DC    | 77  | VAL  |
| 25  | DC    | 141 | HIS  |
| 26  | DD    | 9   | VAL  |
| 26  | DD    | 14  | ILE  |
| 26  | DD    | 74  | GLU  |
| 26  | DD    | 91  | THR  |
| 26  | DD    | 122 | VAL  |
| 26  | DD    | 169 | ARG  |
| 26  | DD    | 170 | VAL  |
| 27  | DK    | 17  | ARG  |
| 27  | DK    | 18  | ARG  |
| 27  | DK    | 31  | ARG  |
| 27  | DK    | 35  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DK    | 72  | PRO  |
| 27  | DK    | 119 | ALA  |
| 27  | DK    | 120 | PRO  |
| 28  | DP    | 25  | VAL  |
| 28  | DP    | 50  | ARG  |
| 28  | DP    | 64  | SER  |
| 28  | DP    | 65  | ASN  |
| 28  | DP    | 75  | THR  |
| 28  | DP    | 100 | ARG  |
| 29  | DE    | 60  | TRP  |
| 29  | DE    | 165 | HIS  |
| 29  | DE    | 167 | VAL  |
| 30  | DY    | 2   | LYS  |
| 31  | D0    | 42  | ILE  |
| 31  | D0    | 48  | TYR  |
| 31  | D0    | 51  | ARG  |
| 33  | D1    | 4   | ILE  |
| 37  | DL    | 89  | VAL  |
| 37  | DL    | 100 | ILE  |
| 37  | DL    | 111 | ILE  |
| 37  | DL    | 116 | VAL  |
| 38  | DM    | 13  | HIS  |
| 38  | DM    | 36  | VAL  |
| 38  | DM    | 78  | LEU  |
| 39  | DX    | 2   | LYS  |
| 40  | DH    | 3   | VAL  |
| 40  | DH    | 10  | ALA  |
| 40  | DH    | 31  | VAL  |
| 40  | DH    | 32  | PRO  |
| 40  | DH    | 33  | GLN  |
| 40  | DH    | 86  | ASP  |
| 40  | DH    | 121 | VAL  |
| 40  | DH    | 136 | SER  |
| 41  | DJ    | 4   | PHE  |
| 41  | DJ    | 44  | TYR  |
| 41  | DJ    | 45  | THR  |
| 41  | DJ    | 81  | ILE  |
| 41  | DJ    | 124 | VAL  |
| 44  | DQ    | 30  | VAL  |
| 44  | DQ    | 31  | TYR  |
| 45  | DS    | 3   | THR  |
| 45  | DS    | 13  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | DS    | 27  | LYS  |
| 45  | DS    | 61  | ASN  |
| 46  | DU    | 6   | ARG  |
| 46  | DU    | 18  | LYS  |
| 46  | DU    | 42  | LYS  |
| 46  | DU    | 59  | GLU  |
| 46  | DU    | 85  | ARG  |
| 47  | DF    | 32  | LYS  |
| 47  | DF    | 41  | GLU  |
| 47  | DF    | 43  | ILE  |
| 47  | DF    | 77  | LYS  |
| 47  | DF    | 92  | GLY  |
| 47  | DF    | 112 | ASP  |
| 47  | DF    | 135 | ILE  |
| 47  | DF    | 138 | PRO  |
| 47  | DF    | 148 | VAL  |
| 47  | DF    | 149 | ARG  |
| 48  | DG    | 9   | VAL  |
| 48  | DG    | 11  | PRO  |
| 48  | DG    | 84  | LYS  |
| 48  | DG    | 85  | LYS  |
| 48  | DG    | 91  | VAL  |
| 48  | DG    | 94  | ARG  |
| 48  | DG    | 117 | PRO  |
| 48  | DG    | 172 | GLU  |
| 50  | DT    | 38  | ALA  |
| 50  | DT    | 39  | THR  |
| 50  | DT    | 58  | VAL  |
| 50  | DT    | 88  | LYS  |
| 51  | DZ    | 33  | LEU  |
| 51  | DZ    | 77  | LYS  |
| 52  | DW    | 9   | THR  |
| 52  | DW    | 14  | ASP  |
| 52  | DW    | 30  | VAL  |
| 52  | DW    | 36  | ILE  |
| 52  | DW    | 50  | VAL  |
| 52  | DW    | 59  | PHE  |
| 52  | DW    | 60  | ALA  |
| 53  | D6    | 84  | ARG  |
| 53  | D6    | 88  | LEU  |
| 2   | AC    | 14  | VAL  |
| 2   | AC    | 60  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 180 | ASP  |
| 3   | AD    | 24  | VAL  |
| 3   | AD    | 82  | LYS  |
| 4   | AE    | 20  | VAL  |
| 5   | AF    | 69  | GLU  |
| 5   | AF    | 85  | ILE  |
| 5   | AF    | 92  | THR  |
| 5   | AF    | 98  | GLU  |
| 6   | AG    | 112 | ASP  |
| 7   | AH    | 59  | GLU  |
| 7   | AH    | 65  | PHE  |
| 7   | AH    | 82  | LEU  |
| 8   | AI    | 127 | SER  |
| 9   | AJ    | 74  | VAL  |
| 10  | AK    | 88  | PRO  |
| 10  | AK    | 126 | ARG  |
| 11  | AL    | 13  | ARG  |
| 11  | AL    | 16  | ALA  |
| 11  | AL    | 23  | LEU  |
| 11  | AL    | 24  | GLU  |
| 11  | AL    | 42  | LYS  |
| 11  | AL    | 117 | GLY  |
| 13  | AN    | 2   | LYS  |
| 13  | AN    | 29  | ILE  |
| 13  | AN    | 71  | GLY  |
| 15  | AP    | 52  | LEU  |
| 18  | AS    | 27  | LYS  |
| 19  | AT    | 76  | ALA  |
| 20  | AB    | 86  | CYS  |
| 20  | AB    | 94  | ARG  |
| 20  | AB    | 163 | ILE  |
| 20  | AB    | 188 | THR  |
| 21  | AU    | 7   | GLU  |
| 24  | BI    | 14  | ALA  |
| 24  | BI    | 64  | ARG  |
| 25  | BC    | 3   | VAL  |
| 25  | BC    | 36  | ASN  |
| 25  | BC    | 51  | ARG  |
| 25  | BC    | 52  | HIS  |
| 25  | BC    | 53  | ILE  |
| 25  | BC    | 64  | VAL  |
| 25  | BC    | 88  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BC    | 93  | VAL  |
| 25  | BC    | 107 | LYS  |
| 25  | BC    | 145 | MET  |
| 25  | BC    | 222 | THR  |
| 25  | BC    | 239 | PHE  |
| 25  | BC    | 250 | GLN  |
| 25  | BC    | 255 | LYS  |
| 26  | BD    | 53  | GLY  |
| 26  | BD    | 93  | GLY  |
| 26  | BD    | 106 | LYS  |
| 26  | BD    | 107 | VAL  |
| 26  | BD    | 121 | THR  |
| 26  | BD    | 131 | ASP  |
| 26  | BD    | 136 | ASN  |
| 26  | BD    | 145 | SER  |
| 26  | BD    | 149 | ASN  |
| 26  | BD    | 159 | LYS  |
| 26  | BD    | 197 | THR  |
| 27  | BK    | 6   | THR  |
| 27  | BK    | 92  | GLU  |
| 27  | BK    | 119 | ALA  |
| 29  | BE    | 42  | GLY  |
| 29  | BE    | 79  | ARG  |
| 29  | BE    | 86  | ALA  |
| 30  | BY    | 4   | ILE  |
| 32  | B4    | 4   | ARG  |
| 33  | B1    | 4   | ILE  |
| 34  | B3    | 22  | LYS  |
| 35  | BV    | 25  | LYS  |
| 36  | B2    | 45  | SER  |
| 37  | BL    | 9   | ALA  |
| 37  | BL    | 28  | GLY  |
| 37  | BL    | 36  | LYS  |
| 37  | BL    | 54  | GLN  |
| 37  | BL    | 99  | ASN  |
| 37  | BL    | 143 | GLU  |
| 38  | BM    | 20  | LEU  |
| 38  | BM    | 43  | ALA  |
| 38  | BM    | 69  | PRO  |
| 38  | BM    | 79  | ALA  |
| 38  | BM    | 134 | THR  |
| 39  | BX    | 9   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BX    | 61  | ALA  |
| 40  | BH    | 73  | ASN  |
| 40  | BH    | 77  | THR  |
| 40  | BH    | 125 | THR  |
| 41  | BJ    | 2   | LYS  |
| 41  | BJ    | 43  | GLU  |
| 41  | BJ    | 73  | VAL  |
| 41  | BJ    | 124 | VAL  |
| 41  | BJ    | 134 | ALA  |
| 42  | BN    | 98  | LEU  |
| 42  | BN    | 100 | CYS  |
| 42  | BN    | 101 | GLY  |
| 43  | BO    | 51  | ALA  |
| 43  | BO    | 100 | HIS  |
| 44  | BQ    | 17  | LEU  |
| 44  | BQ    | 18  | LYS  |
| 44  | BQ    | 89  | ILE  |
| 44  | BQ    | 91  | ARG  |
| 45  | BS    | 3   | THR  |
| 45  | BS    | 14  | ALA  |
| 45  | BS    | 25  | ARG  |
| 45  | BS    | 96  | ILE  |
| 46  | BU    | 19  | GLY  |
| 46  | BU    | 41  | VAL  |
| 46  | BU    | 50  | ALA  |
| 46  | BU    | 59  | GLU  |
| 46  | BU    | 82  | VAL  |
| 46  | BU    | 89  | GLY  |
| 46  | BU    | 92  | VAL  |
| 47  | BF    | 11  | VAL  |
| 47  | BF    | 36  | ASN  |
| 47  | BF    | 78  | ILE  |
| 47  | BF    | 87  | LYS  |
| 47  | BF    | 103 | ILE  |
| 47  | BF    | 110 | ILE  |
| 47  | BF    | 142 | TYR  |
| 48  | BG    | 31  | GLU  |
| 48  | BG    | 38  | ASP  |
| 48  | BG    | 46  | ASP  |
| 48  | BG    | 83  | THR  |
| 48  | BG    | 97  | VAL  |
| 48  | BG    | 164 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | BG    | 170 | THR  |
| 49  | BR    | 24  | LYS  |
| 49  | BR    | 43  | ASN  |
| 49  | BR    | 55  | ASP  |
| 49  | BR    | 57  | GLY  |
| 49  | BR    | 70  | GLU  |
| 50  | BT    | 2   | ILE  |
| 50  | BT    | 19  | LYS  |
| 51  | BZ    | 71  | LEU  |
| 52  | BW    | 12  | GLY  |
| 52  | BW    | 13  | ARG  |
| 52  | BW    | 17  | ALA  |
| 52  | BW    | 32  | ALA  |
| 52  | BW    | 34  | SER  |
| 52  | BW    | 53  | GLY  |
| 52  | BW    | 61  | LYS  |
| 52  | BW    | 62  | ALA  |
| 53  | B6    | 41  | LEU  |
| 2   | CC    | 14  | VAL  |
| 2   | CC    | 60  | ALA  |
| 2   | CC    | 180 | ASP  |
| 3   | CD    | 24  | VAL  |
| 3   | CD    | 82  | LYS  |
| 4   | CE    | 20  | VAL  |
| 5   | CF    | 69  | GLU  |
| 5   | CF    | 85  | ILE  |
| 5   | CF    | 92  | THR  |
| 5   | CF    | 98  | GLU  |
| 6   | CG    | 112 | ASP  |
| 7   | CH    | 59  | GLU  |
| 7   | CH    | 65  | PHE  |
| 7   | CH    | 82  | LEU  |
| 8   | CI    | 127 | SER  |
| 9   | CJ    | 74  | VAL  |
| 10  | CK    | 88  | PRO  |
| 10  | CK    | 126 | ARG  |
| 11  | CL    | 13  | ARG  |
| 11  | CL    | 16  | ALA  |
| 11  | CL    | 23  | LEU  |
| 11  | CL    | 24  | GLU  |
| 11  | CL    | 42  | LYS  |
| 11  | CL    | 117 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CM    | 49  | GLU  |
| 13  | CN    | 29  | ILE  |
| 13  | CN    | 71  | GLY  |
| 15  | CP    | 52  | LEU  |
| 18  | CS    | 27  | LYS  |
| 19  | CT    | 76  | ALA  |
| 20  | CB    | 18  | GLN  |
| 20  | CB    | 86  | CYS  |
| 20  | CB    | 163 | ILE  |
| 20  | CB    | 188 | THR  |
| 25  | DC    | 3   | VAL  |
| 25  | DC    | 36  | ASN  |
| 25  | DC    | 52  | HIS  |
| 25  | DC    | 53  | ILE  |
| 25  | DC    | 64  | VAL  |
| 25  | DC    | 88  | ALA  |
| 25  | DC    | 93  | VAL  |
| 25  | DC    | 94  | LEU  |
| 25  | DC    | 107 | LYS  |
| 25  | DC    | 145 | MET  |
| 25  | DC    | 222 | THR  |
| 25  | DC    | 239 | PHE  |
| 25  | DC    | 250 | GLN  |
| 25  | DC    | 255 | LYS  |
| 26  | DD    | 93  | GLY  |
| 26  | DD    | 106 | LYS  |
| 26  | DD    | 107 | VAL  |
| 26  | DD    | 121 | THR  |
| 26  | DD    | 145 | SER  |
| 26  | DD    | 149 | ASN  |
| 26  | DD    | 159 | LYS  |
| 26  | DD    | 196 | ALA  |
| 26  | DD    | 197 | THR  |
| 27  | DK    | 6   | THR  |
| 27  | DK    | 92  | GLU  |
| 28  | DP    | 38  | ARG  |
| 29  | DE    | 42  | GLY  |
| 29  | DE    | 43  | THR  |
| 29  | DE    | 78  | TRP  |
| 29  | DE    | 79  | ARG  |
| 29  | DE    | 86  | ALA  |
| 30  | DY    | 4   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DY    | 34  | THR  |
| 32  | D4    | 4   | ARG  |
| 32  | D4    | 8   | LYS  |
| 34  | D3    | 20  | GLY  |
| 34  | D3    | 22  | LYS  |
| 34  | D3    | 29  | ARG  |
| 35  | DV    | 25  | LYS  |
| 36  | D2    | 45  | SER  |
| 37  | DL    | 9   | ALA  |
| 37  | DL    | 28  | GLY  |
| 37  | DL    | 54  | GLN  |
| 37  | DL    | 99  | ASN  |
| 37  | DL    | 143 | GLU  |
| 38  | DM    | 20  | LEU  |
| 38  | DM    | 43  | ALA  |
| 38  | DM    | 69  | PRO  |
| 38  | DM    | 79  | ALA  |
| 38  | DM    | 134 | THR  |
| 39  | DX    | 9   | LYS  |
| 39  | DX    | 61  | ALA  |
| 40  | DH    | 12  | LEU  |
| 40  | DH    | 96  | THR  |
| 40  | DH    | 113 | SER  |
| 40  | DH    | 114 | GLU  |
| 41  | DJ    | 2   | LYS  |
| 41  | DJ    | 41  | LYS  |
| 41  | DJ    | 43  | GLU  |
| 41  | DJ    | 73  | VAL  |
| 41  | DJ    | 112 | GLY  |
| 42  | DN    | 11  | ASN  |
| 42  | DN    | 98  | LEU  |
| 42  | DN    | 100 | CYS  |
| 42  | DN    | 101 | GLY  |
| 43  | DO    | 51  | ALA  |
| 43  | DO    | 100 | HIS  |
| 44  | DQ    | 18  | LYS  |
| 44  | DQ    | 89  | ILE  |
| 44  | DQ    | 91  | ARG  |
| 45  | DS    | 14  | ALA  |
| 45  | DS    | 25  | ARG  |
| 45  | DS    | 96  | ILE  |
| 46  | DU    | 19  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | DU    | 41  | VAL  |
| 46  | DU    | 50  | ALA  |
| 46  | DU    | 82  | VAL  |
| 46  | DU    | 89  | GLY  |
| 46  | DU    | 92  | VAL  |
| 47  | DF    | 11  | VAL  |
| 47  | DF    | 36  | ASN  |
| 47  | DF    | 78  | ILE  |
| 47  | DF    | 87  | LYS  |
| 47  | DF    | 103 | ILE  |
| 47  | DF    | 142 | TYR  |
| 48  | DG    | 31  | GLU  |
| 48  | DG    | 38  | ASP  |
| 48  | DG    | 46  | ASP  |
| 48  | DG    | 83  | THR  |
| 48  | DG    | 97  | VAL  |
| 48  | DG    | 164 | ALA  |
| 48  | DG    | 170 | THR  |
| 49  | DR    | 24  | LYS  |
| 49  | DR    | 43  | ASN  |
| 49  | DR    | 57  | GLY  |
| 49  | DR    | 70  | GLU  |
| 50  | DT    | 2   | ILE  |
| 50  | DT    | 19  | LYS  |
| 51  | DZ    | 71  | LEU  |
| 52  | DW    | 12  | GLY  |
| 52  | DW    | 13  | ARG  |
| 52  | DW    | 17  | ALA  |
| 52  | DW    | 32  | ALA  |
| 52  | DW    | 34  | SER  |
| 52  | DW    | 53  | GLY  |
| 52  | DW    | 61  | LYS  |
| 52  | DW    | 62  | ALA  |
| 53  | D6    | 39  | LEU  |
| 53  | D6    | 41  | LEU  |
| 2   | AC    | 3   | LYS  |
| 2   | AC    | 59  | PRO  |
| 2   | AC    | 112 | ALA  |
| 3   | AD    | 22  | SER  |
| 3   | AD    | 25  | ARG  |
| 3   | AD    | 31  | CYS  |
| 3   | AD    | 191 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AF    | 54  | LEU  |
| 5   | AF    | 82  | ASP  |
| 8   | AI    | 24  | ASN  |
| 9   | AJ    | 34  | ALA  |
| 9   | AJ    | 56  | HIS  |
| 9   | AJ    | 75  | ASP  |
| 10  | AK    | 46  | ALA  |
| 10  | AK    | 124 | LYS  |
| 11  | AL    | 15  | VAL  |
| 11  | AL    | 47  | ALA  |
| 11  | AL    | 121 | PRO  |
| 12  | AM    | 49  | GLU  |
| 12  | AM    | 104 | ASN  |
| 13  | AN    | 27  | LYS  |
| 13  | AN    | 34  | ASN  |
| 20  | AB    | 14  | HIS  |
| 20  | AB    | 18  | GLN  |
| 20  | AB    | 36  | LYS  |
| 20  | AB    | 58  | LYS  |
| 21  | AU    | 25  | ALA  |
| 24  | BI    | 23  | VAL  |
| 25  | BC    | 37  | SER  |
| 25  | BC    | 59  | GLN  |
| 25  | BC    | 70  | LYS  |
| 25  | BC    | 94  | LEU  |
| 25  | BC    | 121 | ALA  |
| 25  | BC    | 140 | VAL  |
| 25  | BC    | 237 | ARG  |
| 25  | BC    | 246 | PRO  |
| 26  | BD    | 54  | ALA  |
| 26  | BD    | 113 | SER  |
| 26  | BD    | 144 | GLY  |
| 26  | BD    | 162 | ALA  |
| 26  | BD    | 167 | ASN  |
| 26  | BD    | 181 | ASP  |
| 26  | BD    | 194 | PRO  |
| 26  | BD    | 196 | ALA  |
| 27  | BK    | 14  | SER  |
| 27  | BK    | 43  | ILE  |
| 27  | BK    | 73  | ASP  |
| 27  | BK    | 89  | ASN  |
| 27  | BK    | 110 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BP    | 37  | LYS  |
| 28  | BP    | 101 | GLU  |
| 29  | BE    | 27  | LEU  |
| 29  | BE    | 46  | GLN  |
| 29  | BE    | 69  | ARG  |
| 29  | BE    | 70  | SER  |
| 29  | BE    | 188 | MET  |
| 30  | BY    | 34  | THR  |
| 30  | BY    | 50  | VAL  |
| 31  | B0    | 54  | ILE  |
| 32  | B4    | 8   | LYS  |
| 32  | B4    | 21  | GLY  |
| 32  | B4    | 36  | ARG  |
| 33  | B1    | 36  | LYS  |
| 33  | B1    | 50  | GLU  |
| 34  | B3    | 31  | ILE  |
| 34  | B3    | 58  | ILE  |
| 37  | BL    | 15  | ALA  |
| 37  | BL    | 19  | LEU  |
| 37  | BL    | 29  | LYS  |
| 37  | BL    | 51  | GLU  |
| 37  | BL    | 62  | PRO  |
| 37  | BL    | 65  | GLY  |
| 37  | BL    | 81  | ASP  |
| 38  | BM    | 21  | ALA  |
| 38  | BM    | 72  | PRO  |
| 38  | BM    | 77  | PRO  |
| 39  | BX    | 62  | GLY  |
| 40  | BH    | 7   | ASP  |
| 40  | BH    | 9   | VAL  |
| 40  | BH    | 11  | ASN  |
| 40  | BH    | 28  | ASN  |
| 40  | BH    | 45  | GLU  |
| 40  | BH    | 54  | LEU  |
| 40  | BH    | 64  | ALA  |
| 40  | BH    | 83  | LYS  |
| 41  | BJ    | 84  | ILE  |
| 41  | BJ    | 112 | GLY  |
| 42  | BN    | 10  | LEU  |
| 42  | BN    | 11  | ASN  |
| 42  | BN    | 68  | ALA  |
| 42  | BN    | 82  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | BN    | 119 | SER  |
| 44  | BQ    | 10  | ARG  |
| 46  | BU    | 12  | VAL  |
| 46  | BU    | 47  | PRO  |
| 46  | BU    | 49  | PRO  |
| 47  | BF    | 9   | ASP  |
| 47  | BF    | 121 | PHE  |
| 47  | BF    | 136 | ILE  |
| 47  | BF    | 176 | PHE  |
| 48  | BG    | 2   | ARG  |
| 48  | BG    | 61  | TRP  |
| 48  | BG    | 89  | VAL  |
| 49  | BR    | 7   | SER  |
| 49  | BR    | 40  | MET  |
| 49  | BR    | 46  | GLU  |
| 49  | BR    | 56  | GLY  |
| 49  | BR    | 79  | ARG  |
| 49  | BR    | 98  | ILE  |
| 50  | BT    | 11  | LEU  |
| 51  | BZ    | 70  | GLU  |
| 52  | BW    | 29  | SER  |
| 53  | B6    | 30  | THR  |
| 53  | B6    | 69  | GLN  |
| 2   | CC    | 3   | LYS  |
| 2   | CC    | 59  | PRO  |
| 2   | CC    | 112 | ALA  |
| 3   | CD    | 22  | SER  |
| 3   | CD    | 25  | ARG  |
| 3   | CD    | 31  | CYS  |
| 3   | CD    | 68  | GLU  |
| 3   | CD    | 191 | SER  |
| 5   | CF    | 54  | LEU  |
| 5   | CF    | 82  | ASP  |
| 8   | CI    | 24  | ASN  |
| 9   | CJ    | 34  | ALA  |
| 9   | CJ    | 56  | HIS  |
| 9   | CJ    | 75  | ASP  |
| 10  | CK    | 51  | PHE  |
| 10  | CK    | 124 | LYS  |
| 11  | CL    | 47  | ALA  |
| 11  | CL    | 121 | PRO  |
| 12  | CM    | 104 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CN    | 2   | LYS  |
| 18  | CS    | 2   | ARG  |
| 20  | CB    | 14  | HIS  |
| 20  | CB    | 36  | LYS  |
| 20  | CB    | 58  | LYS  |
| 20  | CB    | 141 | GLU  |
| 21  | CU    | 7   | GLU  |
| 21  | CU    | 25  | ALA  |
| 24  | DI    | 23  | VAL  |
| 25  | DC    | 37  | SER  |
| 25  | DC    | 59  | GLN  |
| 25  | DC    | 70  | LYS  |
| 25  | DC    | 121 | ALA  |
| 25  | DC    | 123 | ILE  |
| 25  | DC    | 140 | VAL  |
| 25  | DC    | 195 | GLY  |
| 25  | DC    | 237 | ARG  |
| 25  | DC    | 246 | PRO  |
| 25  | DC    | 254 | LYS  |
| 26  | DD    | 53  | GLY  |
| 26  | DD    | 54  | ALA  |
| 26  | DD    | 127 | PHE  |
| 26  | DD    | 131 | ASP  |
| 26  | DD    | 136 | ASN  |
| 26  | DD    | 144 | GLY  |
| 26  | DD    | 162 | ALA  |
| 26  | DD    | 167 | ASN  |
| 26  | DD    | 181 | ASP  |
| 26  | DD    | 194 | PRO  |
| 27  | DK    | 14  | SER  |
| 27  | DK    | 43  | ILE  |
| 27  | DK    | 46  | ALA  |
| 27  | DK    | 73  | ASP  |
| 27  | DK    | 89  | ASN  |
| 27  | DK    | 110 | GLU  |
| 28  | DP    | 101 | GLU  |
| 29  | DE    | 46  | GLN  |
| 29  | DE    | 69  | ARG  |
| 29  | DE    | 70  | SER  |
| 30  | DY    | 50  | VAL  |
| 31  | D0    | 54  | ILE  |
| 32  | D4    | 21  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | D4    | 36  | ARG  |
| 33  | D1    | 36  | LYS  |
| 33  | D1    | 50  | GLU  |
| 33  | D1    | 51  | ALA  |
| 34  | D3    | 31  | ILE  |
| 34  | D3    | 58  | ILE  |
| 37  | DL    | 3   | LEU  |
| 37  | DL    | 15  | ALA  |
| 37  | DL    | 19  | LEU  |
| 37  | DL    | 31  | GLY  |
| 37  | DL    | 36  | LYS  |
| 37  | DL    | 51  | GLU  |
| 37  | DL    | 81  | ASP  |
| 37  | DL    | 117 | THR  |
| 38  | DM    | 2   | LEU  |
| 38  | DM    | 21  | ALA  |
| 38  | DM    | 72  | PRO  |
| 38  | DM    | 77  | PRO  |
| 39  | DX    | 62  | GLY  |
| 40  | DH    | 7   | ASP  |
| 40  | DH    | 9   | VAL  |
| 40  | DH    | 11  | ASN  |
| 40  | DH    | 28  | ASN  |
| 40  | DH    | 40  | THR  |
| 41  | DJ    | 84  | ILE  |
| 41  | DJ    | 134 | ALA  |
| 42  | DN    | 10  | LEU  |
| 42  | DN    | 68  | ALA  |
| 42  | DN    | 82  | GLU  |
| 42  | DN    | 119 | SER  |
| 43  | DO    | 98  | GLN  |
| 44  | DQ    | 10  | ARG  |
| 44  | DQ    | 17  | LEU  |
| 46  | DU    | 12  | VAL  |
| 46  | DU    | 47  | PRO  |
| 46  | DU    | 49  | PRO  |
| 47  | DF    | 136 | ILE  |
| 47  | DF    | 176 | PHE  |
| 48  | DG    | 2   | ARG  |
| 48  | DG    | 18  | ILE  |
| 48  | DG    | 61  | TRP  |
| 48  | DG    | 89  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | DG    | 109 | SER  |
| 49  | DR    | 7   | SER  |
| 49  | DR    | 46  | GLU  |
| 49  | DR    | 55  | ASP  |
| 49  | DR    | 56  | GLY  |
| 49  | DR    | 79  | ARG  |
| 49  | DR    | 98  | ILE  |
| 50  | DT    | 11  | LEU  |
| 51  | DZ    | 70  | GLU  |
| 52  | DW    | 10  | ARG  |
| 52  | DW    | 23  | LYS  |
| 52  | DW    | 29  | SER  |
| 53  | D6    | 70  | SER  |
| 2   | AC    | 100 | ILE  |
| 2   | AC    | 107 | LYS  |
| 3   | AD    | 68  | GLU  |
| 4   | AE    | 77  | ASN  |
| 4   | AE    | 156 | ARG  |
| 5   | AF    | 95  | ALA  |
| 8   | AI    | 44  | ARG  |
| 8   | AI    | 55  | ASP  |
| 10  | AK    | 51  | PHE  |
| 13  | AN    | 48  | GLN  |
| 13  | AN    | 51  | PRO  |
| 13  | AN    | 52  | ARG  |
| 13  | AN    | 67  | GLY  |
| 16  | AQ    | 70  | LYS  |
| 16  | AQ    | 81  | ALA  |
| 20  | AB    | 119 | GLN  |
| 20  | AB    | 121 | GLN  |
| 20  | AB    | 141 | GLU  |
| 20  | AB    | 149 | GLY  |
| 20  | AB    | 153 | MET  |
| 20  | AB    | 200 | PRO  |
| 20  | AB    | 205 | ALA  |
| 21  | AU    | 9   | GLU  |
| 21  | AU    | 11  | PHE  |
| 21  | AU    | 17  | ARG  |
| 21  | AU    | 22  | CYS  |
| 25  | BC    | 35  | LYS  |
| 25  | BC    | 105 | ALA  |
| 25  | BC    | 123 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BC    | 196 | ASN  |
| 25  | BC    | 257 | ARG  |
| 26  | BD    | 56  | LYS  |
| 26  | BD    | 127 | PHE  |
| 27  | BK    | 4   | GLU  |
| 27  | BK    | 46  | ALA  |
| 28  | BP    | 113 | LEU  |
| 29  | BE    | 78  | TRP  |
| 29  | BE    | 96  | VAL  |
| 29  | BE    | 131 | THR  |
| 30  | BY    | 9   | THR  |
| 32  | B4    | 9   | LYS  |
| 32  | B4    | 10  | LEU  |
| 33  | B1    | 51  | ALA  |
| 34  | B3    | 20  | GLY  |
| 35  | BV    | 71  | LYS  |
| 36  | B2    | 14  | ARG  |
| 37  | BL    | 31  | GLY  |
| 37  | BL    | 117 | THR  |
| 38  | BM    | 2   | LEU  |
| 39  | BX    | 37  | LEU  |
| 40  | BH    | 44  | ILE  |
| 40  | BH    | 62  | LEU  |
| 40  | BH    | 86  | ASP  |
| 40  | BH    | 97  | ARG  |
| 40  | BH    | 126 | GLY  |
| 42  | BN    | 70  | THR  |
| 43  | BO    | 65  | THR  |
| 43  | BO    | 68  | LYS  |
| 43  | BO    | 98  | GLN  |
| 44  | BQ    | 26  | ALA  |
| 44  | BQ    | 86  | SER  |
| 44  | BQ    | 88  | GLU  |
| 45  | BS    | 71  | VAL  |
| 45  | BS    | 80  | PRO  |
| 46  | BU    | 51  | LEU  |
| 46  | BU    | 63  | ALA  |
| 46  | BU    | 67  | SER  |
| 46  | BU    | 78  | LYS  |
| 46  | BU    | 101 | THR  |
| 48  | BG    | 18  | ILE  |
| 48  | BG    | 109 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | BT    | 28  | ASN  |
| 50  | BT    | 29  | THR  |
| 50  | BT    | 69  | ARG  |
| 50  | BT    | 86  | THR  |
| 51  | BZ    | 35  | SER  |
| 52  | BW    | 10  | ARG  |
| 52  | BW    | 23  | LYS  |
| 52  | BW    | 28  | GLU  |
| 52  | BW    | 56  | HIS  |
| 52  | BW    | 68  | PHE  |
| 52  | BW    | 77  | LYS  |
| 53  | B6    | 44  | GLU  |
| 2   | CC    | 100 | ILE  |
| 2   | CC    | 107 | LYS  |
| 3   | CD    | 192 | ALA  |
| 4   | CE    | 77  | ASN  |
| 4   | CE    | 156 | ARG  |
| 5   | CF    | 95  | ALA  |
| 6   | CG    | 152 | HIS  |
| 8   | CI    | 42  | THR  |
| 8   | CI    | 55  | ASP  |
| 10  | CK    | 46  | ALA  |
| 11  | CL    | 15  | VAL  |
| 13  | CN    | 27  | LYS  |
| 13  | CN    | 34  | ASN  |
| 13  | CN    | 48  | GLN  |
| 13  | CN    | 51  | PRO  |
| 13  | CN    | 52  | ARG  |
| 13  | CN    | 67  | GLY  |
| 20  | CB    | 129 | THR  |
| 20  | CB    | 130 | LYS  |
| 20  | CB    | 153 | MET  |
| 20  | CB    | 200 | PRO  |
| 20  | CB    | 205 | ALA  |
| 21  | CU    | 9   | GLU  |
| 21  | CU    | 11  | PHE  |
| 21  | CU    | 17  | ARG  |
| 25  | DC    | 196 | ASN  |
| 25  | DC    | 257 | ARG  |
| 26  | DD    | 56  | LYS  |
| 26  | DD    | 109 | VAL  |
| 26  | DD    | 113 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DK    | 4   | GLU  |
| 28  | DP    | 37  | LYS  |
| 28  | DP    | 113 | LEU  |
| 29  | DE    | 27  | LEU  |
| 29  | DE    | 188 | MET  |
| 30  | DY    | 9   | THR  |
| 31  | D0    | 17  | SER  |
| 32  | D4    | 9   | LYS  |
| 32  | D4    | 10  | LEU  |
| 33  | D1    | 35  | LEU  |
| 34  | D3    | 50  | SER  |
| 35  | DV    | 45  | ASP  |
| 35  | DV    | 71  | LYS  |
| 36  | D2    | 14  | ARG  |
| 37  | DL    | 62  | PRO  |
| 39  | DX    | 37  | LEU  |
| 40  | DH    | 41  | LYS  |
| 40  | DH    | 148 | ALA  |
| 42  | DN    | 70  | THR  |
| 43  | DO    | 65  | THR  |
| 43  | DO    | 68  | LYS  |
| 44  | DQ    | 26  | ALA  |
| 45  | DS    | 80  | PRO  |
| 46  | DU    | 51  | LEU  |
| 46  | DU    | 63  | ALA  |
| 46  | DU    | 67  | SER  |
| 46  | DU    | 78  | LYS  |
| 47  | DF    | 9   | ASP  |
| 47  | DF    | 110 | ILE  |
| 47  | DF    | 121 | PHE  |
| 48  | DG    | 29  | ASN  |
| 49  | DR    | 40  | MET  |
| 50  | DT    | 28  | ASN  |
| 50  | DT    | 29  | THR  |
| 50  | DT    | 69  | ARG  |
| 50  | DT    | 86  | THR  |
| 51  | DZ    | 35  | SER  |
| 52  | DW    | 28  | GLU  |
| 52  | DW    | 51  | GLY  |
| 52  | DW    | 77  | LYS  |
| 53  | D6    | 69  | GLN  |
| 53  | D6    | 106 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 167 | TYR  |
| 3   | AD    | 29  | THR  |
| 3   | AD    | 192 | ALA  |
| 8   | AI    | 42  | THR  |
| 10  | AK    | 14  | GLN  |
| 11  | AL    | 70  | GLY  |
| 12  | AM    | 67  | ASP  |
| 13  | AN    | 31  | SER  |
| 14  | AO    | 74  | ASP  |
| 19  | AT    | 4   | LYS  |
| 20  | AB    | 50  | ASN  |
| 20  | AB    | 64  | GLY  |
| 24  | BI    | 49  | GLU  |
| 25  | BC    | 190 | THR  |
| 25  | BC    | 195 | GLY  |
| 25  | BC    | 200 | MET  |
| 25  | BC    | 254 | LYS  |
| 26  | BD    | 31  | ALA  |
| 26  | BD    | 109 | VAL  |
| 26  | BD    | 114 | LYS  |
| 27  | BK    | 93  | GLN  |
| 29  | BE    | 83  | VAL  |
| 31  | B0    | 26  | SER  |
| 33  | B1    | 35  | LEU  |
| 34  | B3    | 6   | VAL  |
| 35  | BV    | 45  | ASP  |
| 35  | BV    | 61  | LEU  |
| 36  | B2    | 44  | VAL  |
| 37  | BL    | 66  | PHE  |
| 38  | BM    | 56  | ALA  |
| 39  | BX    | 36  | GLN  |
| 40  | BH    | 29  | PHE  |
| 40  | BH    | 40  | THR  |
| 41  | BJ    | 13  | ARG  |
| 41  | BJ    | 58  | ASN  |
| 43  | BO    | 62  | LEU  |
| 43  | BO    | 99  | TYR  |
| 45  | BS    | 30  | SER  |
| 45  | BS    | 40  | ASN  |
| 45  | BS    | 65  | ASP  |
| 46  | BU    | 83  | GLY  |
| 47  | BF    | 156 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | BG    | 29  | ASN  |
| 48  | BG    | 155 | PRO  |
| 49  | BR    | 101 | ILE  |
| 50  | BT    | 8   | LEU  |
| 51  | BZ    | 28  | ARG  |
| 52  | BW    | 51  | GLY  |
| 2   | CC    | 153 | SER  |
| 2   | CC    | 167 | TYR  |
| 8   | CI    | 44  | ARG  |
| 9   | CJ    | 62  | ARG  |
| 11  | CL    | 70  | GLY  |
| 12  | CM    | 67  | ASP  |
| 15  | CP    | 46  | LYS  |
| 16  | CQ    | 70  | LYS  |
| 16  | CQ    | 81  | ALA  |
| 16  | CQ    | 82  | VAL  |
| 19  | CT    | 4   | LYS  |
| 20  | CB    | 9   | LEU  |
| 20  | CB    | 50  | ASN  |
| 20  | CB    | 64  | GLY  |
| 20  | CB    | 128 | LEU  |
| 20  | CB    | 149 | GLY  |
| 21  | CU    | 22  | CYS  |
| 21  | CU    | 41  | THR  |
| 24  | DI    | 14  | ALA  |
| 25  | DC    | 69  | ASN  |
| 25  | DC    | 105 | ALA  |
| 25  | DC    | 200 | MET  |
| 26  | DD    | 95  | SER  |
| 26  | DD    | 168 | GLU  |
| 26  | DD    | 184 | ARG  |
| 27  | DK    | 16  | ALA  |
| 27  | DK    | 93  | GLN  |
| 28  | DP    | 23  | ASP  |
| 29  | DE    | 72  | SER  |
| 29  | DE    | 83  | VAL  |
| 29  | DE    | 96  | VAL  |
| 29  | DE    | 131 | THR  |
| 31  | D0    | 26  | SER  |
| 35  | DV    | 15  | GLY  |
| 37  | DL    | 5   | THR  |
| 37  | DL    | 29  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DL    | 65  | GLY  |
| 37  | DL    | 66  | PHE  |
| 38  | DM    | 56  | ALA  |
| 39  | DX    | 36  | GLN  |
| 39  | DX    | 45  | GLN  |
| 40  | DH    | 29  | PHE  |
| 41  | DJ    | 13  | ARG  |
| 41  | DJ    | 14  | ASP  |
| 42  | DN    | 88  | ALA  |
| 43  | DO    | 62  | LEU  |
| 43  | DO    | 99  | TYR  |
| 44  | DQ    | 86  | SER  |
| 44  | DQ    | 88  | GLU  |
| 45  | DS    | 30  | SER  |
| 45  | DS    | 40  | ASN  |
| 45  | DS    | 65  | ASP  |
| 45  | DS    | 71  | VAL  |
| 46  | DU    | 101 | THR  |
| 47  | DF    | 40  | GLY  |
| 47  | DF    | 156 | THR  |
| 48  | DG    | 155 | PRO  |
| 48  | DG    | 157 | LYS  |
| 49  | DR    | 101 | ILE  |
| 50  | DT    | 8   | LEU  |
| 51  | DZ    | 28  | ARG  |
| 52  | DW    | 68  | PHE  |
| 53  | D6    | 42  | LYS  |
| 53  | D6    | 51  | PRO  |
| 2   | AC    | 47  | ALA  |
| 2   | AC    | 153 | SER  |
| 3   | AD    | 27  | ILE  |
| 7   | AH    | 47  | ASP  |
| 9   | AJ    | 62  | ARG  |
| 25  | BC    | 18  | VAL  |
| 25  | BC    | 31  | PRO  |
| 25  | BC    | 69  | ASN  |
| 26  | BD    | 33  | ARG  |
| 26  | BD    | 95  | SER  |
| 26  | BD    | 184 | ARG  |
| 28  | BP    | 83  | ILE  |
| 28  | BP    | 108 | ARG  |
| 32  | B4    | 16  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BV    | 15  | GLY  |
| 35  | BV    | 84  | PRO  |
| 37  | BL    | 52  | GLY  |
| 37  | BL    | 58  | TYR  |
| 38  | BM    | 73  | ILE  |
| 39  | BX    | 45  | GLN  |
| 41  | BJ    | 5   | THR  |
| 41  | BJ    | 14  | ASP  |
| 42  | BN    | 61  | ALA  |
| 45  | BS    | 18  | ARG  |
| 47  | BF    | 2   | LYS  |
| 47  | BF    | 40  | GLY  |
| 48  | BG    | 168 | VAL  |
| 53  | B6    | 49  | HIS  |
| 53  | B6    | 52  | LEU  |
| 2   | CC    | 104 | GLU  |
| 3   | CD    | 27  | ILE  |
| 3   | CD    | 29  | THR  |
| 3   | CD    | 165 | GLU  |
| 8   | CI    | 71  | ILE  |
| 10  | CK    | 14  | GLN  |
| 14  | CO    | 6   | GLU  |
| 25  | DC    | 18  | VAL  |
| 25  | DC    | 31  | PRO  |
| 25  | DC    | 135 | PRO  |
| 25  | DC    | 151 | GLY  |
| 26  | DD    | 114 | LYS  |
| 28  | DP    | 108 | ARG  |
| 32  | D4    | 16  | ILE  |
| 34  | D3    | 6   | VAL  |
| 35  | DV    | 84  | PRO  |
| 36  | D2    | 44  | VAL  |
| 38  | DM    | 73  | ILE  |
| 40  | DH    | 85  | GLY  |
| 40  | DH    | 107 | GLY  |
| 42  | DN    | 61  | ALA  |
| 45  | DS    | 18  | ARG  |
| 46  | DU    | 5   | ARG  |
| 47  | DF    | 2   | LYS  |
| 52  | DW    | 56  | HIS  |
| 53  | D6    | 95  | LYS  |
| 10  | AK    | 89  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | AL    | 10  | PRO  |
| 13  | AN    | 94  | GLY  |
| 19  | AT    | 3   | ILE  |
| 28  | BP    | 4   | ILE  |
| 29  | BE    | 129 | PRO  |
| 29  | BE    | 148 | ILE  |
| 38  | BM    | 83  | GLY  |
| 41  | BJ    | 64  | VAL  |
| 45  | BS    | 29  | VAL  |
| 47  | BF    | 88  | VAL  |
| 50  | BT    | 55  | VAL  |
| 10  | CK    | 89  | GLY  |
| 11  | CL    | 10  | PRO  |
| 12  | CM    | 3   | ILE  |
| 13  | CN    | 94  | GLY  |
| 25  | DC    | 15  | VAL  |
| 28  | DP    | 83  | ILE  |
| 29  | DE    | 73  | ILE  |
| 29  | DE    | 129 | PRO  |
| 29  | DE    | 148 | ILE  |
| 37  | DL    | 22  | GLY  |
| 38  | DM    | 83  | GLY  |
| 41  | DJ    | 64  | VAL  |
| 43  | DO    | 8   | ILE  |
| 45  | DS    | 29  | VAL  |
| 47  | DF    | 88  | VAL  |
| 48  | DG    | 168 | VAL  |
| 50  | DT    | 55  | VAL  |
| 12  | AM    | 3   | ILE  |
| 16  | AQ    | 31  | PRO  |
| 25  | BC    | 15  | VAL  |
| 25  | BC    | 63  | ILE  |
| 25  | BC    | 135 | PRO  |
| 25  | BC    | 151 | GLY  |
| 25  | BC    | 232 | GLY  |
| 29  | BE    | 73  | ILE  |
| 37  | BL    | 43  | GLY  |
| 40  | BH    | 34  | GLY  |
| 43  | BO    | 8   | ILE  |
| 44  | BQ    | 87  | VAL  |
| 48  | BG    | 16  | VAL  |
| 48  | BG    | 152 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | BR    | 52  | PRO  |
| 53  | B6    | 55  | ILE  |
| 3   | CD    | 107 | GLY  |
| 16  | CQ    | 31  | PRO  |
| 19  | CT    | 3   | ILE  |
| 25  | DC    | 63  | ILE  |
| 28  | DP    | 4   | ILE  |
| 40  | DH    | 34  | GLY  |
| 43  | DO    | 28  | VAL  |
| 44  | DQ    | 87  | VAL  |
| 46  | DU    | 83  | GLY  |
| 48  | DG    | 16  | VAL  |
| 48  | DG    | 152 | ARG  |
| 49  | DR    | 52  | PRO  |
| 52  | DW    | 33  | GLY  |
| 3   | AD    | 107 | GLY  |
| 9   | AJ    | 41  | PRO  |
| 31  | B0    | 24  | VAL  |
| 42  | BN    | 47  | VAL  |
| 43  | BO    | 28  | VAL  |
| 47  | BF    | 81  | GLY  |
| 52  | BW    | 70  | VAL  |
| 12  | CM    | 6   | ILE  |
| 25  | DC    | 232 | GLY  |
| 37  | DL    | 43  | GLY  |
| 37  | DL    | 52  | GLY  |
| 52  | DW    | 70  | VAL  |
| 6   | AG    | 15  | PRO  |
| 6   | AG    | 68  | VAL  |
| 12  | AM    | 6   | ILE  |
| 50  | BT    | 16  | VAL  |
| 52  | BW    | 33  | GLY  |
| 2   | CC    | 65  | VAL  |
| 4   | CE    | 107 | GLY  |
| 6   | CG    | 68  | VAL  |
| 9   | CJ    | 41  | PRO  |
| 31  | D0    | 24  | VAL  |
| 41  | DJ    | 139 | VAL  |
| 42  | DN    | 47  | VAL  |
| 47  | DF    | 12  | VAL  |
| 47  | DF    | 81  | GLY  |
| 50  | DT    | 16  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | D6    | 105 | PRO  |
| 40  | BH    | 103 | VAL  |
| 47  | BF    | 12  | VAL  |
| 6   | CG    | 15  | PRO  |
| 38  | DM    | 19  | GLY  |

### 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   | AC    | 170/189 (90%)  | 142 (84%) | 28 (16%) | 3           | 25 |
| 2   | CC    | 170/189 (90%)  | 142 (84%) | 28 (16%) | 3           | 25 |
| 3   | AD    | 172/172 (100%) | 147 (86%) | 25 (14%) | 5           | 31 |
| 3   | CD    | 172/172 (100%) | 148 (86%) | 24 (14%) | 5           | 33 |
| 4   | AE    | 113/125 (90%)  | 96 (85%)  | 17 (15%) | 4           | 30 |
| 4   | CE    | 113/125 (90%)  | 96 (85%)  | 17 (15%) | 4           | 30 |
| 5   | AF    | 87/116 (75%)   | 71 (82%)  | 16 (18%) | 2           | 18 |
| 5   | CF    | 87/116 (75%)   | 70 (80%)  | 17 (20%) | 2           | 15 |
| 6   | AG    | 123/146 (84%)  | 106 (86%) | 17 (14%) | 5           | 34 |
| 6   | CG    | 125/146 (86%)  | 109 (87%) | 16 (13%) | 6           | 38 |
| 7   | AH    | 104/104 (100%) | 96 (92%)  | 8 (8%)   | 18          | 64 |
| 7   | CH    | 104/104 (100%) | 96 (92%)  | 8 (8%)   | 18          | 64 |
| 8   | AI    | 105/106 (99%)  | 88 (84%)  | 17 (16%) | 3           | 26 |
| 8   | CI    | 105/106 (99%)  | 88 (84%)  | 17 (16%) | 3           | 26 |
| 9   | AJ    | 86/90 (96%)    | 73 (85%)  | 13 (15%) | 4           | 29 |
| 9   | CJ    | 86/90 (96%)    | 73 (85%)  | 13 (15%) | 4           | 29 |
| 10  | AK    | 90/98 (92%)    | 76 (84%)  | 14 (16%) | 4           | 28 |
| 10  | CK    | 90/98 (92%)    | 76 (84%)  | 14 (16%) | 4           | 28 |
| 11  | AL    | 103/103 (100%) | 92 (89%)  | 11 (11%) | 10          | 48 |
| 11  | CL    | 103/103 (100%) | 91 (88%)  | 12 (12%) | 8           | 42 |
| 12  | AM    | 92/95 (97%)    | 78 (85%)  | 14 (15%) | 4           | 29 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 12  | CM    | 91/95 (96%)    | 77 (85%)  | 14 (15%) | 4           | 28 |
| 13  | AN    | 79/83 (95%)    | 66 (84%)  | 13 (16%) | 3           | 25 |
| 13  | CN    | 79/83 (95%)    | 66 (84%)  | 13 (16%) | 3           | 25 |
| 14  | AO    | 76/77 (99%)    | 64 (84%)  | 12 (16%) | 4           | 27 |
| 14  | CO    | 76/77 (99%)    | 64 (84%)  | 12 (16%) | 4           | 27 |
| 15  | AP    | 65/65 (100%)   | 60 (92%)  | 5 (8%)   | 18          | 64 |
| 15  | CP    | 65/65 (100%)   | 60 (92%)  | 5 (8%)   | 18          | 64 |
| 16  | AQ    | 74/77 (96%)    | 66 (89%)  | 8 (11%)  | 9           | 47 |
| 16  | CQ    | 75/77 (97%)    | 67 (89%)  | 8 (11%)  | 10          | 48 |
| 17  | AR    | 48/64 (75%)    | 45 (94%)  | 3 (6%)   | 25          | 73 |
| 17  | CR    | 48/64 (75%)    | 45 (94%)  | 3 (6%)   | 25          | 73 |
| 18  | AS    | 70/78 (90%)    | 54 (77%)  | 16 (23%) | 1           | 10 |
| 18  | CS    | 71/78 (91%)    | 55 (78%)  | 16 (22%) | 1           | 11 |
| 19  | AT    | 65/65 (100%)   | 56 (86%)  | 9 (14%)  | 5           | 34 |
| 19  | CT    | 65/65 (100%)   | 56 (86%)  | 9 (14%)  | 5           | 34 |
| 20  | AB    | 180/198 (91%)  | 150 (83%) | 30 (17%) | 3           | 24 |
| 20  | CB    | 180/198 (91%)  | 149 (83%) | 31 (17%) | 3           | 22 |
| 21  | AU    | 44/60 (73%)    | 31 (70%)  | 13 (30%) | 0           | 5  |
| 21  | CU    | 44/60 (73%)    | 31 (70%)  | 13 (30%) | 0           | 5  |
| 24  | BI    | 109/109 (100%) | 107 (98%) | 2 (2%)   | 71          | 93 |
| 24  | DI    | 109/109 (100%) | 103 (94%) | 6 (6%)   | 30          | 77 |
| 25  | BC    | 216/217 (100%) | 178 (82%) | 38 (18%) | 3           | 20 |
| 25  | DC    | 216/217 (100%) | 179 (83%) | 37 (17%) | 3           | 22 |
| 26  | BD    | 164/164 (100%) | 142 (87%) | 22 (13%) | 6           | 35 |
| 26  | DD    | 164/164 (100%) | 140 (85%) | 24 (15%) | 5           | 31 |
| 27  | BK    | 102/104 (98%)  | 75 (74%)  | 27 (26%) | 1           | 7  |
| 27  | DK    | 102/104 (98%)  | 75 (74%)  | 27 (26%) | 1           | 7  |
| 28  | BP    | 99/99 (100%)   | 82 (83%)  | 17 (17%) | 3           | 22 |
| 28  | DP    | 99/99 (100%)   | 82 (83%)  | 17 (17%) | 3           | 22 |
| 29  | BE    | 165/165 (100%) | 141 (86%) | 24 (14%) | 5           | 31 |
| 29  | DE    | 165/165 (100%) | 140 (85%) | 25 (15%) | 4           | 29 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30  | BY    | 48/48 (100%)   | 38 (79%)  | 10 (21%) | 2           | 13 |
| 30  | DY    | 48/48 (100%)   | 38 (79%)  | 10 (21%) | 2           | 13 |
| 31  | B0    | 47/47 (100%)   | 39 (83%)  | 8 (17%)  | 3           | 23 |
| 31  | D0    | 47/47 (100%)   | 39 (83%)  | 8 (17%)  | 3           | 23 |
| 32  | B4    | 34/34 (100%)   | 28 (82%)  | 6 (18%)  | 3           | 20 |
| 32  | D4    | 34/34 (100%)   | 28 (82%)  | 6 (18%)  | 3           | 20 |
| 33  | B1    | 45/48 (94%)    | 42 (93%)  | 3 (7%)   | 23          | 70 |
| 33  | D1    | 45/48 (94%)    | 42 (93%)  | 3 (7%)   | 23          | 70 |
| 34  | B3    | 51/51 (100%)   | 47 (92%)  | 4 (8%)   | 18          | 64 |
| 34  | D3    | 51/51 (100%)   | 47 (92%)  | 4 (8%)   | 18          | 64 |
| 35  | BV    | 78/78 (100%)   | 66 (85%)  | 12 (15%) | 4           | 28 |
| 35  | DV    | 78/78 (100%)   | 67 (86%)  | 11 (14%) | 5           | 33 |
| 36  | B2    | 38/38 (100%)   | 34 (90%)  | 4 (10%)  | 10          | 48 |
| 36  | D2    | 38/38 (100%)   | 34 (90%)  | 4 (10%)  | 10          | 48 |
| 37  | BL    | 102/103 (99%)  | 87 (85%)  | 15 (15%) | 4           | 30 |
| 37  | DL    | 102/103 (99%)  | 88 (86%)  | 14 (14%) | 5           | 34 |
| 38  | BM    | 109/109 (100%) | 88 (81%)  | 21 (19%) | 2           | 16 |
| 38  | DM    | 109/109 (100%) | 89 (82%)  | 20 (18%) | 2           | 18 |
| 39  | BX    | 55/55 (100%)   | 40 (73%)  | 15 (27%) | 0           | 6  |
| 39  | DX    | 55/55 (100%)   | 42 (76%)  | 13 (24%) | 1           | 9  |
| 40  | BH    | 114/114 (100%) | 68 (60%)  | 46 (40%) | 0           | 1  |
| 40  | DH    | 114/114 (100%) | 91 (80%)  | 23 (20%) | 2           | 14 |
| 41  | BJ    | 116/116 (100%) | 99 (85%)  | 17 (15%) | 4           | 30 |
| 41  | DJ    | 116/116 (100%) | 99 (85%)  | 17 (15%) | 4           | 30 |
| 42  | BN    | 100/103 (97%)  | 86 (86%)  | 14 (14%) | 5           | 33 |
| 42  | DN    | 100/103 (97%)  | 86 (86%)  | 14 (14%) | 5           | 33 |
| 43  | BO    | 86/87 (99%)    | 73 (85%)  | 13 (15%) | 4           | 29 |
| 43  | DO    | 86/87 (99%)    | 74 (86%)  | 12 (14%) | 5           | 33 |
| 44  | BQ    | 89/89 (100%)   | 76 (85%)  | 13 (15%) | 5           | 31 |
| 44  | DQ    | 89/89 (100%)   | 75 (84%)  | 14 (16%) | 4           | 27 |
| 45  | BS    | 93/93 (100%)   | 79 (85%)  | 14 (15%) | 4           | 29 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 45  | DS    | 93/93 (100%)     | 80 (86%)   | 13 (14%)   | 5           | 33 |
| 46  | BU    | 83/84 (99%)      | 69 (83%)   | 14 (17%)   | 3           | 23 |
| 46  | DU    | 83/84 (99%)      | 69 (83%)   | 14 (17%)   | 3           | 23 |
| 47  | BF    | 149/149 (100%)   | 114 (76%)  | 35 (24%)   | 1           | 9  |
| 47  | DF    | 149/149 (100%)   | 116 (78%)  | 33 (22%)   | 1           | 11 |
| 48  | BG    | 137/137 (100%)   | 114 (83%)  | 23 (17%)   | 3           | 24 |
| 48  | DG    | 137/137 (100%)   | 115 (84%)  | 22 (16%)   | 3           | 26 |
| 49  | BR    | 84/84 (100%)     | 72 (86%)   | 12 (14%)   | 5           | 32 |
| 49  | DR    | 84/84 (100%)     | 72 (86%)   | 12 (14%)   | 5           | 32 |
| 50  | BT    | 80/84 (95%)      | 65 (81%)   | 15 (19%)   | 2           | 17 |
| 50  | DT    | 80/84 (95%)      | 68 (85%)   | 12 (15%)   | 4           | 30 |
| 51  | BZ    | 67/68 (98%)      | 53 (79%)   | 14 (21%)   | 1           | 13 |
| 51  | DZ    | 67/68 (98%)      | 54 (81%)   | 13 (19%)   | 2           | 16 |
| 52  | BW    | 59/62 (95%)      | 47 (80%)   | 12 (20%)   | 2           | 14 |
| 52  | DW    | 59/62 (95%)      | 46 (78%)   | 13 (22%)   | 1           | 11 |
| 53  | B6    | 157/157 (100%)   | 119 (76%)  | 38 (24%)   | 1           | 9  |
| 53  | D6    | 157/157 (100%)   | 123 (78%)  | 34 (22%)   | 1           | 11 |
| All | All   | 9647/10014 (96%) | 8085 (84%) | 1562 (16%) | 3           | 26 |

All (1562) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 2   | GLN  |
| 2   | AC    | 13  | ILE  |
| 2   | AC    | 17  | TRP  |
| 2   | AC    | 19  | SER  |
| 2   | AC    | 27  | GLU  |
| 2   | AC    | 35  | ASP  |
| 2   | AC    | 41  | TYR  |
| 2   | AC    | 44  | LYS  |
| 2   | AC    | 48  | LYS  |
| 2   | AC    | 61  | LYS  |
| 2   | AC    | 62  | SER  |
| 2   | AC    | 69  | THR  |
| 2   | AC    | 71  | ARG  |
| 2   | AC    | 78  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 84  | GLU  |
| 2   | AC    | 87  | ARG  |
| 2   | AC    | 88  | LYS  |
| 2   | AC    | 106 | ARG  |
| 2   | AC    | 125 | ARG  |
| 2   | AC    | 128 | MET  |
| 2   | AC    | 131 | ARG  |
| 2   | AC    | 138 | GLN  |
| 2   | AC    | 168 | ARG  |
| 2   | AC    | 171 | ARG  |
| 2   | AC    | 180 | ASP  |
| 2   | AC    | 184 | ASN  |
| 2   | AC    | 192 | TYR  |
| 2   | AC    | 206 | ILE  |
| 3   | AD    | 4   | LEU  |
| 3   | AD    | 18  | LEU  |
| 3   | AD    | 25  | ARG  |
| 3   | AD    | 28  | ASP  |
| 3   | AD    | 32  | LYS  |
| 3   | AD    | 35  | GLN  |
| 3   | AD    | 39  | GLN  |
| 3   | AD    | 55  | ARG  |
| 3   | AD    | 61  | ARG  |
| 3   | AD    | 84  | ASN  |
| 3   | AD    | 87  | GLU  |
| 3   | AD    | 114 | ARG  |
| 3   | AD    | 146 | GLU  |
| 3   | AD    | 147 | LYS  |
| 3   | AD    | 155 | LYS  |
| 3   | AD    | 160 | LEU  |
| 3   | AD    | 164 | ARG  |
| 3   | AD    | 176 | LYS  |
| 3   | AD    | 183 | ARG  |
| 3   | AD    | 189 | ASP  |
| 3   | AD    | 190 | LEU  |
| 3   | AD    | 196 | GLU  |
| 3   | AD    | 197 | HIS  |
| 3   | AD    | 198 | LEU  |
| 3   | AD    | 203 | TYR  |
| 4   | AE    | 9   | GLU  |
| 4   | AE    | 23  | THR  |
| 4   | AE    | 28  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AE    | 30  | PHE  |
| 4   | AE    | 45  | VAL  |
| 4   | AE    | 51  | LYS  |
| 4   | AE    | 55  | VAL  |
| 4   | AE    | 61  | LYS  |
| 4   | AE    | 64  | GLU  |
| 4   | AE    | 81  | GLN  |
| 4   | AE    | 95  | MET  |
| 4   | AE    | 115 | GLU  |
| 4   | AE    | 123 | LEU  |
| 4   | AE    | 127 | TYR  |
| 4   | AE    | 147 | ASN  |
| 4   | AE    | 151 | MET  |
| 4   | AE    | 156 | ARG  |
| 5   | AF    | 1   | MET  |
| 5   | AF    | 6   | ILE  |
| 5   | AF    | 13  | ASP  |
| 5   | AF    | 16  | GLU  |
| 5   | AF    | 39  | LEU  |
| 5   | AF    | 53  | LYS  |
| 5   | AF    | 54  | LEU  |
| 5   | AF    | 55  | HIS  |
| 5   | AF    | 61  | LEU  |
| 5   | AF    | 64  | VAL  |
| 5   | AF    | 71  | ILE  |
| 5   | AF    | 77  | THR  |
| 5   | AF    | 86  | ARG  |
| 5   | AF    | 87  | SER  |
| 5   | AF    | 90  | MET  |
| 5   | AF    | 98  | GLU  |
| 6   | AG    | 6   | ILE  |
| 6   | AG    | 8   | GLN  |
| 6   | AG    | 10  | LYS  |
| 6   | AG    | 12  | LEU  |
| 6   | AG    | 21  | LEU  |
| 6   | AG    | 22  | LEU  |
| 6   | AG    | 26  | VAL  |
| 6   | AG    | 49  | LEU  |
| 6   | AG    | 55  | LYS  |
| 6   | AG    | 58  | LEU  |
| 6   | AG    | 62  | GLU  |
| 6   | AG    | 75  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AG    | 78  | ARG  |
| 6   | AG    | 109 | LYS  |
| 6   | AG    | 110 | ARG  |
| 6   | AG    | 117 | LEU  |
| 6   | AG    | 129 | ASN  |
| 7   | AH    | 17  | GLN  |
| 7   | AH    | 55  | LYS  |
| 7   | AH    | 72  | GLU  |
| 7   | AH    | 76  | ARG  |
| 7   | AH    | 88  | LYS  |
| 7   | AH    | 107 | LYS  |
| 7   | AH    | 111 | THR  |
| 7   | AH    | 113 | ARG  |
| 8   | AI    | 36  | GLN  |
| 8   | AI    | 45  | MET  |
| 8   | AI    | 58  | GLU  |
| 8   | AI    | 59  | LYS  |
| 8   | AI    | 60  | LEU  |
| 8   | AI    | 61  | ASP  |
| 8   | AI    | 62  | LEU  |
| 8   | AI    | 67  | LYS  |
| 8   | AI    | 74  | GLN  |
| 8   | AI    | 84  | ARG  |
| 8   | AI    | 87  | MET  |
| 8   | AI    | 91  | GLU  |
| 8   | AI    | 94  | ARG  |
| 8   | AI    | 105 | ARG  |
| 8   | AI    | 106 | ASP  |
| 8   | AI    | 108 | ARG  |
| 8   | AI    | 109 | GLN  |
| 9   | AJ    | 14  | ASP  |
| 9   | AJ    | 17  | LEU  |
| 9   | AJ    | 31  | ARG  |
| 9   | AJ    | 35  | GLN  |
| 9   | AJ    | 45  | ARG  |
| 9   | AJ    | 47  | GLU  |
| 9   | AJ    | 59  | LYS  |
| 9   | AJ    | 85  | ASP  |
| 9   | AJ    | 87  | LEU  |
| 9   | AJ    | 88  | MET  |
| 9   | AJ    | 89  | ARG  |
| 9   | AJ    | 90  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | AJ    | 92  | LEU  |
| 10  | AK    | 28  | ASN  |
| 10  | AK    | 29  | THR  |
| 10  | AK    | 34  | THR  |
| 10  | AK    | 51  | PHE  |
| 10  | AK    | 52  | ARG  |
| 10  | AK    | 55  | ARG  |
| 10  | AK    | 56  | LYS  |
| 10  | AK    | 80  | ASN  |
| 10  | AK    | 84  | MET  |
| 10  | AK    | 92  | ARG  |
| 10  | AK    | 100 | ASN  |
| 10  | AK    | 105 | ARG  |
| 10  | AK    | 117 | HIS  |
| 10  | AK    | 128 | VAL  |
| 11  | AL    | 13  | ARG  |
| 11  | AL    | 14  | LYS  |
| 11  | AL    | 15  | VAL  |
| 11  | AL    | 17  | LYS  |
| 11  | AL    | 19  | ASN  |
| 11  | AL    | 28  | GLN  |
| 11  | AL    | 43  | LYS  |
| 11  | AL    | 49  | ARG  |
| 11  | AL    | 93  | ARG  |
| 11  | AL    | 107 | LYS  |
| 11  | AL    | 114 | SER  |
| 12  | AM    | 2   | ARG  |
| 12  | AM    | 15  | VAL  |
| 12  | AM    | 28  | ARG  |
| 12  | AM    | 43  | LYS  |
| 12  | AM    | 44  | ILE  |
| 12  | AM    | 46  | GLU  |
| 12  | AM    | 57  | ASP  |
| 12  | AM    | 64  | VAL  |
| 12  | AM    | 67  | ASP  |
| 12  | AM    | 71  | GLU  |
| 12  | AM    | 79  | LEU  |
| 12  | AM    | 82  | LEU  |
| 12  | AM    | 92  | ARG  |
| 12  | AM    | 102 | LYS  |
| 13  | AN    | 17  | ASP  |
| 13  | AN    | 19  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | AN    | 26  | LEU  |
| 13  | AN    | 30  | ILE  |
| 13  | AN    | 34  | ASN  |
| 13  | AN    | 40  | ARG  |
| 13  | AN    | 41  | TRP  |
| 13  | AN    | 45  | LEU  |
| 13  | AN    | 57  | SER  |
| 13  | AN    | 59  | GLN  |
| 13  | AN    | 65  | GLN  |
| 13  | AN    | 68  | ARG  |
| 13  | AN    | 97  | LYS  |
| 14  | AO    | 18  | ASP  |
| 14  | AO    | 25  | THR  |
| 14  | AO    | 37  | ASN  |
| 14  | AO    | 42  | HIS  |
| 14  | AO    | 54  | ARG  |
| 14  | AO    | 59  | MET  |
| 14  | AO    | 64  | ARG  |
| 14  | AO    | 68  | ASP  |
| 14  | AO    | 70  | LEU  |
| 14  | AO    | 71  | LYS  |
| 14  | AO    | 88  | ARG  |
| 14  | AO    | 89  | ARG  |
| 15  | AP    | 28  | ARG  |
| 15  | AP    | 31  | ARG  |
| 15  | AP    | 45  | GLU  |
| 15  | AP    | 51  | ARG  |
| 15  | AP    | 79  | ASN  |
| 16  | AQ    | 24  | ILE  |
| 16  | AQ    | 39  | ARG  |
| 16  | AQ    | 56  | ASP  |
| 16  | AQ    | 60  | ILE  |
| 16  | AQ    | 61  | ARG  |
| 16  | AQ    | 67  | SER  |
| 16  | AQ    | 71  | SER  |
| 16  | AQ    | 80  | LYS  |
| 17  | AR    | 33  | THR  |
| 17  | AR    | 38  | ILE  |
| 17  | AR    | 73  | HIS  |
| 18  | AS    | 2   | ARG  |
| 18  | AS    | 4   | LEU  |
| 18  | AS    | 5   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | AS    | 12  | LEU  |
| 18  | AS    | 13  | HIS  |
| 18  | AS    | 14  | LEU  |
| 18  | AS    | 15  | LEU  |
| 18  | AS    | 17  | LYS  |
| 18  | AS    | 20  | LYS  |
| 18  | AS    | 23  | GLU  |
| 18  | AS    | 27  | LYS  |
| 18  | AS    | 28  | LYS  |
| 18  | AS    | 42  | ASN  |
| 18  | AS    | 43  | MET  |
| 18  | AS    | 46  | LEU  |
| 18  | AS    | 64  | GLU  |
| 19  | AT    | 4   | LYS  |
| 19  | AT    | 35  | TYR  |
| 19  | AT    | 38  | ILE  |
| 19  | AT    | 43  | LYS  |
| 19  | AT    | 51  | ASN  |
| 19  | AT    | 53  | MET  |
| 19  | AT    | 69  | ASN  |
| 19  | AT    | 74  | HIS  |
| 19  | AT    | 85  | LEU  |
| 20  | AB    | 20  | ARG  |
| 20  | AB    | 27  | LYS  |
| 20  | AB    | 35  | ASN  |
| 20  | AB    | 36  | LYS  |
| 20  | AB    | 38  | HIS  |
| 20  | AB    | 43  | GLU  |
| 20  | AB    | 46  | VAL  |
| 20  | AB    | 53  | LEU  |
| 20  | AB    | 57  | ASN  |
| 20  | AB    | 62  | ARG  |
| 20  | AB    | 67  | LEU  |
| 20  | AB    | 84  | LEU  |
| 20  | AB    | 87  | ASP  |
| 20  | AB    | 88  | GLN  |
| 20  | AB    | 94  | ARG  |
| 20  | AB    | 95  | TRP  |
| 20  | AB    | 100 | LEU  |
| 20  | AB    | 104 | LYS  |
| 20  | AB    | 124 | THR  |
| 20  | AB    | 127 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AB    | 128 | LEU  |
| 20  | AB    | 138 | ARG  |
| 20  | AB    | 166 | ASP  |
| 20  | AB    | 176 | ASN  |
| 20  | AB    | 196 | ASP  |
| 20  | AB    | 202 | ASN  |
| 20  | AB    | 203 | ASP  |
| 20  | AB    | 211 | LEU  |
| 20  | AB    | 213 | LEU  |
| 20  | AB    | 221 | ARG  |
| 21  | AU    | 7   | GLU  |
| 21  | AU    | 11  | PHE  |
| 21  | AU    | 15  | LEU  |
| 21  | AU    | 16  | ARG  |
| 21  | AU    | 20  | ARG  |
| 21  | AU    | 22  | CYS  |
| 21  | AU    | 24  | LYS  |
| 21  | AU    | 33  | ARG  |
| 21  | AU    | 34  | ARG  |
| 21  | AU    | 35  | GLU  |
| 21  | AU    | 38  | GLU  |
| 21  | AU    | 44  | ARG  |
| 21  | AU    | 48  | LYS  |
| 24  | BI    | 63  | ASP  |
| 24  | BI    | 96  | LYS  |
| 25  | BC    | 4   | LYS  |
| 25  | BC    | 12  | ARG  |
| 25  | BC    | 37  | SER  |
| 25  | BC    | 43  | ASN  |
| 25  | BC    | 44  | ASN  |
| 25  | BC    | 45  | ASN  |
| 25  | BC    | 47  | ARG  |
| 25  | BC    | 52  | HIS  |
| 25  | BC    | 62  | ARG  |
| 25  | BC    | 65  | ASP  |
| 25  | BC    | 86  | ARG  |
| 25  | BC    | 89  | ASN  |
| 25  | BC    | 90  | ILE  |
| 25  | BC    | 100 | ARG  |
| 25  | BC    | 109 | LEU  |
| 25  | BC    | 123 | ILE  |
| 25  | BC    | 129 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BC    | 134 | ILE  |
| 25  | BC    | 142 | ASN  |
| 25  | BC    | 155 | ARG  |
| 25  | BC    | 167 | ASP  |
| 25  | BC    | 172 | THR  |
| 25  | BC    | 173 | LEU  |
| 25  | BC    | 176 | ARG  |
| 25  | BC    | 180 | MET  |
| 25  | BC    | 181 | ARG  |
| 25  | BC    | 191 | LEU  |
| 25  | BC    | 196 | ASN  |
| 25  | BC    | 203 | VAL  |
| 25  | BC    | 211 | ARG  |
| 25  | BC    | 212 | TRP  |
| 25  | BC    | 224 | MET  |
| 25  | BC    | 239 | PHE  |
| 25  | BC    | 245 | THR  |
| 25  | BC    | 249 | VAL  |
| 25  | BC    | 250 | GLN  |
| 25  | BC    | 251 | THR  |
| 25  | BC    | 257 | ARG  |
| 26  | BD    | 16  | THR  |
| 26  | BD    | 30  | GLU  |
| 26  | BD    | 40  | LEU  |
| 26  | BD    | 56  | LYS  |
| 26  | BD    | 79  | LEU  |
| 26  | BD    | 81  | GLU  |
| 26  | BD    | 82  | PHE  |
| 26  | BD    | 84  | LEU  |
| 26  | BD    | 88  | GLU  |
| 26  | BD    | 95  | SER  |
| 26  | BD    | 99  | GLU  |
| 26  | BD    | 114 | LYS  |
| 26  | BD    | 124 | ARG  |
| 26  | BD    | 137 | SER  |
| 26  | BD    | 138 | LEU  |
| 26  | BD    | 142 | VAL  |
| 26  | BD    | 148 | GLN  |
| 26  | BD    | 159 | LYS  |
| 26  | BD    | 179 | ARG  |
| 26  | BD    | 186 | LEU  |
| 26  | BD    | 197 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | BD    | 204 | LYS  |
| 27  | BK    | 2   | ILE  |
| 27  | BK    | 8   | LEU  |
| 27  | BK    | 18  | ARG  |
| 27  | BK    | 21  | CYS  |
| 27  | BK    | 25  | LEU  |
| 27  | BK    | 32  | TYR  |
| 27  | BK    | 47  | ILE  |
| 27  | BK    | 53  | LYS  |
| 27  | BK    | 54  | LYS  |
| 27  | BK    | 58  | LEU  |
| 27  | BK    | 64  | ARG  |
| 27  | BK    | 67  | LYS  |
| 27  | BK    | 70  | ARG  |
| 27  | BK    | 72  | PRO  |
| 27  | BK    | 73  | ASP  |
| 27  | BK    | 79  | PHE  |
| 27  | BK    | 80  | ASP  |
| 27  | BK    | 86  | LEU  |
| 27  | BK    | 87  | LEU  |
| 27  | BK    | 88  | ASN  |
| 27  | BK    | 89  | ASN  |
| 27  | BK    | 98  | ARG  |
| 27  | BK    | 104 | THR  |
| 27  | BK    | 105 | ARG  |
| 27  | BK    | 107 | LEU  |
| 27  | BK    | 111 | LYS  |
| 27  | BK    | 120 | PRO  |
| 28  | BP    | 3   | ILE  |
| 28  | BP    | 6   | GLN  |
| 28  | BP    | 19  | PHE  |
| 28  | BP    | 25  | VAL  |
| 28  | BP    | 33  | GLU  |
| 28  | BP    | 38  | ARG  |
| 28  | BP    | 43  | GLU  |
| 28  | BP    | 61  | ARG  |
| 28  | BP    | 65  | ASN  |
| 28  | BP    | 80  | VAL  |
| 28  | BP    | 83  | ILE  |
| 28  | BP    | 99  | LEU  |
| 28  | BP    | 100 | ARG  |
| 28  | BP    | 101 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BP    | 111 | GLU  |
| 28  | BP    | 112 | ARG  |
| 28  | BP    | 114 | ASN  |
| 29  | BE    | 2   | GLU  |
| 29  | BE    | 3   | LEU  |
| 29  | BE    | 5   | LEU  |
| 29  | BE    | 7   | ASP  |
| 29  | BE    | 22  | ASP  |
| 29  | BE    | 24  | ASN  |
| 29  | BE    | 58  | LYS  |
| 29  | BE    | 60  | TRP  |
| 29  | BE    | 62  | GLN  |
| 29  | BE    | 67  | ARG  |
| 29  | BE    | 70  | SER  |
| 29  | BE    | 75  | SER  |
| 29  | BE    | 80  | SER  |
| 29  | BE    | 97  | ASN  |
| 29  | BE    | 107 | SER  |
| 29  | BE    | 108 | ILE  |
| 29  | BE    | 111 | GLU  |
| 29  | BE    | 116 | ASP  |
| 29  | BE    | 118 | LEU  |
| 29  | BE    | 122 | GLU  |
| 29  | BE    | 133 | LEU  |
| 29  | BE    | 150 | THR  |
| 29  | BE    | 159 | LEU  |
| 29  | BE    | 163 | ASN  |
| 30  | BY    | 2   | LYS  |
| 30  | BY    | 6   | ILE  |
| 30  | BY    | 8   | GLN  |
| 30  | BY    | 15  | ARG  |
| 30  | BY    | 16  | LEU  |
| 30  | BY    | 19  | HIS  |
| 30  | BY    | 23  | LEU  |
| 30  | BY    | 30  | ARG  |
| 30  | BY    | 37  | ARG  |
| 30  | BY    | 43  | ILE  |
| 31  | B0    | 5   | ASN  |
| 31  | B0    | 27  | LEU  |
| 31  | B0    | 31  | LYS  |
| 31  | B0    | 38  | LEU  |
| 31  | B0    | 41  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | B0    | 51  | ARG  |
| 31  | B0    | 53  | VAL  |
| 31  | B0    | 56  | LYS  |
| 32  | B4    | 2   | LYS  |
| 32  | B4    | 9   | LYS  |
| 32  | B4    | 15  | LYS  |
| 32  | B4    | 22  | VAL  |
| 32  | B4    | 24  | ARG  |
| 32  | B4    | 35  | GLN  |
| 33  | B1    | 6   | GLU  |
| 33  | B1    | 9   | LYS  |
| 33  | B1    | 35  | LEU  |
| 34  | B3    | 7   | ARG  |
| 34  | B3    | 18  | LYS  |
| 34  | B3    | 49  | VAL  |
| 34  | B3    | 61  | LEU  |
| 35  | BV    | 35  | GLU  |
| 35  | BV    | 40  | ILE  |
| 35  | BV    | 41  | GLU  |
| 35  | BV    | 42  | LEU  |
| 35  | BV    | 45  | ASP  |
| 35  | BV    | 46  | LYS  |
| 35  | BV    | 51  | GLN  |
| 35  | BV    | 53  | LYS  |
| 35  | BV    | 66  | ASP  |
| 35  | BV    | 69  | GLU  |
| 35  | BV    | 70  | ILE  |
| 35  | BV    | 75  | GLN  |
| 36  | B2    | 19  | ARG  |
| 36  | B2    | 33  | ARG  |
| 36  | B2    | 35  | ARG  |
| 36  | B2    | 39  | ARG  |
| 37  | BL    | 10  | GLU  |
| 37  | BL    | 39  | LYS  |
| 37  | BL    | 47  | ARG  |
| 37  | BL    | 55  | MET  |
| 37  | BL    | 60  | ARG  |
| 37  | BL    | 67  | THR  |
| 37  | BL    | 69  | ARG  |
| 37  | BL    | 82  | LEU  |
| 37  | BL    | 91  | ASP  |
| 37  | BL    | 92  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BL    | 95  | LEU  |
| 37  | BL    | 99  | ASN  |
| 37  | BL    | 112 | LEU  |
| 37  | BL    | 118 | THR  |
| 37  | BL    | 123 | ARG  |
| 38  | BM    | 1   | MET  |
| 38  | BM    | 2   | LEU  |
| 38  | BM    | 7   | THR  |
| 38  | BM    | 10  | ARG  |
| 38  | BM    | 18  | ARG  |
| 38  | BM    | 20  | LEU  |
| 38  | BM    | 26  | VAL  |
| 38  | BM    | 47  | GLU  |
| 38  | BM    | 55  | ARG  |
| 38  | BM    | 65  | ILE  |
| 38  | BM    | 70  | ASP  |
| 38  | BM    | 78  | LEU  |
| 38  | BM    | 81  | ARG  |
| 38  | BM    | 88  | ASN  |
| 38  | BM    | 90  | GLU  |
| 38  | BM    | 108 | VAL  |
| 38  | BM    | 110 | GLU  |
| 38  | BM    | 111 | GLU  |
| 38  | BM    | 114 | ARG  |
| 38  | BM    | 115 | GLU  |
| 38  | BM    | 123 | LYS  |
| 39  | BX    | 1   | MET  |
| 39  | BX    | 7   | ARG  |
| 39  | BX    | 10  | SER  |
| 39  | BX    | 15  | ASN  |
| 39  | BX    | 18  | LEU  |
| 39  | BX    | 20  | ASN  |
| 39  | BX    | 21  | LEU  |
| 39  | BX    | 28  | LEU  |
| 39  | BX    | 29  | ARG  |
| 39  | BX    | 30  | MET  |
| 39  | BX    | 38  | GLN  |
| 39  | BX    | 41  | HIS  |
| 39  | BX    | 48  | ARG  |
| 39  | BX    | 49  | ASP  |
| 39  | BX    | 59  | GLU  |
| 40  | BH    | 3   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BH    | 4   | ILE  |
| 40  | BH    | 12  | LEU  |
| 40  | BH    | 15  | LEU  |
| 40  | BH    | 19  | VAL  |
| 40  | BH    | 28  | ASN  |
| 40  | BH    | 31  | VAL  |
| 40  | BH    | 32  | PRO  |
| 40  | BH    | 33  | GLN  |
| 40  | BH    | 41  | LYS  |
| 40  | BH    | 43  | ASN  |
| 40  | BH    | 44  | ILE  |
| 40  | BH    | 45  | GLU  |
| 40  | BH    | 46  | PHE  |
| 40  | BH    | 48  | GLU  |
| 40  | BH    | 50  | ARG  |
| 40  | BH    | 51  | ARG  |
| 40  | BH    | 54  | LEU  |
| 40  | BH    | 57  | LYS  |
| 40  | BH    | 58  | LEU  |
| 40  | BH    | 60  | GLU  |
| 40  | BH    | 62  | LEU  |
| 40  | BH    | 68  | ARG  |
| 40  | BH    | 70  | GLU  |
| 40  | BH    | 71  | LYS  |
| 40  | BH    | 73  | ASN  |
| 40  | BH    | 75  | LEU  |
| 40  | BH    | 79  | THR  |
| 40  | BH    | 82  | SER  |
| 40  | BH    | 87  | GLU  |
| 40  | BH    | 89  | LYS  |
| 40  | BH    | 110 | VAL  |
| 40  | BH    | 112 | LYS  |
| 40  | BH    | 114 | GLU  |
| 40  | BH    | 116 | ARG  |
| 40  | BH    | 119 | ASN  |
| 40  | BH    | 125 | THR  |
| 40  | BH    | 128 | HIS  |
| 40  | BH    | 130 | VAL  |
| 40  | BH    | 134 | VAL  |
| 40  | BH    | 135 | HIS  |
| 40  | BH    | 138 | VAL  |
| 40  | BH    | 139 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BH    | 141 | LYS  |
| 40  | BH    | 142 | VAL  |
| 40  | BH    | 147 | VAL  |
| 41  | BJ    | 3   | THR  |
| 41  | BJ    | 5   | THR  |
| 41  | BJ    | 9   | GLU  |
| 41  | BJ    | 12  | LYS  |
| 41  | BJ    | 28  | LEU  |
| 41  | BJ    | 30  | THR  |
| 41  | BJ    | 44  | TYR  |
| 41  | BJ    | 65  | THR  |
| 41  | BJ    | 71  | ASP  |
| 41  | BJ    | 73  | VAL  |
| 41  | BJ    | 95  | ARG  |
| 41  | BJ    | 106 | LYS  |
| 41  | BJ    | 120 | ARG  |
| 41  | BJ    | 124 | VAL  |
| 41  | BJ    | 129 | GLU  |
| 41  | BJ    | 131 | ASN  |
| 41  | BJ    | 138 | GLN  |
| 42  | BN    | 1   | MET  |
| 42  | BN    | 9   | GLN  |
| 42  | BN    | 11  | ASN  |
| 42  | BN    | 20  | MET  |
| 42  | BN    | 31  | HIS  |
| 42  | BN    | 35  | LYS  |
| 42  | BN    | 46  | ARG  |
| 42  | BN    | 51  | LEU  |
| 42  | BN    | 69  | ARG  |
| 42  | BN    | 71  | ARG  |
| 42  | BN    | 82  | GLU  |
| 42  | BN    | 96  | ARG  |
| 42  | BN    | 114 | GLU  |
| 42  | BN    | 120 | GLU  |
| 43  | BO    | 31  | THR  |
| 43  | BO    | 35  | ILE  |
| 43  | BO    | 36  | TYR  |
| 43  | BO    | 43  | ASN  |
| 43  | BO    | 58  | ILE  |
| 43  | BO    | 62  | LEU  |
| 43  | BO    | 69  | ASP  |
| 43  | BO    | 74  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | BO    | 81  | ARG  |
| 43  | BO    | 89  | ASP  |
| 43  | BO    | 106 | LEU  |
| 43  | BO    | 115 | LEU  |
| 43  | BO    | 116 | GLN  |
| 44  | BQ    | 4   | LYS  |
| 44  | BQ    | 5   | ARG  |
| 44  | BQ    | 10  | ARG  |
| 44  | BQ    | 13  | HIS  |
| 44  | BQ    | 63  | ARG  |
| 44  | BQ    | 69  | ARG  |
| 44  | BQ    | 79  | ILE  |
| 44  | BQ    | 83  | LYS  |
| 44  | BQ    | 84  | LYS  |
| 44  | BQ    | 89  | ILE  |
| 44  | BQ    | 90  | ASP  |
| 44  | BQ    | 91  | ARG  |
| 44  | BQ    | 96  | ASP  |
| 45  | BS    | 7   | HIS  |
| 45  | BS    | 15  | GLN  |
| 45  | BS    | 22  | ASP  |
| 45  | BS    | 27  | LYS  |
| 45  | BS    | 57  | ASN  |
| 45  | BS    | 61  | ASN  |
| 45  | BS    | 66  | ILE  |
| 45  | BS    | 72  | THR  |
| 45  | BS    | 84  | ARG  |
| 45  | BS    | 86  | MET  |
| 45  | BS    | 88  | ARG  |
| 45  | BS    | 92  | ARG  |
| 45  | BS    | 99  | ARG  |
| 45  | BS    | 101 | SER  |
| 46  | BU    | 11  | ILE  |
| 46  | BU    | 13  | LEU  |
| 46  | BU    | 20  | LYS  |
| 46  | BU    | 26  | ASN  |
| 46  | BU    | 45  | GLN  |
| 46  | BU    | 49  | PRO  |
| 46  | BU    | 51  | LEU  |
| 46  | BU    | 53  | GLN  |
| 46  | BU    | 60  | LYS  |
| 46  | BU    | 73  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | BU    | 78  | LYS  |
| 46  | BU    | 81  | ARG  |
| 46  | BU    | 85  | ARG  |
| 46  | BU    | 88  | ASP  |
| 47  | BF    | 2   | LYS  |
| 47  | BF    | 13  | LYS  |
| 47  | BF    | 19  | PHE  |
| 47  | BF    | 22  | ASN  |
| 47  | BF    | 29  | ARG  |
| 47  | BF    | 32  | LYS  |
| 47  | BF    | 46  | LYS  |
| 47  | BF    | 50  | ASP  |
| 47  | BF    | 55  | ASP  |
| 47  | BF    | 56  | LEU  |
| 47  | BF    | 68  | LYS  |
| 47  | BF    | 70  | ARG  |
| 47  | BF    | 76  | PHE  |
| 47  | BF    | 79  | ARG  |
| 47  | BF    | 91  | ARG  |
| 47  | BF    | 96  | TRP  |
| 47  | BF    | 97  | GLU  |
| 47  | BF    | 100 | GLU  |
| 47  | BF    | 102 | LEU  |
| 47  | BF    | 103 | ILE  |
| 47  | BF    | 109 | ARG  |
| 47  | BF    | 111 | ARG  |
| 47  | BF    | 120 | SER  |
| 47  | BF    | 121 | PHE  |
| 47  | BF    | 124 | ARG  |
| 47  | BF    | 129 | MET  |
| 47  | BF    | 134 | GLN  |
| 47  | BF    | 137 | PHE  |
| 47  | BF    | 138 | PRO  |
| 47  | BF    | 142 | TYR  |
| 47  | BF    | 149 | ARG  |
| 47  | BF    | 168 | LEU  |
| 47  | BF    | 173 | ASP  |
| 47  | BF    | 174 | PHE  |
| 47  | BF    | 178 | LYS  |
| 48  | BG    | 2   | ARG  |
| 48  | BG    | 14  | VAL  |
| 48  | BG    | 24  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | BG    | 26  | LYS  |
| 48  | BG    | 31  | GLU  |
| 48  | BG    | 34  | ARG  |
| 48  | BG    | 46  | ASP  |
| 48  | BG    | 54  | ARG  |
| 48  | BG    | 61  | TRP  |
| 48  | BG    | 66  | THR  |
| 48  | BG    | 68  | ARG  |
| 48  | BG    | 70  | LEU  |
| 48  | BG    | 84  | LYS  |
| 48  | BG    | 94  | ARG  |
| 48  | BG    | 106 | LEU  |
| 48  | BG    | 120 | ILE  |
| 48  | BG    | 132 | LEU  |
| 48  | BG    | 133 | LYS  |
| 48  | BG    | 138 | GLN  |
| 48  | BG    | 152 | ARG  |
| 48  | BG    | 162 | ARG  |
| 48  | BG    | 166 | GLU  |
| 48  | BG    | 176 | LYS  |
| 49  | BR    | 4   | VAL  |
| 49  | BR    | 19  | THR  |
| 49  | BR    | 22  | LEU  |
| 49  | BR    | 39  | LEU  |
| 49  | BR    | 53  | PHE  |
| 49  | BR    | 55  | ASP  |
| 49  | BR    | 70  | GLU  |
| 49  | BR    | 71  | LYS  |
| 49  | BR    | 72  | VAL  |
| 49  | BR    | 79  | ARG  |
| 49  | BR    | 82  | HIS  |
| 49  | BR    | 86  | GLN  |
| 50  | BT    | 2   | ILE  |
| 50  | BT    | 3   | ARG  |
| 50  | BT    | 4   | GLU  |
| 50  | BT    | 9   | LYS  |
| 50  | BT    | 11  | LEU  |
| 50  | BT    | 12  | ARG  |
| 50  | BT    | 25  | GLU  |
| 50  | BT    | 29  | THR  |
| 50  | BT    | 32  | LEU  |
| 50  | BT    | 50  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | BT    | 64  | LYS  |
| 50  | BT    | 68  | LYS  |
| 50  | BT    | 69  | ARG  |
| 50  | BT    | 70  | HIS  |
| 50  | BT    | 81  | LYS  |
| 51  | BZ    | 2   | SER  |
| 51  | BZ    | 14  | THR  |
| 51  | BZ    | 25  | THR  |
| 51  | BZ    | 27  | ARG  |
| 51  | BZ    | 28  | ARG  |
| 51  | BZ    | 30  | LEU  |
| 51  | BZ    | 33  | LEU  |
| 51  | BZ    | 37  | ARG  |
| 51  | BZ    | 46  | PHE  |
| 51  | BZ    | 50  | ARG  |
| 51  | BZ    | 60  | ASP  |
| 51  | BZ    | 66  | THR  |
| 51  | BZ    | 77  | LYS  |
| 51  | BZ    | 78  | TYR  |
| 52  | BW    | 10  | ARG  |
| 52  | BW    | 16  | GLU  |
| 52  | BW    | 19  | ARG  |
| 52  | BW    | 24  | ARG  |
| 52  | BW    | 25  | PHE  |
| 52  | BW    | 39  | GLN  |
| 52  | BW    | 44  | PHE  |
| 52  | BW    | 49  | ASN  |
| 52  | BW    | 50  | VAL  |
| 52  | BW    | 75  | ASN  |
| 52  | BW    | 77  | LYS  |
| 52  | BW    | 82  | GLU  |
| 53  | B6    | 1   | MET  |
| 53  | B6    | 10  | THR  |
| 53  | B6    | 12  | SER  |
| 53  | B6    | 16  | LYS  |
| 53  | B6    | 22  | GLU  |
| 53  | B6    | 24  | ASN  |
| 53  | B6    | 39  | LEU  |
| 53  | B6    | 46  | TYR  |
| 53  | B6    | 50  | VAL  |
| 53  | B6    | 59  | THR  |
| 53  | B6    | 62  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | B6    | 64  | ARG  |
| 53  | B6    | 66  | LEU  |
| 53  | B6    | 71  | TRP  |
| 53  | B6    | 73  | GLN  |
| 53  | B6    | 77  | LYS  |
| 53  | B6    | 84  | ARG  |
| 53  | B6    | 86  | SER  |
| 53  | B6    | 88  | LEU  |
| 53  | B6    | 90  | LEU  |
| 53  | B6    | 97  | ASP  |
| 53  | B6    | 102 | ASN  |
| 53  | B6    | 106 | LEU  |
| 53  | B6    | 111 | ARG  |
| 53  | B6    | 112 | LYS  |
| 53  | B6    | 113 | ASP  |
| 53  | B6    | 134 | ARG  |
| 53  | B6    | 137 | LEU  |
| 53  | B6    | 141 | LYS  |
| 53  | B6    | 142 | LYS  |
| 53  | B6    | 147 | LEU  |
| 53  | B6    | 156 | ARG  |
| 53  | B6    | 162 | GLN  |
| 53  | B6    | 169 | ILE  |
| 53  | B6    | 174 | GLN  |
| 53  | B6    | 177 | GLU  |
| 53  | B6    | 180 | GLU  |
| 53  | B6    | 181 | GLN  |
| 2   | CC    | 2   | GLN  |
| 2   | CC    | 13  | ILE  |
| 2   | CC    | 17  | TRP  |
| 2   | CC    | 19  | SER  |
| 2   | CC    | 27  | GLU  |
| 2   | CC    | 35  | ASP  |
| 2   | CC    | 41  | TYR  |
| 2   | CC    | 44  | LYS  |
| 2   | CC    | 48  | LYS  |
| 2   | CC    | 61  | LYS  |
| 2   | CC    | 62  | SER  |
| 2   | CC    | 69  | THR  |
| 2   | CC    | 71  | ARG  |
| 2   | CC    | 78  | LYS  |
| 2   | CC    | 84  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CC    | 87  | ARG  |
| 2   | CC    | 88  | LYS  |
| 2   | CC    | 106 | ARG  |
| 2   | CC    | 125 | ARG  |
| 2   | CC    | 128 | MET  |
| 2   | CC    | 131 | ARG  |
| 2   | CC    | 138 | GLN  |
| 2   | CC    | 168 | ARG  |
| 2   | CC    | 171 | ARG  |
| 2   | CC    | 180 | ASP  |
| 2   | CC    | 184 | ASN  |
| 2   | CC    | 192 | TYR  |
| 2   | CC    | 206 | ILE  |
| 3   | CD    | 4   | LEU  |
| 3   | CD    | 18  | LEU  |
| 3   | CD    | 25  | ARG  |
| 3   | CD    | 28  | ASP  |
| 3   | CD    | 32  | LYS  |
| 3   | CD    | 35  | GLN  |
| 3   | CD    | 39  | GLN  |
| 3   | CD    | 55  | ARG  |
| 3   | CD    | 61  | ARG  |
| 3   | CD    | 84  | ASN  |
| 3   | CD    | 87  | GLU  |
| 3   | CD    | 114 | ARG  |
| 3   | CD    | 146 | GLU  |
| 3   | CD    | 147 | LYS  |
| 3   | CD    | 155 | LYS  |
| 3   | CD    | 160 | LEU  |
| 3   | CD    | 164 | ARG  |
| 3   | CD    | 176 | LYS  |
| 3   | CD    | 183 | ARG  |
| 3   | CD    | 189 | ASP  |
| 3   | CD    | 190 | LEU  |
| 3   | CD    | 196 | GLU  |
| 3   | CD    | 198 | LEU  |
| 3   | CD    | 203 | TYR  |
| 4   | CE    | 9   | GLU  |
| 4   | CE    | 23  | THR  |
| 4   | CE    | 28  | ARG  |
| 4   | CE    | 30  | PHE  |
| 4   | CE    | 45  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CE    | 51  | LYS  |
| 4   | CE    | 55  | VAL  |
| 4   | CE    | 61  | LYS  |
| 4   | CE    | 64  | GLU  |
| 4   | CE    | 81  | GLN  |
| 4   | CE    | 95  | MET  |
| 4   | CE    | 115 | GLU  |
| 4   | CE    | 123 | LEU  |
| 4   | CE    | 127 | TYR  |
| 4   | CE    | 147 | ASN  |
| 4   | CE    | 151 | MET  |
| 4   | CE    | 156 | ARG  |
| 5   | CF    | 1   | MET  |
| 5   | CF    | 6   | ILE  |
| 5   | CF    | 13  | ASP  |
| 5   | CF    | 16  | GLU  |
| 5   | CF    | 39  | LEU  |
| 5   | CF    | 53  | LYS  |
| 5   | CF    | 54  | LEU  |
| 5   | CF    | 55  | HIS  |
| 5   | CF    | 61  | LEU  |
| 5   | CF    | 62  | MET  |
| 5   | CF    | 64  | VAL  |
| 5   | CF    | 71  | ILE  |
| 5   | CF    | 77  | THR  |
| 5   | CF    | 86  | ARG  |
| 5   | CF    | 87  | SER  |
| 5   | CF    | 90  | MET  |
| 5   | CF    | 98  | GLU  |
| 6   | CG    | 2   | ARG  |
| 6   | CG    | 8   | GLN  |
| 6   | CG    | 10  | LYS  |
| 6   | CG    | 12  | LEU  |
| 6   | CG    | 21  | LEU  |
| 6   | CG    | 22  | LEU  |
| 6   | CG    | 26  | VAL  |
| 6   | CG    | 49  | LEU  |
| 6   | CG    | 55  | LYS  |
| 6   | CG    | 58  | LEU  |
| 6   | CG    | 62  | GLU  |
| 6   | CG    | 75  | LYS  |
| 6   | CG    | 78  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | CG    | 109 | LYS  |
| 6   | CG    | 117 | LEU  |
| 6   | CG    | 129 | ASN  |
| 7   | CH    | 17  | GLN  |
| 7   | CH    | 55  | LYS  |
| 7   | CH    | 72  | GLU  |
| 7   | CH    | 76  | ARG  |
| 7   | CH    | 88  | LYS  |
| 7   | CH    | 107 | LYS  |
| 7   | CH    | 111 | THR  |
| 7   | CH    | 113 | ARG  |
| 8   | CI    | 36  | GLN  |
| 8   | CI    | 45  | MET  |
| 8   | CI    | 58  | GLU  |
| 8   | CI    | 59  | LYS  |
| 8   | CI    | 60  | LEU  |
| 8   | CI    | 61  | ASP  |
| 8   | CI    | 62  | LEU  |
| 8   | CI    | 67  | LYS  |
| 8   | CI    | 74  | GLN  |
| 8   | CI    | 84  | ARG  |
| 8   | CI    | 87  | MET  |
| 8   | CI    | 91  | GLU  |
| 8   | CI    | 94  | ARG  |
| 8   | CI    | 105 | ARG  |
| 8   | CI    | 106 | ASP  |
| 8   | CI    | 108 | ARG  |
| 8   | CI    | 109 | GLN  |
| 9   | CJ    | 14  | ASP  |
| 9   | CJ    | 17  | LEU  |
| 9   | CJ    | 31  | ARG  |
| 9   | CJ    | 35  | GLN  |
| 9   | CJ    | 45  | ARG  |
| 9   | CJ    | 47  | GLU  |
| 9   | CJ    | 59  | LYS  |
| 9   | CJ    | 85  | ASP  |
| 9   | CJ    | 87  | LEU  |
| 9   | CJ    | 88  | MET  |
| 9   | CJ    | 89  | ARG  |
| 9   | CJ    | 90  | LEU  |
| 9   | CJ    | 92  | LEU  |
| 10  | CK    | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | CK    | 29  | THR  |
| 10  | CK    | 34  | THR  |
| 10  | CK    | 51  | PHE  |
| 10  | CK    | 52  | ARG  |
| 10  | CK    | 55  | ARG  |
| 10  | CK    | 56  | LYS  |
| 10  | CK    | 80  | ASN  |
| 10  | CK    | 84  | MET  |
| 10  | CK    | 92  | ARG  |
| 10  | CK    | 100 | ASN  |
| 10  | CK    | 105 | ARG  |
| 10  | CK    | 117 | HIS  |
| 10  | CK    | 128 | VAL  |
| 11  | CL    | 13  | ARG  |
| 11  | CL    | 14  | LYS  |
| 11  | CL    | 15  | VAL  |
| 11  | CL    | 17  | LYS  |
| 11  | CL    | 19  | ASN  |
| 11  | CL    | 28  | GLN  |
| 11  | CL    | 33  | CYS  |
| 11  | CL    | 43  | LYS  |
| 11  | CL    | 49  | ARG  |
| 11  | CL    | 93  | ARG  |
| 11  | CL    | 107 | LYS  |
| 11  | CL    | 114 | SER  |
| 12  | CM    | 2   | ARG  |
| 12  | CM    | 15  | VAL  |
| 12  | CM    | 28  | ARG  |
| 12  | CM    | 43  | LYS  |
| 12  | CM    | 44  | ILE  |
| 12  | CM    | 46  | GLU  |
| 12  | CM    | 57  | ASP  |
| 12  | CM    | 64  | VAL  |
| 12  | CM    | 67  | ASP  |
| 12  | CM    | 71  | GLU  |
| 12  | CM    | 79  | LEU  |
| 12  | CM    | 82  | LEU  |
| 12  | CM    | 92  | ARG  |
| 12  | CM    | 102 | LYS  |
| 13  | CN    | 17  | ASP  |
| 13  | CN    | 19  | TYR  |
| 13  | CN    | 26  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CN    | 30  | ILE  |
| 13  | CN    | 34  | ASN  |
| 13  | CN    | 40  | ARG  |
| 13  | CN    | 41  | TRP  |
| 13  | CN    | 45  | LEU  |
| 13  | CN    | 57  | SER  |
| 13  | CN    | 59  | GLN  |
| 13  | CN    | 65  | GLN  |
| 13  | CN    | 68  | ARG  |
| 13  | CN    | 97  | LYS  |
| 14  | CO    | 18  | ASP  |
| 14  | CO    | 25  | THR  |
| 14  | CO    | 37  | ASN  |
| 14  | CO    | 42  | HIS  |
| 14  | CO    | 54  | ARG  |
| 14  | CO    | 59  | MET  |
| 14  | CO    | 64  | ARG  |
| 14  | CO    | 68  | ASP  |
| 14  | CO    | 70  | LEU  |
| 14  | CO    | 71  | LYS  |
| 14  | CO    | 88  | ARG  |
| 14  | CO    | 89  | ARG  |
| 15  | CP    | 28  | ARG  |
| 15  | CP    | 31  | ARG  |
| 15  | CP    | 45  | GLU  |
| 15  | CP    | 51  | ARG  |
| 15  | CP    | 79  | ASN  |
| 16  | CQ    | 24  | ILE  |
| 16  | CQ    | 39  | ARG  |
| 16  | CQ    | 56  | ASP  |
| 16  | CQ    | 60  | ILE  |
| 16  | CQ    | 61  | ARG  |
| 16  | CQ    | 67  | SER  |
| 16  | CQ    | 71  | SER  |
| 16  | CQ    | 80  | LYS  |
| 17  | CR    | 33  | THR  |
| 17  | CR    | 38  | ILE  |
| 17  | CR    | 73  | HIS  |
| 18  | CS    | 2   | ARG  |
| 18  | CS    | 4   | LEU  |
| 18  | CS    | 5   | LYS  |
| 18  | CS    | 12  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | CS    | 13  | HIS  |
| 18  | CS    | 14  | LEU  |
| 18  | CS    | 15  | LEU  |
| 18  | CS    | 17  | LYS  |
| 18  | CS    | 20  | LYS  |
| 18  | CS    | 23  | GLU  |
| 18  | CS    | 27  | LYS  |
| 18  | CS    | 28  | LYS  |
| 18  | CS    | 42  | ASN  |
| 18  | CS    | 43  | MET  |
| 18  | CS    | 46  | LEU  |
| 18  | CS    | 64  | GLU  |
| 19  | CT    | 4   | LYS  |
| 19  | CT    | 35  | TYR  |
| 19  | CT    | 38  | ILE  |
| 19  | CT    | 43  | LYS  |
| 19  | CT    | 51  | ASN  |
| 19  | CT    | 53  | MET  |
| 19  | CT    | 69  | ASN  |
| 19  | CT    | 74  | HIS  |
| 19  | CT    | 85  | LEU  |
| 20  | CB    | 20  | ARG  |
| 20  | CB    | 27  | LYS  |
| 20  | CB    | 35  | ASN  |
| 20  | CB    | 36  | LYS  |
| 20  | CB    | 38  | HIS  |
| 20  | CB    | 43  | GLU  |
| 20  | CB    | 46  | VAL  |
| 20  | CB    | 53  | LEU  |
| 20  | CB    | 57  | ASN  |
| 20  | CB    | 62  | ARG  |
| 20  | CB    | 67  | LEU  |
| 20  | CB    | 76  | SER  |
| 20  | CB    | 84  | LEU  |
| 20  | CB    | 87  | ASP  |
| 20  | CB    | 88  | GLN  |
| 20  | CB    | 94  | ARG  |
| 20  | CB    | 95  | TRP  |
| 20  | CB    | 100 | LEU  |
| 20  | CB    | 104 | LYS  |
| 20  | CB    | 125 | PHE  |
| 20  | CB    | 127 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | CB    | 130 | LYS  |
| 20  | CB    | 138 | ARG  |
| 20  | CB    | 166 | ASP  |
| 20  | CB    | 176 | ASN  |
| 20  | CB    | 196 | ASP  |
| 20  | CB    | 202 | ASN  |
| 20  | CB    | 203 | ASP  |
| 20  | CB    | 211 | LEU  |
| 20  | CB    | 213 | LEU  |
| 20  | CB    | 221 | ARG  |
| 21  | CU    | 11  | PHE  |
| 21  | CU    | 15  | LEU  |
| 21  | CU    | 16  | ARG  |
| 21  | CU    | 18  | PHE  |
| 21  | CU    | 20  | ARG  |
| 21  | CU    | 22  | CYS  |
| 21  | CU    | 24  | LYS  |
| 21  | CU    | 33  | ARG  |
| 21  | CU    | 34  | ARG  |
| 21  | CU    | 35  | GLU  |
| 21  | CU    | 38  | GLU  |
| 21  | CU    | 44  | ARG  |
| 21  | CU    | 48  | LYS  |
| 24  | DI    | 2   | LYS  |
| 24  | DI    | 54  | ILE  |
| 24  | DI    | 91  | LYS  |
| 24  | DI    | 99  | LYS  |
| 24  | DI    | 121 | ILE  |
| 24  | DI    | 140 | GLU  |
| 25  | DC    | 4   | LYS  |
| 25  | DC    | 12  | ARG  |
| 25  | DC    | 37  | SER  |
| 25  | DC    | 43  | ASN  |
| 25  | DC    | 44  | ASN  |
| 25  | DC    | 45  | ASN  |
| 25  | DC    | 47  | ARG  |
| 25  | DC    | 52  | HIS  |
| 25  | DC    | 62  | ARG  |
| 25  | DC    | 65  | ASP  |
| 25  | DC    | 86  | ARG  |
| 25  | DC    | 89  | ASN  |
| 25  | DC    | 90  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | DC    | 100 | ARG  |
| 25  | DC    | 109 | LEU  |
| 25  | DC    | 123 | ILE  |
| 25  | DC    | 129 | LEU  |
| 25  | DC    | 134 | ILE  |
| 25  | DC    | 142 | ASN  |
| 25  | DC    | 155 | ARG  |
| 25  | DC    | 167 | ASP  |
| 25  | DC    | 172 | THR  |
| 25  | DC    | 173 | LEU  |
| 25  | DC    | 176 | ARG  |
| 25  | DC    | 180 | MET  |
| 25  | DC    | 181 | ARG  |
| 25  | DC    | 191 | LEU  |
| 25  | DC    | 203 | VAL  |
| 25  | DC    | 211 | ARG  |
| 25  | DC    | 212 | TRP  |
| 25  | DC    | 224 | MET  |
| 25  | DC    | 239 | PHE  |
| 25  | DC    | 245 | THR  |
| 25  | DC    | 249 | VAL  |
| 25  | DC    | 250 | GLN  |
| 25  | DC    | 251 | THR  |
| 25  | DC    | 257 | ARG  |
| 26  | DD    | 16  | THR  |
| 26  | DD    | 30  | GLU  |
| 26  | DD    | 40  | LEU  |
| 26  | DD    | 56  | LYS  |
| 26  | DD    | 79  | LEU  |
| 26  | DD    | 81  | GLU  |
| 26  | DD    | 82  | PHE  |
| 26  | DD    | 84  | LEU  |
| 26  | DD    | 88  | GLU  |
| 26  | DD    | 91  | THR  |
| 26  | DD    | 95  | SER  |
| 26  | DD    | 99  | GLU  |
| 26  | DD    | 114 | LYS  |
| 26  | DD    | 124 | ARG  |
| 26  | DD    | 137 | SER  |
| 26  | DD    | 138 | LEU  |
| 26  | DD    | 141 | ARG  |
| 26  | DD    | 142 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 148 | GLN  |
| 26  | DD    | 159 | LYS  |
| 26  | DD    | 179 | ARG  |
| 26  | DD    | 186 | LEU  |
| 26  | DD    | 197 | THR  |
| 26  | DD    | 204 | LYS  |
| 27  | DK    | 2   | ILE  |
| 27  | DK    | 8   | LEU  |
| 27  | DK    | 18  | ARG  |
| 27  | DK    | 21  | CYS  |
| 27  | DK    | 25  | LEU  |
| 27  | DK    | 32  | TYR  |
| 27  | DK    | 47  | ILE  |
| 27  | DK    | 53  | LYS  |
| 27  | DK    | 54  | LYS  |
| 27  | DK    | 58  | LEU  |
| 27  | DK    | 64  | ARG  |
| 27  | DK    | 67  | LYS  |
| 27  | DK    | 70  | ARG  |
| 27  | DK    | 72  | PRO  |
| 27  | DK    | 73  | ASP  |
| 27  | DK    | 79  | PHE  |
| 27  | DK    | 80  | ASP  |
| 27  | DK    | 86  | LEU  |
| 27  | DK    | 87  | LEU  |
| 27  | DK    | 88  | ASN  |
| 27  | DK    | 89  | ASN  |
| 27  | DK    | 98  | ARG  |
| 27  | DK    | 104 | THR  |
| 27  | DK    | 105 | ARG  |
| 27  | DK    | 107 | LEU  |
| 27  | DK    | 111 | LYS  |
| 27  | DK    | 120 | PRO  |
| 28  | DP    | 3   | ILE  |
| 28  | DP    | 6   | GLN  |
| 28  | DP    | 19  | PHE  |
| 28  | DP    | 25  | VAL  |
| 28  | DP    | 33  | GLU  |
| 28  | DP    | 38  | ARG  |
| 28  | DP    | 43  | GLU  |
| 28  | DP    | 61  | ARG  |
| 28  | DP    | 65  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DP    | 80  | VAL  |
| 28  | DP    | 83  | ILE  |
| 28  | DP    | 99  | LEU  |
| 28  | DP    | 100 | ARG  |
| 28  | DP    | 101 | GLU  |
| 28  | DP    | 111 | GLU  |
| 28  | DP    | 112 | ARG  |
| 28  | DP    | 114 | ASN  |
| 29  | DE    | 2   | GLU  |
| 29  | DE    | 3   | LEU  |
| 29  | DE    | 5   | LEU  |
| 29  | DE    | 7   | ASP  |
| 29  | DE    | 22  | ASP  |
| 29  | DE    | 24  | ASN  |
| 29  | DE    | 58  | LYS  |
| 29  | DE    | 60  | TRP  |
| 29  | DE    | 62  | GLN  |
| 29  | DE    | 67  | ARG  |
| 29  | DE    | 70  | SER  |
| 29  | DE    | 75  | SER  |
| 29  | DE    | 80  | SER  |
| 29  | DE    | 97  | ASN  |
| 29  | DE    | 98  | LYS  |
| 29  | DE    | 107 | SER  |
| 29  | DE    | 108 | ILE  |
| 29  | DE    | 111 | GLU  |
| 29  | DE    | 116 | ASP  |
| 29  | DE    | 118 | LEU  |
| 29  | DE    | 122 | GLU  |
| 29  | DE    | 133 | LEU  |
| 29  | DE    | 150 | THR  |
| 29  | DE    | 159 | LEU  |
| 29  | DE    | 163 | ASN  |
| 30  | DY    | 2   | LYS  |
| 30  | DY    | 6   | ILE  |
| 30  | DY    | 8   | GLN  |
| 30  | DY    | 15  | ARG  |
| 30  | DY    | 16  | LEU  |
| 30  | DY    | 19  | HIS  |
| 30  | DY    | 23  | LEU  |
| 30  | DY    | 30  | ARG  |
| 30  | DY    | 37  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DY    | 43  | ILE  |
| 31  | D0    | 5   | ASN  |
| 31  | D0    | 27  | LEU  |
| 31  | D0    | 31  | LYS  |
| 31  | D0    | 38  | LEU  |
| 31  | D0    | 41  | HIS  |
| 31  | D0    | 51  | ARG  |
| 31  | D0    | 53  | VAL  |
| 31  | D0    | 56  | LYS  |
| 32  | D4    | 2   | LYS  |
| 32  | D4    | 9   | LYS  |
| 32  | D4    | 15  | LYS  |
| 32  | D4    | 22  | VAL  |
| 32  | D4    | 24  | ARG  |
| 32  | D4    | 35  | GLN  |
| 33  | D1    | 6   | GLU  |
| 33  | D1    | 9   | LYS  |
| 33  | D1    | 35  | LEU  |
| 34  | D3    | 7   | ARG  |
| 34  | D3    | 18  | LYS  |
| 34  | D3    | 49  | VAL  |
| 34  | D3    | 61  | LEU  |
| 35  | DV    | 35  | GLU  |
| 35  | DV    | 40  | ILE  |
| 35  | DV    | 42  | LEU  |
| 35  | DV    | 45  | ASP  |
| 35  | DV    | 46  | LYS  |
| 35  | DV    | 51  | GLN  |
| 35  | DV    | 53  | LYS  |
| 35  | DV    | 66  | ASP  |
| 35  | DV    | 69  | GLU  |
| 35  | DV    | 70  | ILE  |
| 35  | DV    | 75  | GLN  |
| 36  | D2    | 19  | ARG  |
| 36  | D2    | 33  | ARG  |
| 36  | D2    | 35  | ARG  |
| 36  | D2    | 39  | ARG  |
| 37  | DL    | 10  | GLU  |
| 37  | DL    | 39  | LYS  |
| 37  | DL    | 47  | ARG  |
| 37  | DL    | 55  | MET  |
| 37  | DL    | 67  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DL    | 69  | ARG  |
| 37  | DL    | 82  | LEU  |
| 37  | DL    | 91  | ASP  |
| 37  | DL    | 92  | LEU  |
| 37  | DL    | 95  | LEU  |
| 37  | DL    | 99  | ASN  |
| 37  | DL    | 112 | LEU  |
| 37  | DL    | 118 | THR  |
| 37  | DL    | 123 | ARG  |
| 38  | DM    | 1   | MET  |
| 38  | DM    | 7   | THR  |
| 38  | DM    | 10  | ARG  |
| 38  | DM    | 18  | ARG  |
| 38  | DM    | 20  | LEU  |
| 38  | DM    | 26  | VAL  |
| 38  | DM    | 47  | GLU  |
| 38  | DM    | 55  | ARG  |
| 38  | DM    | 65  | ILE  |
| 38  | DM    | 70  | ASP  |
| 38  | DM    | 78  | LEU  |
| 38  | DM    | 81  | ARG  |
| 38  | DM    | 88  | ASN  |
| 38  | DM    | 90  | GLU  |
| 38  | DM    | 108 | VAL  |
| 38  | DM    | 111 | GLU  |
| 38  | DM    | 114 | ARG  |
| 38  | DM    | 115 | GLU  |
| 38  | DM    | 123 | LYS  |
| 38  | DM    | 126 | ILE  |
| 39  | DX    | 1   | MET  |
| 39  | DX    | 7   | ARG  |
| 39  | DX    | 10  | SER  |
| 39  | DX    | 15  | ASN  |
| 39  | DX    | 18  | LEU  |
| 39  | DX    | 20  | ASN  |
| 39  | DX    | 21  | LEU  |
| 39  | DX    | 28  | LEU  |
| 39  | DX    | 29  | ARG  |
| 39  | DX    | 30  | MET  |
| 39  | DX    | 41  | HIS  |
| 39  | DX    | 49  | ASP  |
| 39  | DX    | 59  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | DH    | 3   | VAL  |
| 40  | DH    | 4   | ILE  |
| 40  | DH    | 12  | LEU  |
| 40  | DH    | 15  | LEU  |
| 40  | DH    | 19  | VAL  |
| 40  | DH    | 28  | ASN  |
| 40  | DH    | 31  | VAL  |
| 40  | DH    | 32  | PRO  |
| 40  | DH    | 33  | GLN  |
| 40  | DH    | 47  | PHE  |
| 40  | DH    | 50  | ARG  |
| 40  | DH    | 55  | GLU  |
| 40  | DH    | 70  | GLU  |
| 40  | DH    | 83  | LYS  |
| 40  | DH    | 97  | ARG  |
| 40  | DH    | 112 | LYS  |
| 40  | DH    | 113 | SER  |
| 40  | DH    | 121 | VAL  |
| 40  | DH    | 124 | THR  |
| 40  | DH    | 129 | GLU  |
| 40  | DH    | 133 | GLN  |
| 40  | DH    | 137 | GLU  |
| 40  | DH    | 141 | LYS  |
| 41  | DJ    | 3   | THR  |
| 41  | DJ    | 5   | THR  |
| 41  | DJ    | 9   | GLU  |
| 41  | DJ    | 12  | LYS  |
| 41  | DJ    | 28  | LEU  |
| 41  | DJ    | 30  | THR  |
| 41  | DJ    | 44  | TYR  |
| 41  | DJ    | 65  | THR  |
| 41  | DJ    | 71  | ASP  |
| 41  | DJ    | 92  | MET  |
| 41  | DJ    | 95  | ARG  |
| 41  | DJ    | 106 | LYS  |
| 41  | DJ    | 120 | ARG  |
| 41  | DJ    | 124 | VAL  |
| 41  | DJ    | 129 | GLU  |
| 41  | DJ    | 131 | ASN  |
| 41  | DJ    | 138 | GLN  |
| 42  | DN    | 1   | MET  |
| 42  | DN    | 9   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DN    | 11  | ASN  |
| 42  | DN    | 20  | MET  |
| 42  | DN    | 31  | HIS  |
| 42  | DN    | 35  | LYS  |
| 42  | DN    | 46  | ARG  |
| 42  | DN    | 51  | LEU  |
| 42  | DN    | 69  | ARG  |
| 42  | DN    | 71  | ARG  |
| 42  | DN    | 82  | GLU  |
| 42  | DN    | 96  | ARG  |
| 42  | DN    | 114 | GLU  |
| 42  | DN    | 120 | GLU  |
| 43  | DO    | 31  | THR  |
| 43  | DO    | 35  | ILE  |
| 43  | DO    | 36  | TYR  |
| 43  | DO    | 58  | ILE  |
| 43  | DO    | 62  | LEU  |
| 43  | DO    | 69  | ASP  |
| 43  | DO    | 74  | VAL  |
| 43  | DO    | 81  | ARG  |
| 43  | DO    | 89  | ASP  |
| 43  | DO    | 106 | LEU  |
| 43  | DO    | 115 | LEU  |
| 43  | DO    | 116 | GLN  |
| 44  | DQ    | 4   | LYS  |
| 44  | DQ    | 5   | ARG  |
| 44  | DQ    | 10  | ARG  |
| 44  | DQ    | 13  | HIS  |
| 44  | DQ    | 63  | ARG  |
| 44  | DQ    | 69  | ARG  |
| 44  | DQ    | 79  | ILE  |
| 44  | DQ    | 83  | LYS  |
| 44  | DQ    | 84  | LYS  |
| 44  | DQ    | 88  | GLU  |
| 44  | DQ    | 89  | ILE  |
| 44  | DQ    | 90  | ASP  |
| 44  | DQ    | 91  | ARG  |
| 44  | DQ    | 96  | ASP  |
| 45  | DS    | 7   | HIS  |
| 45  | DS    | 15  | GLN  |
| 45  | DS    | 22  | ASP  |
| 45  | DS    | 27  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | DS    | 57  | ASN  |
| 45  | DS    | 61  | ASN  |
| 45  | DS    | 66  | ILE  |
| 45  | DS    | 72  | THR  |
| 45  | DS    | 84  | ARG  |
| 45  | DS    | 86  | MET  |
| 45  | DS    | 88  | ARG  |
| 45  | DS    | 99  | ARG  |
| 45  | DS    | 101 | SER  |
| 46  | DU    | 11  | ILE  |
| 46  | DU    | 13  | LEU  |
| 46  | DU    | 20  | LYS  |
| 46  | DU    | 26  | ASN  |
| 46  | DU    | 45  | GLN  |
| 46  | DU    | 49  | PRO  |
| 46  | DU    | 51  | LEU  |
| 46  | DU    | 53  | GLN  |
| 46  | DU    | 60  | LYS  |
| 46  | DU    | 73  | ASN  |
| 46  | DU    | 78  | LYS  |
| 46  | DU    | 81  | ARG  |
| 46  | DU    | 85  | ARG  |
| 46  | DU    | 88  | ASP  |
| 47  | DF    | 2   | LYS  |
| 47  | DF    | 13  | LYS  |
| 47  | DF    | 19  | PHE  |
| 47  | DF    | 22  | ASN  |
| 47  | DF    | 29  | ARG  |
| 47  | DF    | 32  | LYS  |
| 47  | DF    | 46  | LYS  |
| 47  | DF    | 50  | ASP  |
| 47  | DF    | 55  | ASP  |
| 47  | DF    | 68  | LYS  |
| 47  | DF    | 70  | ARG  |
| 47  | DF    | 76  | PHE  |
| 47  | DF    | 79  | ARG  |
| 47  | DF    | 91  | ARG  |
| 47  | DF    | 96  | TRP  |
| 47  | DF    | 97  | GLU  |
| 47  | DF    | 100 | GLU  |
| 47  | DF    | 102 | LEU  |
| 47  | DF    | 103 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | DF    | 109 | ARG  |
| 47  | DF    | 111 | ARG  |
| 47  | DF    | 120 | SER  |
| 47  | DF    | 121 | PHE  |
| 47  | DF    | 124 | ARG  |
| 47  | DF    | 129 | MET  |
| 47  | DF    | 134 | GLN  |
| 47  | DF    | 137 | PHE  |
| 47  | DF    | 138 | PRO  |
| 47  | DF    | 149 | ARG  |
| 47  | DF    | 168 | LEU  |
| 47  | DF    | 173 | ASP  |
| 47  | DF    | 174 | PHE  |
| 47  | DF    | 178 | LYS  |
| 48  | DG    | 14  | VAL  |
| 48  | DG    | 24  | THR  |
| 48  | DG    | 26  | LYS  |
| 48  | DG    | 31  | GLU  |
| 48  | DG    | 34  | ARG  |
| 48  | DG    | 46  | ASP  |
| 48  | DG    | 54  | ARG  |
| 48  | DG    | 61  | TRP  |
| 48  | DG    | 66  | THR  |
| 48  | DG    | 68  | ARG  |
| 48  | DG    | 70  | LEU  |
| 48  | DG    | 84  | LYS  |
| 48  | DG    | 94  | ARG  |
| 48  | DG    | 106 | LEU  |
| 48  | DG    | 120 | ILE  |
| 48  | DG    | 132 | LEU  |
| 48  | DG    | 133 | LYS  |
| 48  | DG    | 138 | GLN  |
| 48  | DG    | 152 | ARG  |
| 48  | DG    | 162 | ARG  |
| 48  | DG    | 166 | GLU  |
| 48  | DG    | 176 | LYS  |
| 49  | DR    | 4   | VAL  |
| 49  | DR    | 19  | THR  |
| 49  | DR    | 22  | LEU  |
| 49  | DR    | 39  | LEU  |
| 49  | DR    | 53  | PHE  |
| 49  | DR    | 55  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | DR    | 70  | GLU  |
| 49  | DR    | 71  | LYS  |
| 49  | DR    | 72  | VAL  |
| 49  | DR    | 79  | ARG  |
| 49  | DR    | 82  | HIS  |
| 49  | DR    | 86  | GLN  |
| 50  | DT    | 2   | ILE  |
| 50  | DT    | 3   | ARG  |
| 50  | DT    | 4   | GLU  |
| 50  | DT    | 9   | LYS  |
| 50  | DT    | 11  | LEU  |
| 50  | DT    | 12  | ARG  |
| 50  | DT    | 32  | LEU  |
| 50  | DT    | 64  | LYS  |
| 50  | DT    | 68  | LYS  |
| 50  | DT    | 69  | ARG  |
| 50  | DT    | 70  | HIS  |
| 50  | DT    | 81  | LYS  |
| 51  | DZ    | 2   | SER  |
| 51  | DZ    | 25  | THR  |
| 51  | DZ    | 27  | ARG  |
| 51  | DZ    | 28  | ARG  |
| 51  | DZ    | 30  | LEU  |
| 51  | DZ    | 33  | LEU  |
| 51  | DZ    | 37  | ARG  |
| 51  | DZ    | 46  | PHE  |
| 51  | DZ    | 50  | ARG  |
| 51  | DZ    | 60  | ASP  |
| 51  | DZ    | 66  | THR  |
| 51  | DZ    | 77  | LYS  |
| 51  | DZ    | 78  | TYR  |
| 52  | DW    | 10  | ARG  |
| 52  | DW    | 14  | ASP  |
| 52  | DW    | 16  | GLU  |
| 52  | DW    | 19  | ARG  |
| 52  | DW    | 24  | ARG  |
| 52  | DW    | 25  | PHE  |
| 52  | DW    | 39  | GLN  |
| 52  | DW    | 44  | PHE  |
| 52  | DW    | 49  | ASN  |
| 52  | DW    | 50  | VAL  |
| 52  | DW    | 75  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | DW    | 77  | LYS  |
| 52  | DW    | 82  | GLU  |
| 53  | D6    | 1   | MET  |
| 53  | D6    | 6   | LEU  |
| 53  | D6    | 9   | GLU  |
| 53  | D6    | 12  | SER  |
| 53  | D6    | 13  | HIS  |
| 53  | D6    | 16  | LYS  |
| 53  | D6    | 17  | SER  |
| 53  | D6    | 29  | ARG  |
| 53  | D6    | 41  | LEU  |
| 53  | D6    | 44  | GLU  |
| 53  | D6    | 52  | LEU  |
| 53  | D6    | 53  | ASN  |
| 53  | D6    | 54  | GLN  |
| 53  | D6    | 64  | ARG  |
| 53  | D6    | 71  | TRP  |
| 53  | D6    | 73  | GLN  |
| 53  | D6    | 74  | ASN  |
| 53  | D6    | 84  | ARG  |
| 53  | D6    | 85  | ASP  |
| 53  | D6    | 93  | SER  |
| 53  | D6    | 94  | ASN  |
| 53  | D6    | 107 | THR  |
| 53  | D6    | 108 | GLU  |
| 53  | D6    | 110 | ARG  |
| 53  | D6    | 114 | LEU  |
| 53  | D6    | 115 | VAL  |
| 53  | D6    | 121 | TYR  |
| 53  | D6    | 130 | ARG  |
| 53  | D6    | 137 | LEU  |
| 53  | D6    | 138 | ASP  |
| 53  | D6    | 150 | SER  |
| 53  | D6    | 154 | THR  |
| 53  | D6    | 156 | ARG  |
| 53  | D6    | 174 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (336) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 2   | GLN  |
| 2   | AC    | 5   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 68  | HIS  |
| 2   | AC    | 99  | GLN  |
| 2   | AC    | 139 | ASN  |
| 2   | AC    | 184 | ASN  |
| 2   | AC    | 189 | HIS  |
| 3   | AD    | 35  | GLN  |
| 3   | AD    | 84  | ASN  |
| 3   | AD    | 135 | GLN  |
| 3   | AD    | 163 | GLN  |
| 4   | AE    | 18  | ASN  |
| 4   | AE    | 131 | ASN  |
| 5   | AF    | 17  | GLN  |
| 5   | AF    | 37  | HIS  |
| 5   | AF    | 46  | GLN  |
| 6   | AG    | 67  | ASN  |
| 6   | AG    | 121 | ASN  |
| 7   | AH    | 3   | GLN  |
| 7   | AH    | 17  | GLN  |
| 7   | AH    | 117 | GLN  |
| 8   | AI    | 24  | ASN  |
| 8   | AI    | 30  | ASN  |
| 8   | AI    | 31  | GLN  |
| 8   | AI    | 36  | GLN  |
| 8   | AI    | 74  | GLN  |
| 8   | AI    | 80  | HIS  |
| 9   | AJ    | 15  | HIS  |
| 9   | AJ    | 20  | GLN  |
| 9   | AJ    | 58  | ASN  |
| 9   | AJ    | 64  | GLN  |
| 9   | AJ    | 99  | GLN  |
| 10  | AK    | 21  | HIS  |
| 10  | AK    | 28  | ASN  |
| 10  | AK    | 80  | ASN  |
| 10  | AK    | 118 | ASN  |
| 11  | AL    | 5   | GLN  |
| 11  | AL    | 19  | ASN  |
| 11  | AL    | 28  | GLN  |
| 11  | AL    | 45  | ASN  |
| 12  | AM    | 7   | ASN  |
| 12  | AM    | 13  | HIS  |
| 12  | AM    | 90  | HIS  |
| 14  | AO    | 28  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | AO    | 37  | ASN  |
| 14  | AO    | 40  | GLN  |
| 14  | AO    | 62  | GLN  |
| 15  | AP    | 26  | ASN  |
| 15  | AP    | 40  | ASN  |
| 16  | AQ    | 50  | ASN  |
| 17  | AR    | 53  | GLN  |
| 18  | AS    | 42  | ASN  |
| 19  | AT    | 2   | ASN  |
| 19  | AT    | 20  | ASN  |
| 19  | AT    | 67  | HIS  |
| 20  | AB    | 14  | HIS  |
| 20  | AB    | 17  | HIS  |
| 20  | AB    | 18  | GLN  |
| 20  | AB    | 23  | ASN  |
| 20  | AB    | 35  | ASN  |
| 20  | AB    | 41  | ASN  |
| 20  | AB    | 57  | ASN  |
| 20  | AB    | 93  | HIS  |
| 20  | AB    | 119 | GLN  |
| 20  | AB    | 121 | GLN  |
| 20  | AB    | 145 | ASN  |
| 20  | AB    | 169 | HIS  |
| 20  | AB    | 202 | ASN  |
| 24  | BI    | 11  | GLN  |
| 24  | BI    | 29  | GLN  |
| 24  | BI    | 33  | ASN  |
| 25  | BC    | 43  | ASN  |
| 25  | BC    | 45  | ASN  |
| 25  | BC    | 59  | GLN  |
| 25  | BC    | 85  | ASN  |
| 25  | BC    | 114 | GLN  |
| 25  | BC    | 116 | GLN  |
| 25  | BC    | 133 | ASN  |
| 25  | BC    | 152 | GLN  |
| 25  | BC    | 196 | ASN  |
| 25  | BC    | 225 | ASN  |
| 26  | BD    | 32  | ASN  |
| 26  | BD    | 49  | GLN  |
| 26  | BD    | 126 | ASN  |
| 26  | BD    | 136 | ASN  |
| 26  | BD    | 173 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | BK    | 5   | GLN  |
| 27  | BK    | 13  | ASN  |
| 27  | BK    | 88  | ASN  |
| 28  | BP    | 6   | GLN  |
| 28  | BP    | 11  | GLN  |
| 28  | BP    | 114 | ASN  |
| 29  | BE    | 24  | ASN  |
| 29  | BE    | 30  | GLN  |
| 29  | BE    | 62  | GLN  |
| 29  | BE    | 136 | GLN  |
| 29  | BE    | 163 | ASN  |
| 29  | BE    | 195 | GLN  |
| 30  | BY    | 19  | HIS  |
| 30  | BY    | 33  | HIS  |
| 30  | BY    | 48  | ASN  |
| 32  | B4    | 35  | GLN  |
| 32  | B4    | 37  | GLN  |
| 34  | B3    | 30  | HIS  |
| 34  | B3    | 42  | HIS  |
| 35  | BV    | 44  | HIS  |
| 35  | BV    | 49  | ASN  |
| 35  | BV    | 80  | HIS  |
| 35  | BV    | 88  | HIS  |
| 36  | B2    | 6   | GLN  |
| 36  | B2    | 13  | ASN  |
| 37  | BL    | 4   | ASN  |
| 37  | BL    | 54  | GLN  |
| 37  | BL    | 93  | ASN  |
| 37  | BL    | 104 | GLN  |
| 38  | BM    | 17  | ASN  |
| 38  | BM    | 22  | GLN  |
| 39  | BX    | 20  | ASN  |
| 39  | BX    | 25  | GLN  |
| 39  | BX    | 41  | HIS  |
| 40  | BH    | 18  | GLN  |
| 40  | BH    | 28  | ASN  |
| 40  | BH    | 43  | ASN  |
| 40  | BH    | 73  | ASN  |
| 40  | BH    | 133 | GLN  |
| 41  | BJ    | 130 | HIS  |
| 41  | BJ    | 135 | GLN  |
| 41  | BJ    | 136 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BJ    | 138 | GLN  |
| 42  | BN    | 11  | ASN  |
| 42  | BN    | 107 | ASN  |
| 43  | BO    | 19  | GLN  |
| 43  | BO    | 29  | HIS  |
| 43  | BO    | 38  | GLN  |
| 43  | BO    | 61  | GLN  |
| 44  | BQ    | 19  | GLN  |
| 44  | BQ    | 51  | GLN  |
| 44  | BQ    | 58  | GLN  |
| 44  | BQ    | 71  | ASN  |
| 44  | BQ    | 80  | ASN  |
| 46  | BU    | 26  | ASN  |
| 46  | BU    | 45  | GLN  |
| 46  | BU    | 52  | ASN  |
| 46  | BU    | 65  | GLN  |
| 46  | BU    | 73  | ASN  |
| 47  | BF    | 51  | ASN  |
| 47  | BF    | 134 | GLN  |
| 48  | BG    | 29  | ASN  |
| 48  | BG    | 72  | ASN  |
| 48  | BG    | 87  | GLN  |
| 49  | BR    | 6   | GLN  |
| 49  | BR    | 11  | GLN  |
| 49  | BR    | 43  | ASN  |
| 49  | BR    | 86  | GLN  |
| 49  | BR    | 87  | GLN  |
| 50  | BT    | 48  | GLN  |
| 50  | BT    | 91  | GLN  |
| 50  | BT    | 92  | ASN  |
| 51  | BZ    | 6   | GLN  |
| 51  | BZ    | 17  | ASN  |
| 51  | BZ    | 36  | HIS  |
| 52  | BW    | 39  | GLN  |
| 52  | BW    | 49  | ASN  |
| 52  | BW    | 75  | ASN  |
| 53  | B6    | 13  | HIS  |
| 53  | B6    | 24  | ASN  |
| 53  | B6    | 91  | ASN  |
| 53  | B6    | 102 | ASN  |
| 53  | B6    | 162 | GLN  |
| 53  | B6    | 174 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CC    | 2   | GLN  |
| 2   | CC    | 5   | HIS  |
| 2   | CC    | 68  | HIS  |
| 2   | CC    | 99  | GLN  |
| 2   | CC    | 139 | ASN  |
| 2   | CC    | 184 | ASN  |
| 2   | CC    | 189 | HIS  |
| 3   | CD    | 35  | GLN  |
| 3   | CD    | 84  | ASN  |
| 3   | CD    | 135 | GLN  |
| 3   | CD    | 163 | GLN  |
| 4   | CE    | 18  | ASN  |
| 4   | CE    | 81  | GLN  |
| 4   | CE    | 131 | ASN  |
| 5   | CF    | 17  | GLN  |
| 5   | CF    | 37  | HIS  |
| 5   | CF    | 46  | GLN  |
| 5   | CF    | 55  | HIS  |
| 6   | CG    | 67  | ASN  |
| 6   | CG    | 121 | ASN  |
| 7   | CH    | 3   | GLN  |
| 7   | CH    | 17  | GLN  |
| 7   | CH    | 117 | GLN  |
| 8   | CI    | 24  | ASN  |
| 8   | CI    | 30  | ASN  |
| 8   | CI    | 31  | GLN  |
| 8   | CI    | 36  | GLN  |
| 8   | CI    | 74  | GLN  |
| 8   | CI    | 80  | HIS  |
| 9   | CJ    | 20  | GLN  |
| 9   | CJ    | 58  | ASN  |
| 9   | CJ    | 64  | GLN  |
| 9   | CJ    | 99  | GLN  |
| 10  | CK    | 21  | HIS  |
| 10  | CK    | 28  | ASN  |
| 10  | CK    | 80  | ASN  |
| 10  | CK    | 118 | ASN  |
| 11  | CL    | 5   | GLN  |
| 11  | CL    | 19  | ASN  |
| 11  | CL    | 28  | GLN  |
| 11  | CL    | 45  | ASN  |
| 12  | CM    | 7   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CM    | 13  | HIS  |
| 12  | CM    | 90  | HIS  |
| 14  | CO    | 28  | GLN  |
| 14  | CO    | 37  | ASN  |
| 14  | CO    | 40  | GLN  |
| 14  | CO    | 62  | GLN  |
| 15  | CP    | 26  | ASN  |
| 15  | CP    | 40  | ASN  |
| 16  | CQ    | 50  | ASN  |
| 18  | CS    | 42  | ASN  |
| 18  | CS    | 52  | ASN  |
| 19  | CT    | 2   | ASN  |
| 19  | CT    | 20  | ASN  |
| 19  | CT    | 67  | HIS  |
| 20  | CB    | 14  | HIS  |
| 20  | CB    | 17  | HIS  |
| 20  | CB    | 18  | GLN  |
| 20  | CB    | 23  | ASN  |
| 20  | CB    | 35  | ASN  |
| 20  | CB    | 41  | ASN  |
| 20  | CB    | 57  | ASN  |
| 20  | CB    | 93  | HIS  |
| 20  | CB    | 119 | GLN  |
| 20  | CB    | 145 | ASN  |
| 20  | CB    | 169 | HIS  |
| 20  | CB    | 202 | ASN  |
| 24  | DI    | 5   | GLN  |
| 24  | DI    | 11  | GLN  |
| 24  | DI    | 33  | ASN  |
| 25  | DC    | 43  | ASN  |
| 25  | DC    | 45  | ASN  |
| 25  | DC    | 59  | GLN  |
| 25  | DC    | 85  | ASN  |
| 25  | DC    | 114 | GLN  |
| 25  | DC    | 116 | GLN  |
| 25  | DC    | 133 | ASN  |
| 25  | DC    | 152 | GLN  |
| 25  | DC    | 196 | ASN  |
| 26  | DD    | 32  | ASN  |
| 26  | DD    | 49  | GLN  |
| 26  | DD    | 126 | ASN  |
| 26  | DD    | 136 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 173 | GLN  |
| 27  | DK    | 5   | GLN  |
| 27  | DK    | 13  | ASN  |
| 27  | DK    | 88  | ASN  |
| 28  | DP    | 6   | GLN  |
| 28  | DP    | 11  | GLN  |
| 28  | DP    | 114 | ASN  |
| 29  | DE    | 24  | ASN  |
| 29  | DE    | 29  | HIS  |
| 29  | DE    | 30  | GLN  |
| 29  | DE    | 62  | GLN  |
| 29  | DE    | 136 | GLN  |
| 29  | DE    | 163 | ASN  |
| 29  | DE    | 195 | GLN  |
| 30  | DY    | 33  | HIS  |
| 30  | DY    | 48  | ASN  |
| 32  | D4    | 35  | GLN  |
| 32  | D4    | 37  | GLN  |
| 34  | D3    | 30  | HIS  |
| 34  | D3    | 42  | HIS  |
| 35  | DV    | 44  | HIS  |
| 35  | DV    | 49  | ASN  |
| 35  | DV    | 80  | HIS  |
| 36  | D2    | 6   | GLN  |
| 36  | D2    | 13  | ASN  |
| 37  | DL    | 4   | ASN  |
| 37  | DL    | 54  | GLN  |
| 37  | DL    | 93  | ASN  |
| 37  | DL    | 104 | GLN  |
| 38  | DM    | 17  | ASN  |
| 39  | DX    | 20  | ASN  |
| 39  | DX    | 25  | GLN  |
| 39  | DX    | 41  | HIS  |
| 40  | DH    | 28  | ASN  |
| 40  | DH    | 66  | ASN  |
| 40  | DH    | 133 | GLN  |
| 40  | DH    | 135 | HIS  |
| 41  | DJ    | 130 | HIS  |
| 41  | DJ    | 136 | GLN  |
| 41  | DJ    | 138 | GLN  |
| 42  | DN    | 11  | ASN  |
| 42  | DN    | 16  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DN    | 107 | ASN  |
| 43  | DO    | 19  | GLN  |
| 43  | DO    | 29  | HIS  |
| 43  | DO    | 38  | GLN  |
| 43  | DO    | 61  | GLN  |
| 44  | DQ    | 19  | GLN  |
| 44  | DQ    | 51  | GLN  |
| 44  | DQ    | 58  | GLN  |
| 44  | DQ    | 71  | ASN  |
| 44  | DQ    | 80  | ASN  |
| 46  | DU    | 26  | ASN  |
| 46  | DU    | 45  | GLN  |
| 46  | DU    | 52  | ASN  |
| 46  | DU    | 65  | GLN  |
| 46  | DU    | 73  | ASN  |
| 47  | DF    | 51  | ASN  |
| 47  | DF    | 134 | GLN  |
| 48  | DG    | 29  | ASN  |
| 48  | DG    | 63  | GLN  |
| 48  | DG    | 72  | ASN  |
| 48  | DG    | 87  | GLN  |
| 49  | DR    | 6   | GLN  |
| 49  | DR    | 11  | GLN  |
| 49  | DR    | 43  | ASN  |
| 49  | DR    | 86  | GLN  |
| 49  | DR    | 87  | GLN  |
| 50  | DT    | 48  | GLN  |
| 50  | DT    | 72  | GLN  |
| 50  | DT    | 91  | GLN  |
| 50  | DT    | 92  | ASN  |
| 51  | DZ    | 6   | GLN  |
| 51  | DZ    | 17  | ASN  |
| 51  | DZ    | 36  | HIS  |
| 52  | DW    | 39  | GLN  |
| 52  | DW    | 49  | ASN  |
| 52  | DW    | 75  | ASN  |
| 53  | D6    | 53  | ASN  |
| 53  | D6    | 54  | GLN  |
| 53  | D6    | 74  | ASN  |
| 53  | D6    | 174 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1529/1542 (99%) | 246 (16%)         | 16 (1%)         |
| 1   | CA    | 1529/1542 (99%) | 244 (15%)         | 16 (1%)         |
| 22  | BA    | 116/120 (96%)   | 18 (15%)          | 0               |
| 22  | DA    | 116/120 (96%)   | 18 (15%)          | 0               |
| 23  | BB    | 2837/2904 (97%) | 446 (15%)         | 14 (0%)         |
| 23  | DB    | 2837/2904 (97%) | 447 (15%)         | 16 (0%)         |
| All | All   | 8964/9132 (98%) | 1419 (15%)        | 62 (0%)         |

All (1419) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 7   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 14  | U    |
| 1   | AA    | 31  | G    |
| 1   | AA    | 32  | A    |
| 1   | AA    | 39  | G    |
| 1   | AA    | 47  | C    |
| 1   | AA    | 48  | C    |
| 1   | AA    | 51  | A    |
| 1   | AA    | 52  | C    |
| 1   | AA    | 55  | A    |
| 1   | AA    | 65  | A    |
| 1   | AA    | 71  | A    |
| 1   | AA    | 72  | A    |
| 1   | AA    | 79  | G    |
| 1   | AA    | 83  | C    |
| 1   | AA    | 84  | U    |
| 1   | AA    | 85  | U    |
| 1   | AA    | 86  | G    |
| 1   | AA    | 88  | U    |
| 1   | AA    | 89  | U    |
| 1   | AA    | 91  | U    |
| 1   | AA    | 93  | U    |
| 1   | AA    | 94  | G    |
| 1   | AA    | 95  | C    |
| 1   | AA    | 96  | U    |
| 1   | AA    | 119 | A    |
| 1   | AA    | 121 | U    |
| 1   | AA    | 131 | A    |
| 1   | AA    | 151 | A    |
| 1   | AA    | 182 | A    |
| 1   | AA    | 183 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 191 | G    |
| 1   | AA    | 197 | A    |
| 1   | AA    | 202 | G    |
| 1   | AA    | 209 | U    |
| 1   | AA    | 210 | C    |
| 1   | AA    | 211 | G    |
| 1   | AA    | 213 | G    |
| 1   | AA    | 239 | U    |
| 1   | AA    | 240 | G    |
| 1   | AA    | 243 | A    |
| 1   | AA    | 244 | U    |
| 1   | AA    | 245 | U    |
| 1   | AA    | 247 | G    |
| 1   | AA    | 250 | A    |
| 1   | AA    | 251 | G    |
| 1   | AA    | 253 | A    |
| 1   | AA    | 257 | G    |
| 1   | AA    | 258 | G    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 267 | C    |
| 1   | AA    | 280 | C    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 301 | G    |
| 1   | AA    | 316 | C    |
| 1   | AA    | 321 | A    |
| 1   | AA    | 328 | C    |
| 1   | AA    | 329 | A    |
| 1   | AA    | 330 | C    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 345 | C    |
| 1   | AA    | 346 | G    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 353 | A    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 372 | C    |
| 1   | AA    | 373 | A    |
| 1   | AA    | 381 | C    |
| 1   | AA    | 382 | A    |
| 1   | AA    | 384 | G    |
| 1   | AA    | 397 | A    |
| 1   | AA    | 398 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 406 | G    |
| 1   | AA    | 408 | A    |
| 1   | AA    | 409 | U    |
| 1   | AA    | 411 | A    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 421 | U    |
| 1   | AA    | 422 | C    |
| 1   | AA    | 423 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | A    |
| 1   | AA    | 438 | U    |
| 1   | AA    | 461 | A    |
| 1   | AA    | 462 | G    |
| 1   | AA    | 463 | U    |
| 1   | AA    | 464 | U    |
| 1   | AA    | 465 | A    |
| 1   | AA    | 466 | A    |
| 1   | AA    | 467 | U    |
| 1   | AA    | 468 | A    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | U    |
| 1   | AA    | 486 | U    |
| 1   | AA    | 493 | A    |
| 1   | AA    | 500 | G    |
| 1   | AA    | 511 | C    |
| 1   | AA    | 518 | C    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 532 | A    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 562 | U    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 576 | C    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 607 | A    |
| 1   | AA    | 633 | G    |
| 1   | AA    | 653 | U    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 687 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 695 | A    |
| 1   | AA    | 700 | G    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 724 | G    |
| 1   | AA    | 731 | G    |
| 1   | AA    | 747 | A    |
| 1   | AA    | 748 | G    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 777 | A    |
| 1   | AA    | 781 | A    |
| 1   | AA    | 782 | A    |
| 1   | AA    | 793 | U    |
| 1   | AA    | 794 | A    |
| 1   | AA    | 812 | G    |
| 1   | AA    | 813 | U    |
| 1   | AA    | 814 | A    |
| 1   | AA    | 815 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 819 | A    |
| 1   | AA    | 821 | G    |
| 1   | AA    | 828 | U    |
| 1   | AA    | 829 | G    |
| 1   | AA    | 841 | C    |
| 1   | AA    | 843 | U    |
| 1   | AA    | 844 | G    |
| 1   | AA    | 845 | A    |
| 1   | AA    | 907 | A    |
| 1   | AA    | 926 | G    |
| 1   | AA    | 927 | G    |
| 1   | AA    | 934 | C    |
| 1   | AA    | 935 | A    |
| 1   | AA    | 960 | U    |
| 1   | AA    | 961 | U    |
| 1   | AA    | 969 | A    |
| 1   | AA    | 971 | G    |
| 1   | AA    | 974 | A    |
| 1   | AA    | 976 | G    |
| 1   | AA    | 977 | A    |
| 1   | AA    | 991 | U    |
| 1   | AA    | 992 | U    |
| 1   | AA    | 993 | G    |
| 1   | AA    | 994 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1004 | A    |
| 1   | AA    | 1009 | U    |
| 1   | AA    | 1010 | U    |
| 1   | AA    | 1020 | G    |
| 1   | AA    | 1022 | A    |
| 1   | AA    | 1028 | C    |
| 1   | AA    | 1029 | U    |
| 1   | AA    | 1030 | U    |
| 1   | AA    | 1031 | C    |
| 1   | AA    | 1034 | G    |
| 1   | AA    | 1035 | A    |
| 1   | AA    | 1037 | C    |
| 1   | AA    | 1038 | C    |
| 1   | AA    | 1049 | U    |
| 1   | AA    | 1050 | G    |
| 1   | AA    | 1054 | C    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1066 | C    |
| 1   | AA    | 1081 | A    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1095 | U    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1136 | C    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1138 | G    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1158 | C    |
| 1   | AA    | 1168 | U    |
| 1   | AA    | 1171 | A    |
| 1   | AA    | 1181 | G    |
| 1   | AA    | 1183 | U    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1196 | A    |
| 1   | AA    | 1197 | A    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1202 | U    |
| 1   | AA    | 1209 | C    |
| 1   | AA    | 1211 | U    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1213 | A    |
| 1   | AA    | 1214 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1215 | G    |
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1240 | U    |
| 1   | AA    | 1250 | A    |
| 1   | AA    | 1256 | A    |
| 1   | AA    | 1279 | G    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1281 | C    |
| 1   | AA    | 1285 | A    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1301 | U    |
| 1   | AA    | 1302 | C    |
| 1   | AA    | 1303 | C    |
| 1   | AA    | 1305 | G    |
| 1   | AA    | 1316 | G    |
| 1   | AA    | 1317 | C    |
| 1   | AA    | 1319 | A    |
| 1   | AA    | 1320 | C    |
| 1   | AA    | 1323 | G    |
| 1   | AA    | 1336 | C    |
| 1   | AA    | 1363 | A    |
| 1   | AA    | 1364 | U    |
| 1   | AA    | 1381 | U    |
| 1   | AA    | 1398 | A    |
| 1   | AA    | 1409 | C    |
| 1   | AA    | 1410 | A    |
| 1   | AA    | 1432 | G    |
| 1   | AA    | 1446 | A    |
| 1   | AA    | 1448 | C    |
| 1   | AA    | 1451 | U    |
| 1   | AA    | 1452 | C    |
| 1   | AA    | 1453 | G    |
| 1   | AA    | 1491 | G    |
| 1   | AA    | 1492 | A    |
| 1   | AA    | 1497 | G    |
| 1   | AA    | 1503 | A    |
| 1   | AA    | 1506 | U    |
| 1   | AA    | 1517 | G    |
| 1   | AA    | 1519 | A    |
| 1   | AA    | 1520 | C    |
| 1   | AA    | 1529 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1530 | G    |
| 1   | AA    | 1532 | U    |
| 1   | AA    | 1533 | C    |
| 1   | AA    | 1534 | A    |
| 22  | BA    | 16   | G    |
| 22  | BA    | 24   | G    |
| 22  | BA    | 25   | U    |
| 22  | BA    | 26   | C    |
| 22  | BA    | 30   | C    |
| 22  | BA    | 35   | C    |
| 22  | BA    | 42   | C    |
| 22  | BA    | 43   | C    |
| 22  | BA    | 44   | G    |
| 22  | BA    | 53   | A    |
| 22  | BA    | 88   | C    |
| 22  | BA    | 89   | U    |
| 22  | BA    | 90   | C    |
| 22  | BA    | 96   | G    |
| 22  | BA    | 99   | A    |
| 22  | BA    | 109  | A    |
| 22  | BA    | 112  | G    |
| 22  | BA    | 116  | G    |
| 23  | BB    | 2    | G    |
| 23  | BB    | 4    | U    |
| 23  | BB    | 34   | U    |
| 23  | BB    | 46   | G    |
| 23  | BB    | 51   | G    |
| 23  | BB    | 63   | A    |
| 23  | BB    | 71   | A    |
| 23  | BB    | 72   | U    |
| 23  | BB    | 74   | A    |
| 23  | BB    | 75   | G    |
| 23  | BB    | 79   | C    |
| 23  | BB    | 91   | A    |
| 23  | BB    | 99   | U    |
| 23  | BB    | 101  | A    |
| 23  | BB    | 102  | U    |
| 23  | BB    | 103  | A    |
| 23  | BB    | 118  | A    |
| 23  | BB    | 119  | A    |
| 23  | BB    | 120  | U    |
| 23  | BB    | 125  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BB    | 126 | A    |
| 23  | BB    | 128 | C    |
| 23  | BB    | 140 | C    |
| 23  | BB    | 141 | G    |
| 23  | BB    | 142 | A    |
| 23  | BB    | 144 | A    |
| 23  | BB    | 149 | A    |
| 23  | BB    | 160 | A    |
| 23  | BB    | 162 | U    |
| 23  | BB    | 163 | C    |
| 23  | BB    | 180 | G    |
| 23  | BB    | 181 | A    |
| 23  | BB    | 196 | A    |
| 23  | BB    | 199 | A    |
| 23  | BB    | 203 | A    |
| 23  | BB    | 215 | G    |
| 23  | BB    | 216 | A    |
| 23  | BB    | 221 | A    |
| 23  | BB    | 222 | A    |
| 23  | BB    | 230 | G    |
| 23  | BB    | 233 | A    |
| 23  | BB    | 248 | G    |
| 23  | BB    | 250 | G    |
| 23  | BB    | 255 | A    |
| 23  | BB    | 265 | A    |
| 23  | BB    | 266 | G    |
| 23  | BB    | 267 | C    |
| 23  | BB    | 271 | G    |
| 23  | BB    | 278 | A    |
| 23  | BB    | 279 | A    |
| 23  | BB    | 281 | C    |
| 23  | BB    | 299 | A    |
| 23  | BB    | 302 | C    |
| 23  | BB    | 311 | A    |
| 23  | BB    | 323 | C    |
| 23  | BB    | 329 | G    |
| 23  | BB    | 330 | A    |
| 23  | BB    | 333 | G    |
| 23  | BB    | 346 | A    |
| 23  | BB    | 349 | U    |
| 23  | BB    | 353 | C    |
| 23  | BB    | 369 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BB    | 371 | A    |
| 23  | BB    | 372 | G    |
| 23  | BB    | 386 | G    |
| 23  | BB    | 387 | U    |
| 23  | BB    | 395 | U    |
| 23  | BB    | 396 | G    |
| 23  | BB    | 405 | U    |
| 23  | BB    | 411 | G    |
| 23  | BB    | 412 | A    |
| 23  | BB    | 424 | G    |
| 23  | BB    | 435 | C    |
| 23  | BB    | 455 | C    |
| 23  | BB    | 456 | C    |
| 23  | BB    | 457 | A    |
| 23  | BB    | 479 | A    |
| 23  | BB    | 480 | A    |
| 23  | BB    | 481 | G    |
| 23  | BB    | 491 | G    |
| 23  | BB    | 504 | A    |
| 23  | BB    | 505 | A    |
| 23  | BB    | 508 | A    |
| 23  | BB    | 509 | C    |
| 23  | BB    | 510 | C    |
| 23  | BB    | 512 | G    |
| 23  | BB    | 527 | C    |
| 23  | BB    | 531 | C    |
| 23  | BB    | 532 | A    |
| 23  | BB    | 546 | U    |
| 23  | BB    | 547 | A    |
| 23  | BB    | 548 | G    |
| 23  | BB    | 549 | G    |
| 23  | BB    | 550 | C    |
| 23  | BB    | 563 | A    |
| 23  | BB    | 572 | A    |
| 23  | BB    | 573 | U    |
| 23  | BB    | 574 | A    |
| 23  | BB    | 575 | A    |
| 23  | BB    | 603 | A    |
| 23  | BB    | 613 | A    |
| 23  | BB    | 614 | A    |
| 23  | BB    | 615 | U    |
| 23  | BB    | 616 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BB    | 627 | A    |
| 23  | BB    | 632 | A    |
| 23  | BB    | 637 | A    |
| 23  | BB    | 645 | C    |
| 23  | BB    | 646 | U    |
| 23  | BB    | 647 | G    |
| 23  | BB    | 654 | A    |
| 23  | BB    | 655 | A    |
| 23  | BB    | 671 | C    |
| 23  | BB    | 686 | U    |
| 23  | BB    | 718 | A    |
| 23  | BB    | 719 | C    |
| 23  | BB    | 730 | A    |
| 23  | BB    | 746 | U    |
| 23  | BB    | 747 | U    |
| 23  | BB    | 764 | A    |
| 23  | BB    | 775 | G    |
| 23  | BB    | 782 | A    |
| 23  | BB    | 784 | G    |
| 23  | BB    | 785 | G    |
| 23  | BB    | 789 | A    |
| 23  | BB    | 805 | G    |
| 23  | BB    | 812 | C    |
| 23  | BB    | 819 | A    |
| 23  | BB    | 827 | U    |
| 23  | BB    | 828 | U    |
| 23  | BB    | 847 | U    |
| 23  | BB    | 859 | G    |
| 23  | BB    | 876 | C    |
| 23  | BB    | 877 | A    |
| 23  | BB    | 899 | A    |
| 23  | BB    | 910 | A    |
| 23  | BB    | 912 | C    |
| 23  | BB    | 932 | U    |
| 23  | BB    | 933 | A    |
| 23  | BB    | 941 | A    |
| 23  | BB    | 946 | C    |
| 23  | BB    | 961 | C    |
| 23  | BB    | 962 | G    |
| 23  | BB    | 973 | A    |
| 23  | BB    | 974 | G    |
| 23  | BB    | 983 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 990  | A    |
| 23  | BB    | 991  | C    |
| 23  | BB    | 995  | C    |
| 23  | BB    | 996  | A    |
| 23  | BB    | 1012 | U    |
| 23  | BB    | 1013 | C    |
| 23  | BB    | 1022 | G    |
| 23  | BB    | 1023 | U    |
| 23  | BB    | 1024 | G    |
| 23  | BB    | 1025 | G    |
| 23  | BB    | 1033 | U    |
| 23  | BB    | 1043 | C    |
| 23  | BB    | 1047 | G    |
| 23  | BB    | 1051 | G    |
| 23  | BB    | 1062 | G    |
| 23  | BB    | 1070 | A    |
| 23  | BB    | 1088 | A    |
| 23  | BB    | 1090 | A    |
| 23  | BB    | 1106 | G    |
| 23  | BB    | 1110 | G    |
| 23  | BB    | 1111 | A    |
| 23  | BB    | 1112 | G    |
| 23  | BB    | 1126 | A    |
| 23  | BB    | 1129 | A    |
| 23  | BB    | 1132 | U    |
| 23  | BB    | 1133 | A    |
| 23  | BB    | 1135 | C    |
| 23  | BB    | 1136 | G    |
| 23  | BB    | 1141 | U    |
| 23  | BB    | 1142 | A    |
| 23  | BB    | 1157 | G    |
| 23  | BB    | 1171 | G    |
| 23  | BB    | 1172 | C    |
| 23  | BB    | 1173 | U    |
| 23  | BB    | 1174 | U    |
| 23  | BB    | 1186 | G    |
| 23  | BB    | 1195 | G    |
| 23  | BB    | 1204 | A    |
| 23  | BB    | 1205 | A    |
| 23  | BB    | 1211 | C    |
| 23  | BB    | 1212 | G    |
| 23  | BB    | 1237 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 1238 | G    |
| 23  | BB    | 1247 | A    |
| 23  | BB    | 1248 | G    |
| 23  | BB    | 1250 | G    |
| 23  | BB    | 1251 | C    |
| 23  | BB    | 1253 | A    |
| 23  | BB    | 1256 | G    |
| 23  | BB    | 1266 | G    |
| 23  | BB    | 1271 | G    |
| 23  | BB    | 1272 | A    |
| 23  | BB    | 1273 | U    |
| 23  | BB    | 1275 | A    |
| 23  | BB    | 1276 | A    |
| 23  | BB    | 1301 | A    |
| 23  | BB    | 1302 | A    |
| 23  | BB    | 1321 | A    |
| 23  | BB    | 1324 | G    |
| 23  | BB    | 1325 | U    |
| 23  | BB    | 1330 | C    |
| 23  | BB    | 1337 | G    |
| 23  | BB    | 1341 | G    |
| 23  | BB    | 1345 | C    |
| 23  | BB    | 1365 | A    |
| 23  | BB    | 1368 | G    |
| 23  | BB    | 1378 | A    |
| 23  | BB    | 1379 | U    |
| 23  | BB    | 1383 | A    |
| 23  | BB    | 1384 | A    |
| 23  | BB    | 1386 | C    |
| 23  | BB    | 1396 | U    |
| 23  | BB    | 1397 | U    |
| 23  | BB    | 1416 | G    |
| 23  | BB    | 1419 | A    |
| 23  | BB    | 1427 | A    |
| 23  | BB    | 1428 | C    |
| 23  | BB    | 1451 | C    |
| 23  | BB    | 1453 | A    |
| 23  | BB    | 1454 | C    |
| 23  | BB    | 1455 | G    |
| 23  | BB    | 1459 | G    |
| 23  | BB    | 1460 | U    |
| 23  | BB    | 1461 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 1476 | U    |
| 23  | BB    | 1477 | A    |
| 23  | BB    | 1482 | G    |
| 23  | BB    | 1486 | U    |
| 23  | BB    | 1490 | A    |
| 23  | BB    | 1493 | C    |
| 23  | BB    | 1494 | A    |
| 23  | BB    | 1504 | A    |
| 23  | BB    | 1505 | A    |
| 23  | BB    | 1507 | C    |
| 23  | BB    | 1508 | A    |
| 23  | BB    | 1509 | A    |
| 23  | BB    | 1510 | G    |
| 23  | BB    | 1524 | G    |
| 23  | BB    | 1532 | A    |
| 23  | BB    | 1535 | A    |
| 23  | BB    | 1537 | G    |
| 23  | BB    | 1538 | G    |
| 23  | BB    | 1540 | G    |
| 23  | BB    | 1552 | A    |
| 23  | BB    | 1559 | U    |
| 23  | BB    | 1569 | A    |
| 23  | BB    | 1578 | U    |
| 23  | BB    | 1584 | U    |
| 23  | BB    | 1585 | C    |
| 23  | BB    | 1588 | G    |
| 23  | BB    | 1607 | C    |
| 23  | BB    | 1608 | A    |
| 23  | BB    | 1610 | A    |
| 23  | BB    | 1616 | A    |
| 23  | BB    | 1634 | A    |
| 23  | BB    | 1635 | A    |
| 23  | BB    | 1647 | U    |
| 23  | BB    | 1648 | U    |
| 23  | BB    | 1674 | G    |
| 23  | BB    | 1700 | A    |
| 23  | BB    | 1701 | A    |
| 23  | BB    | 1706 | C    |
| 23  | BB    | 1713 | A    |
| 23  | BB    | 1715 | G    |
| 23  | BB    | 1724 | G    |
| 23  | BB    | 1725 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 1727 | C    |
| 23  | BB    | 1729 | U    |
| 23  | BB    | 1730 | C    |
| 23  | BB    | 1732 | C    |
| 23  | BB    | 1733 | G    |
| 23  | BB    | 1738 | G    |
| 23  | BB    | 1758 | U    |
| 23  | BB    | 1764 | C    |
| 23  | BB    | 1773 | A    |
| 23  | BB    | 1800 | C    |
| 23  | BB    | 1816 | C    |
| 23  | BB    | 1829 | A    |
| 23  | BB    | 1833 | C    |
| 23  | BB    | 1870 | C    |
| 23  | BB    | 1872 | A    |
| 23  | BB    | 1884 | G    |
| 23  | BB    | 1906 | G    |
| 23  | BB    | 1927 | A    |
| 23  | BB    | 1929 | G    |
| 23  | BB    | 1930 | G    |
| 23  | BB    | 1936 | A    |
| 23  | BB    | 1937 | A    |
| 23  | BB    | 1938 | A    |
| 23  | BB    | 1939 | U    |
| 23  | BB    | 1940 | U    |
| 23  | BB    | 1955 | U    |
| 23  | BB    | 1967 | C    |
| 23  | BB    | 1970 | A    |
| 23  | BB    | 1971 | U    |
| 23  | BB    | 1972 | G    |
| 23  | BB    | 1991 | U    |
| 23  | BB    | 1993 | U    |
| 23  | BB    | 1997 | C    |
| 23  | BB    | 2022 | U    |
| 23  | BB    | 2023 | C    |
| 23  | BB    | 2030 | A    |
| 23  | BB    | 2031 | A    |
| 23  | BB    | 2032 | G    |
| 23  | BB    | 2033 | A    |
| 23  | BB    | 2043 | C    |
| 23  | BB    | 2055 | C    |
| 23  | BB    | 2056 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 2060 | A    |
| 23  | BB    | 2061 | G    |
| 23  | BB    | 2062 | A    |
| 23  | BB    | 2069 | G    |
| 23  | BB    | 2072 | C    |
| 23  | BB    | 2096 | C    |
| 23  | BB    | 2102 | G    |
| 23  | BB    | 2103 | C    |
| 23  | BB    | 2109 | U    |
| 23  | BB    | 2137 | U    |
| 23  | BB    | 2138 | G    |
| 23  | BB    | 2143 | C    |
| 23  | BB    | 2144 | G    |
| 23  | BB    | 2145 | C    |
| 23  | BB    | 2147 | A    |
| 23  | BB    | 2148 | G    |
| 23  | BB    | 2149 | U    |
| 23  | BB    | 2151 | U    |
| 23  | BB    | 2153 | C    |
| 23  | BB    | 2154 | A    |
| 23  | BB    | 2155 | U    |
| 23  | BB    | 2157 | G    |
| 23  | BB    | 2181 | U    |
| 23  | BB    | 2183 | A    |
| 23  | BB    | 2184 | A    |
| 23  | BB    | 2192 | U    |
| 23  | BB    | 2198 | A    |
| 23  | BB    | 2199 | A    |
| 23  | BB    | 2203 | U    |
| 23  | BB    | 2204 | G    |
| 23  | BB    | 2211 | A    |
| 23  | BB    | 2212 | A    |
| 23  | BB    | 2213 | U    |
| 23  | BB    | 2225 | A    |
| 23  | BB    | 2238 | G    |
| 23  | BB    | 2239 | G    |
| 23  | BB    | 2250 | G    |
| 23  | BB    | 2266 | A    |
| 23  | BB    | 2283 | C    |
| 23  | BB    | 2287 | A    |
| 23  | BB    | 2288 | A    |
| 23  | BB    | 2305 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 2307 | G    |
| 23  | BB    | 2308 | G    |
| 23  | BB    | 2309 | A    |
| 23  | BB    | 2311 | A    |
| 23  | BB    | 2320 | U    |
| 23  | BB    | 2321 | U    |
| 23  | BB    | 2322 | A    |
| 23  | BB    | 2325 | G    |
| 23  | BB    | 2333 | A    |
| 23  | BB    | 2337 | G    |
| 23  | BB    | 2345 | G    |
| 23  | BB    | 2347 | C    |
| 23  | BB    | 2361 | G    |
| 23  | BB    | 2372 | U    |
| 23  | BB    | 2379 | G    |
| 23  | BB    | 2383 | G    |
| 23  | BB    | 2385 | C    |
| 23  | BB    | 2396 | G    |
| 23  | BB    | 2402 | U    |
| 23  | BB    | 2403 | C    |
| 23  | BB    | 2406 | A    |
| 23  | BB    | 2423 | U    |
| 23  | BB    | 2425 | A    |
| 23  | BB    | 2426 | A    |
| 23  | BB    | 2427 | C    |
| 23  | BB    | 2429 | G    |
| 23  | BB    | 2430 | A    |
| 23  | BB    | 2431 | U    |
| 23  | BB    | 2441 | U    |
| 23  | BB    | 2448 | A    |
| 23  | BB    | 2449 | U    |
| 23  | BB    | 2472 | G    |
| 23  | BB    | 2476 | A    |
| 23  | BB    | 2491 | U    |
| 23  | BB    | 2502 | G    |
| 23  | BB    | 2505 | G    |
| 23  | BB    | 2506 | U    |
| 23  | BB    | 2518 | A    |
| 23  | BB    | 2535 | G    |
| 23  | BB    | 2554 | U    |
| 23  | BB    | 2555 | U    |
| 23  | BB    | 2556 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 2566 | A    |
| 23  | BB    | 2567 | G    |
| 23  | BB    | 2572 | A    |
| 23  | BB    | 2582 | G    |
| 23  | BB    | 2586 | U    |
| 23  | BB    | 2602 | A    |
| 23  | BB    | 2609 | U    |
| 23  | BB    | 2611 | C    |
| 23  | BB    | 2613 | U    |
| 23  | BB    | 2629 | U    |
| 23  | BB    | 2630 | G    |
| 23  | BB    | 2634 | A    |
| 23  | BB    | 2646 | C    |
| 23  | BB    | 2654 | A    |
| 23  | BB    | 2682 | A    |
| 23  | BB    | 2689 | U    |
| 23  | BB    | 2690 | U    |
| 23  | BB    | 2714 | G    |
| 23  | BB    | 2739 | U    |
| 23  | BB    | 2744 | G    |
| 23  | BB    | 2748 | A    |
| 23  | BB    | 2750 | A    |
| 23  | BB    | 2751 | G    |
| 23  | BB    | 2752 | C    |
| 23  | BB    | 2753 | A    |
| 23  | BB    | 2757 | A    |
| 23  | BB    | 2765 | A    |
| 23  | BB    | 2778 | A    |
| 23  | BB    | 2791 | G    |
| 23  | BB    | 2798 | U    |
| 23  | BB    | 2799 | A    |
| 23  | BB    | 2800 | A    |
| 23  | BB    | 2802 | G    |
| 23  | BB    | 2808 | G    |
| 23  | BB    | 2820 | A    |
| 23  | BB    | 2821 | A    |
| 23  | BB    | 2823 | A    |
| 23  | BB    | 2831 | G    |
| 23  | BB    | 2836 | U    |
| 23  | BB    | 2850 | A    |
| 23  | BB    | 2866 | U    |
| 23  | BB    | 2867 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | BB    | 2872 | A    |
| 23  | BB    | 2873 | A    |
| 23  | BB    | 2883 | A    |
| 23  | BB    | 2894 | G    |
| 23  | BB    | 2901 | C    |
| 23  | BB    | 2903 | U    |
| 1   | CA    | 7    | A    |
| 1   | CA    | 9    | G    |
| 1   | CA    | 14   | U    |
| 1   | CA    | 31   | G    |
| 1   | CA    | 32   | A    |
| 1   | CA    | 39   | G    |
| 1   | CA    | 47   | C    |
| 1   | CA    | 48   | C    |
| 1   | CA    | 49   | U    |
| 1   | CA    | 51   | A    |
| 1   | CA    | 52   | C    |
| 1   | CA    | 55   | A    |
| 1   | CA    | 71   | A    |
| 1   | CA    | 72   | A    |
| 1   | CA    | 84   | U    |
| 1   | CA    | 85   | U    |
| 1   | CA    | 86   | G    |
| 1   | CA    | 87   | C    |
| 1   | CA    | 88   | U    |
| 1   | CA    | 93   | U    |
| 1   | CA    | 94   | G    |
| 1   | CA    | 119  | A    |
| 1   | CA    | 121  | U    |
| 1   | CA    | 131  | A    |
| 1   | CA    | 151  | A    |
| 1   | CA    | 182  | A    |
| 1   | CA    | 183  | C    |
| 1   | CA    | 191  | G    |
| 1   | CA    | 197  | A    |
| 1   | CA    | 202  | G    |
| 1   | CA    | 209  | U    |
| 1   | CA    | 210  | C    |
| 1   | CA    | 211  | G    |
| 1   | CA    | 213  | G    |
| 1   | CA    | 239  | U    |
| 1   | CA    | 240  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 243 | A    |
| 1   | CA    | 244 | U    |
| 1   | CA    | 245 | U    |
| 1   | CA    | 247 | G    |
| 1   | CA    | 250 | A    |
| 1   | CA    | 251 | G    |
| 1   | CA    | 253 | A    |
| 1   | CA    | 257 | G    |
| 1   | CA    | 258 | G    |
| 1   | CA    | 266 | G    |
| 1   | CA    | 267 | C    |
| 1   | CA    | 280 | C    |
| 1   | CA    | 289 | G    |
| 1   | CA    | 301 | G    |
| 1   | CA    | 316 | C    |
| 1   | CA    | 321 | A    |
| 1   | CA    | 328 | C    |
| 1   | CA    | 329 | A    |
| 1   | CA    | 330 | C    |
| 1   | CA    | 332 | G    |
| 1   | CA    | 345 | C    |
| 1   | CA    | 346 | G    |
| 1   | CA    | 352 | C    |
| 1   | CA    | 353 | A    |
| 1   | CA    | 354 | G    |
| 1   | CA    | 367 | U    |
| 1   | CA    | 372 | C    |
| 1   | CA    | 373 | A    |
| 1   | CA    | 381 | C    |
| 1   | CA    | 382 | A    |
| 1   | CA    | 384 | G    |
| 1   | CA    | 397 | A    |
| 1   | CA    | 398 | U    |
| 1   | CA    | 406 | G    |
| 1   | CA    | 408 | A    |
| 1   | CA    | 409 | U    |
| 1   | CA    | 411 | A    |
| 1   | CA    | 412 | A    |
| 1   | CA    | 413 | G    |
| 1   | CA    | 421 | U    |
| 1   | CA    | 422 | C    |
| 1   | CA    | 423 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 429 | U    |
| 1   | CA    | 430 | A    |
| 1   | CA    | 435 | A    |
| 1   | CA    | 438 | U    |
| 1   | CA    | 461 | A    |
| 1   | CA    | 462 | G    |
| 1   | CA    | 463 | U    |
| 1   | CA    | 464 | U    |
| 1   | CA    | 465 | A    |
| 1   | CA    | 466 | A    |
| 1   | CA    | 467 | U    |
| 1   | CA    | 468 | A    |
| 1   | CA    | 482 | A    |
| 1   | CA    | 484 | G    |
| 1   | CA    | 485 | U    |
| 1   | CA    | 486 | U    |
| 1   | CA    | 493 | A    |
| 1   | CA    | 500 | G    |
| 1   | CA    | 509 | A    |
| 1   | CA    | 511 | C    |
| 1   | CA    | 518 | C    |
| 1   | CA    | 527 | G    |
| 1   | CA    | 532 | A    |
| 1   | CA    | 547 | A    |
| 1   | CA    | 559 | A    |
| 1   | CA    | 562 | U    |
| 1   | CA    | 572 | A    |
| 1   | CA    | 573 | A    |
| 1   | CA    | 576 | C    |
| 1   | CA    | 577 | G    |
| 1   | CA    | 607 | A    |
| 1   | CA    | 633 | G    |
| 1   | CA    | 653 | U    |
| 1   | CA    | 665 | A    |
| 1   | CA    | 687 | A    |
| 1   | CA    | 695 | A    |
| 1   | CA    | 700 | G    |
| 1   | CA    | 721 | G    |
| 1   | CA    | 724 | G    |
| 1   | CA    | 731 | G    |
| 1   | CA    | 747 | A    |
| 1   | CA    | 748 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 755  | G    |
| 1   | CA    | 777  | A    |
| 1   | CA    | 781  | A    |
| 1   | CA    | 782  | A    |
| 1   | CA    | 793  | U    |
| 1   | CA    | 794  | A    |
| 1   | CA    | 812  | G    |
| 1   | CA    | 813  | U    |
| 1   | CA    | 814  | A    |
| 1   | CA    | 815  | A    |
| 1   | CA    | 817  | C    |
| 1   | CA    | 819  | A    |
| 1   | CA    | 821  | G    |
| 1   | CA    | 828  | U    |
| 1   | CA    | 829  | G    |
| 1   | CA    | 841  | C    |
| 1   | CA    | 843  | U    |
| 1   | CA    | 844  | G    |
| 1   | CA    | 845  | A    |
| 1   | CA    | 907  | A    |
| 1   | CA    | 926  | G    |
| 1   | CA    | 927  | G    |
| 1   | CA    | 934  | C    |
| 1   | CA    | 935  | A    |
| 1   | CA    | 960  | U    |
| 1   | CA    | 961  | U    |
| 1   | CA    | 969  | A    |
| 1   | CA    | 971  | G    |
| 1   | CA    | 974  | A    |
| 1   | CA    | 976  | G    |
| 1   | CA    | 977  | A    |
| 1   | CA    | 991  | U    |
| 1   | CA    | 992  | U    |
| 1   | CA    | 993  | G    |
| 1   | CA    | 994  | A    |
| 1   | CA    | 1004 | A    |
| 1   | CA    | 1009 | U    |
| 1   | CA    | 1010 | U    |
| 1   | CA    | 1020 | G    |
| 1   | CA    | 1022 | A    |
| 1   | CA    | 1028 | C    |
| 1   | CA    | 1029 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1030 | U    |
| 1   | CA    | 1031 | C    |
| 1   | CA    | 1034 | G    |
| 1   | CA    | 1035 | A    |
| 1   | CA    | 1037 | C    |
| 1   | CA    | 1038 | C    |
| 1   | CA    | 1049 | U    |
| 1   | CA    | 1050 | G    |
| 1   | CA    | 1054 | C    |
| 1   | CA    | 1065 | U    |
| 1   | CA    | 1066 | C    |
| 1   | CA    | 1081 | A    |
| 1   | CA    | 1091 | U    |
| 1   | CA    | 1094 | G    |
| 1   | CA    | 1095 | U    |
| 1   | CA    | 1101 | A    |
| 1   | CA    | 1136 | C    |
| 1   | CA    | 1137 | C    |
| 1   | CA    | 1138 | G    |
| 1   | CA    | 1139 | G    |
| 1   | CA    | 1140 | C    |
| 1   | CA    | 1158 | C    |
| 1   | CA    | 1160 | G    |
| 1   | CA    | 1168 | U    |
| 1   | CA    | 1171 | A    |
| 1   | CA    | 1181 | G    |
| 1   | CA    | 1183 | U    |
| 1   | CA    | 1184 | G    |
| 1   | CA    | 1196 | A    |
| 1   | CA    | 1197 | A    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1202 | U    |
| 1   | CA    | 1209 | C    |
| 1   | CA    | 1211 | U    |
| 1   | CA    | 1212 | U    |
| 1   | CA    | 1213 | A    |
| 1   | CA    | 1214 | C    |
| 1   | CA    | 1215 | G    |
| 1   | CA    | 1225 | A    |
| 1   | CA    | 1226 | C    |
| 1   | CA    | 1240 | U    |
| 1   | CA    | 1241 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1250 | A    |
| 1   | CA    | 1256 | A    |
| 1   | CA    | 1279 | G    |
| 1   | CA    | 1280 | A    |
| 1   | CA    | 1281 | C    |
| 1   | CA    | 1285 | A    |
| 1   | CA    | 1300 | G    |
| 1   | CA    | 1301 | U    |
| 1   | CA    | 1302 | C    |
| 1   | CA    | 1303 | C    |
| 1   | CA    | 1305 | G    |
| 1   | CA    | 1316 | G    |
| 1   | CA    | 1317 | C    |
| 1   | CA    | 1319 | A    |
| 1   | CA    | 1320 | C    |
| 1   | CA    | 1323 | G    |
| 1   | CA    | 1336 | C    |
| 1   | CA    | 1363 | A    |
| 1   | CA    | 1364 | U    |
| 1   | CA    | 1381 | U    |
| 1   | CA    | 1398 | A    |
| 1   | CA    | 1419 | G    |
| 1   | CA    | 1432 | G    |
| 1   | CA    | 1446 | A    |
| 1   | CA    | 1448 | C    |
| 1   | CA    | 1451 | U    |
| 1   | CA    | 1452 | C    |
| 1   | CA    | 1453 | G    |
| 1   | CA    | 1490 | U    |
| 1   | CA    | 1492 | A    |
| 1   | CA    | 1494 | G    |
| 1   | CA    | 1497 | G    |
| 1   | CA    | 1503 | A    |
| 1   | CA    | 1506 | U    |
| 1   | CA    | 1517 | G    |
| 1   | CA    | 1519 | A    |
| 1   | CA    | 1520 | C    |
| 1   | CA    | 1529 | G    |
| 1   | CA    | 1530 | G    |
| 1   | CA    | 1534 | A    |
| 22  | DA    | 4    | C    |
| 22  | DA    | 16   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DA    | 24  | G    |
| 22  | DA    | 25  | U    |
| 22  | DA    | 26  | C    |
| 22  | DA    | 30  | C    |
| 22  | DA    | 35  | C    |
| 22  | DA    | 42  | C    |
| 22  | DA    | 43  | C    |
| 22  | DA    | 44  | G    |
| 22  | DA    | 53  | A    |
| 22  | DA    | 88  | C    |
| 22  | DA    | 89  | U    |
| 22  | DA    | 90  | C    |
| 22  | DA    | 96  | G    |
| 22  | DA    | 99  | A    |
| 22  | DA    | 109 | A    |
| 22  | DA    | 112 | G    |
| 23  | DB    | 2   | G    |
| 23  | DB    | 34  | U    |
| 23  | DB    | 46  | G    |
| 23  | DB    | 51  | G    |
| 23  | DB    | 63  | A    |
| 23  | DB    | 71  | A    |
| 23  | DB    | 72  | U    |
| 23  | DB    | 74  | A    |
| 23  | DB    | 75  | G    |
| 23  | DB    | 79  | C    |
| 23  | DB    | 91  | A    |
| 23  | DB    | 99  | U    |
| 23  | DB    | 100 | U    |
| 23  | DB    | 101 | A    |
| 23  | DB    | 102 | U    |
| 23  | DB    | 103 | A    |
| 23  | DB    | 118 | A    |
| 23  | DB    | 119 | A    |
| 23  | DB    | 120 | U    |
| 23  | DB    | 125 | A    |
| 23  | DB    | 126 | A    |
| 23  | DB    | 128 | C    |
| 23  | DB    | 139 | U    |
| 23  | DB    | 140 | C    |
| 23  | DB    | 142 | A    |
| 23  | DB    | 149 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DB    | 160 | A    |
| 23  | DB    | 162 | U    |
| 23  | DB    | 163 | C    |
| 23  | DB    | 180 | G    |
| 23  | DB    | 181 | A    |
| 23  | DB    | 196 | A    |
| 23  | DB    | 199 | A    |
| 23  | DB    | 215 | G    |
| 23  | DB    | 216 | A    |
| 23  | DB    | 221 | A    |
| 23  | DB    | 222 | A    |
| 23  | DB    | 230 | G    |
| 23  | DB    | 233 | A    |
| 23  | DB    | 248 | G    |
| 23  | DB    | 250 | G    |
| 23  | DB    | 255 | A    |
| 23  | DB    | 265 | A    |
| 23  | DB    | 266 | G    |
| 23  | DB    | 267 | C    |
| 23  | DB    | 271 | G    |
| 23  | DB    | 273 | G    |
| 23  | DB    | 276 | U    |
| 23  | DB    | 277 | G    |
| 23  | DB    | 278 | A    |
| 23  | DB    | 281 | C    |
| 23  | DB    | 282 | A    |
| 23  | DB    | 284 | U    |
| 23  | DB    | 287 | G    |
| 23  | DB    | 288 | U    |
| 23  | DB    | 289 | G    |
| 23  | DB    | 299 | A    |
| 23  | DB    | 302 | C    |
| 23  | DB    | 311 | A    |
| 23  | DB    | 323 | C    |
| 23  | DB    | 329 | G    |
| 23  | DB    | 330 | A    |
| 23  | DB    | 333 | G    |
| 23  | DB    | 346 | A    |
| 23  | DB    | 349 | U    |
| 23  | DB    | 352 | A    |
| 23  | DB    | 353 | C    |
| 23  | DB    | 363 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DB    | 369 | U    |
| 23  | DB    | 371 | A    |
| 23  | DB    | 372 | G    |
| 23  | DB    | 386 | G    |
| 23  | DB    | 387 | U    |
| 23  | DB    | 395 | U    |
| 23  | DB    | 396 | G    |
| 23  | DB    | 405 | U    |
| 23  | DB    | 411 | G    |
| 23  | DB    | 412 | A    |
| 23  | DB    | 424 | G    |
| 23  | DB    | 435 | C    |
| 23  | DB    | 455 | C    |
| 23  | DB    | 456 | C    |
| 23  | DB    | 457 | A    |
| 23  | DB    | 479 | A    |
| 23  | DB    | 480 | A    |
| 23  | DB    | 481 | G    |
| 23  | DB    | 491 | G    |
| 23  | DB    | 492 | A    |
| 23  | DB    | 504 | A    |
| 23  | DB    | 505 | A    |
| 23  | DB    | 508 | A    |
| 23  | DB    | 509 | C    |
| 23  | DB    | 510 | C    |
| 23  | DB    | 512 | G    |
| 23  | DB    | 527 | C    |
| 23  | DB    | 531 | C    |
| 23  | DB    | 532 | A    |
| 23  | DB    | 544 | C    |
| 23  | DB    | 545 | U    |
| 23  | DB    | 546 | U    |
| 23  | DB    | 547 | A    |
| 23  | DB    | 548 | G    |
| 23  | DB    | 549 | G    |
| 23  | DB    | 563 | A    |
| 23  | DB    | 572 | A    |
| 23  | DB    | 573 | U    |
| 23  | DB    | 575 | A    |
| 23  | DB    | 586 | A    |
| 23  | DB    | 588 | U    |
| 23  | DB    | 603 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DB    | 613 | A    |
| 23  | DB    | 614 | A    |
| 23  | DB    | 615 | U    |
| 23  | DB    | 616 | A    |
| 23  | DB    | 627 | A    |
| 23  | DB    | 632 | A    |
| 23  | DB    | 637 | A    |
| 23  | DB    | 645 | C    |
| 23  | DB    | 646 | U    |
| 23  | DB    | 647 | G    |
| 23  | DB    | 654 | A    |
| 23  | DB    | 655 | A    |
| 23  | DB    | 671 | C    |
| 23  | DB    | 686 | U    |
| 23  | DB    | 718 | A    |
| 23  | DB    | 719 | C    |
| 23  | DB    | 730 | A    |
| 23  | DB    | 747 | U    |
| 23  | DB    | 764 | A    |
| 23  | DB    | 775 | G    |
| 23  | DB    | 782 | A    |
| 23  | DB    | 784 | G    |
| 23  | DB    | 785 | G    |
| 23  | DB    | 805 | G    |
| 23  | DB    | 812 | C    |
| 23  | DB    | 819 | A    |
| 23  | DB    | 827 | U    |
| 23  | DB    | 828 | U    |
| 23  | DB    | 847 | U    |
| 23  | DB    | 859 | G    |
| 23  | DB    | 899 | A    |
| 23  | DB    | 910 | A    |
| 23  | DB    | 912 | C    |
| 23  | DB    | 932 | U    |
| 23  | DB    | 933 | A    |
| 23  | DB    | 941 | A    |
| 23  | DB    | 946 | C    |
| 23  | DB    | 961 | C    |
| 23  | DB    | 962 | G    |
| 23  | DB    | 973 | A    |
| 23  | DB    | 974 | G    |
| 23  | DB    | 983 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 990  | A    |
| 23  | DB    | 991  | C    |
| 23  | DB    | 995  | C    |
| 23  | DB    | 996  | A    |
| 23  | DB    | 1012 | U    |
| 23  | DB    | 1013 | C    |
| 23  | DB    | 1022 | G    |
| 23  | DB    | 1023 | U    |
| 23  | DB    | 1024 | G    |
| 23  | DB    | 1025 | G    |
| 23  | DB    | 1033 | U    |
| 23  | DB    | 1045 | C    |
| 23  | DB    | 1048 | A    |
| 23  | DB    | 1070 | A    |
| 23  | DB    | 1088 | A    |
| 23  | DB    | 1090 | A    |
| 23  | DB    | 1098 | A    |
| 23  | DB    | 1110 | G    |
| 23  | DB    | 1112 | G    |
| 23  | DB    | 1116 | G    |
| 23  | DB    | 1126 | A    |
| 23  | DB    | 1129 | A    |
| 23  | DB    | 1132 | U    |
| 23  | DB    | 1133 | A    |
| 23  | DB    | 1135 | C    |
| 23  | DB    | 1136 | G    |
| 23  | DB    | 1141 | U    |
| 23  | DB    | 1142 | A    |
| 23  | DB    | 1157 | G    |
| 23  | DB    | 1174 | U    |
| 23  | DB    | 1176 | U    |
| 23  | DB    | 1179 | G    |
| 23  | DB    | 1186 | G    |
| 23  | DB    | 1195 | G    |
| 23  | DB    | 1204 | A    |
| 23  | DB    | 1205 | A    |
| 23  | DB    | 1211 | C    |
| 23  | DB    | 1212 | G    |
| 23  | DB    | 1237 | A    |
| 23  | DB    | 1238 | G    |
| 23  | DB    | 1247 | A    |
| 23  | DB    | 1248 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 1250 | G    |
| 23  | DB    | 1251 | C    |
| 23  | DB    | 1253 | A    |
| 23  | DB    | 1256 | G    |
| 23  | DB    | 1266 | G    |
| 23  | DB    | 1271 | G    |
| 23  | DB    | 1272 | A    |
| 23  | DB    | 1273 | U    |
| 23  | DB    | 1275 | A    |
| 23  | DB    | 1276 | A    |
| 23  | DB    | 1301 | A    |
| 23  | DB    | 1302 | A    |
| 23  | DB    | 1321 | A    |
| 23  | DB    | 1324 | G    |
| 23  | DB    | 1325 | U    |
| 23  | DB    | 1330 | C    |
| 23  | DB    | 1337 | G    |
| 23  | DB    | 1341 | G    |
| 23  | DB    | 1345 | C    |
| 23  | DB    | 1365 | A    |
| 23  | DB    | 1368 | G    |
| 23  | DB    | 1378 | A    |
| 23  | DB    | 1379 | U    |
| 23  | DB    | 1383 | A    |
| 23  | DB    | 1384 | A    |
| 23  | DB    | 1386 | C    |
| 23  | DB    | 1396 | U    |
| 23  | DB    | 1397 | U    |
| 23  | DB    | 1416 | G    |
| 23  | DB    | 1419 | A    |
| 23  | DB    | 1427 | A    |
| 23  | DB    | 1428 | C    |
| 23  | DB    | 1434 | A    |
| 23  | DB    | 1451 | C    |
| 23  | DB    | 1453 | A    |
| 23  | DB    | 1454 | C    |
| 23  | DB    | 1455 | G    |
| 23  | DB    | 1459 | G    |
| 23  | DB    | 1460 | U    |
| 23  | DB    | 1461 | C    |
| 23  | DB    | 1476 | U    |
| 23  | DB    | 1477 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 1482 | G    |
| 23  | DB    | 1486 | U    |
| 23  | DB    | 1490 | A    |
| 23  | DB    | 1493 | C    |
| 23  | DB    | 1494 | A    |
| 23  | DB    | 1504 | A    |
| 23  | DB    | 1505 | A    |
| 23  | DB    | 1507 | C    |
| 23  | DB    | 1508 | A    |
| 23  | DB    | 1509 | A    |
| 23  | DB    | 1510 | G    |
| 23  | DB    | 1524 | G    |
| 23  | DB    | 1532 | A    |
| 23  | DB    | 1535 | A    |
| 23  | DB    | 1537 | G    |
| 23  | DB    | 1538 | G    |
| 23  | DB    | 1540 | G    |
| 23  | DB    | 1552 | A    |
| 23  | DB    | 1559 | U    |
| 23  | DB    | 1569 | A    |
| 23  | DB    | 1578 | U    |
| 23  | DB    | 1584 | U    |
| 23  | DB    | 1585 | C    |
| 23  | DB    | 1588 | G    |
| 23  | DB    | 1607 | C    |
| 23  | DB    | 1608 | A    |
| 23  | DB    | 1610 | A    |
| 23  | DB    | 1616 | A    |
| 23  | DB    | 1634 | A    |
| 23  | DB    | 1635 | A    |
| 23  | DB    | 1647 | U    |
| 23  | DB    | 1648 | U    |
| 23  | DB    | 1674 | G    |
| 23  | DB    | 1700 | A    |
| 23  | DB    | 1701 | A    |
| 23  | DB    | 1706 | C    |
| 23  | DB    | 1713 | A    |
| 23  | DB    | 1715 | G    |
| 23  | DB    | 1724 | G    |
| 23  | DB    | 1725 | U    |
| 23  | DB    | 1727 | C    |
| 23  | DB    | 1729 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 1730 | C    |
| 23  | DB    | 1732 | C    |
| 23  | DB    | 1733 | G    |
| 23  | DB    | 1738 | G    |
| 23  | DB    | 1758 | U    |
| 23  | DB    | 1764 | C    |
| 23  | DB    | 1773 | A    |
| 23  | DB    | 1800 | C    |
| 23  | DB    | 1816 | C    |
| 23  | DB    | 1829 | A    |
| 23  | DB    | 1833 | C    |
| 23  | DB    | 1870 | C    |
| 23  | DB    | 1872 | A    |
| 23  | DB    | 1884 | G    |
| 23  | DB    | 1906 | G    |
| 23  | DB    | 1913 | A    |
| 23  | DB    | 1914 | C    |
| 23  | DB    | 1915 | U    |
| 23  | DB    | 1927 | A    |
| 23  | DB    | 1929 | G    |
| 23  | DB    | 1930 | G    |
| 23  | DB    | 1936 | A    |
| 23  | DB    | 1937 | A    |
| 23  | DB    | 1938 | A    |
| 23  | DB    | 1939 | U    |
| 23  | DB    | 1940 | U    |
| 23  | DB    | 1955 | U    |
| 23  | DB    | 1967 | C    |
| 23  | DB    | 1970 | A    |
| 23  | DB    | 1971 | U    |
| 23  | DB    | 1972 | G    |
| 23  | DB    | 1991 | U    |
| 23  | DB    | 1993 | U    |
| 23  | DB    | 1997 | C    |
| 23  | DB    | 2022 | U    |
| 23  | DB    | 2023 | C    |
| 23  | DB    | 2030 | A    |
| 23  | DB    | 2031 | A    |
| 23  | DB    | 2032 | G    |
| 23  | DB    | 2033 | A    |
| 23  | DB    | 2043 | C    |
| 23  | DB    | 2055 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 2056 | G    |
| 23  | DB    | 2060 | A    |
| 23  | DB    | 2061 | G    |
| 23  | DB    | 2062 | A    |
| 23  | DB    | 2069 | G    |
| 23  | DB    | 2096 | C    |
| 23  | DB    | 2097 | A    |
| 23  | DB    | 2107 | G    |
| 23  | DB    | 2108 | A    |
| 23  | DB    | 2110 | G    |
| 23  | DB    | 2134 | A    |
| 23  | DB    | 2135 | A    |
| 23  | DB    | 2138 | G    |
| 23  | DB    | 2143 | C    |
| 23  | DB    | 2144 | G    |
| 23  | DB    | 2145 | C    |
| 23  | DB    | 2147 | A    |
| 23  | DB    | 2148 | G    |
| 23  | DB    | 2155 | U    |
| 23  | DB    | 2156 | G    |
| 23  | DB    | 2157 | G    |
| 23  | DB    | 2180 | U    |
| 23  | DB    | 2183 | A    |
| 23  | DB    | 2189 | U    |
| 23  | DB    | 2190 | G    |
| 23  | DB    | 2193 | G    |
| 23  | DB    | 2198 | A    |
| 23  | DB    | 2199 | A    |
| 23  | DB    | 2203 | U    |
| 23  | DB    | 2204 | G    |
| 23  | DB    | 2211 | A    |
| 23  | DB    | 2212 | A    |
| 23  | DB    | 2213 | U    |
| 23  | DB    | 2225 | A    |
| 23  | DB    | 2238 | G    |
| 23  | DB    | 2239 | G    |
| 23  | DB    | 2250 | G    |
| 23  | DB    | 2266 | A    |
| 23  | DB    | 2283 | C    |
| 23  | DB    | 2287 | A    |
| 23  | DB    | 2288 | A    |
| 23  | DB    | 2305 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 2307 | G    |
| 23  | DB    | 2308 | G    |
| 23  | DB    | 2309 | A    |
| 23  | DB    | 2311 | A    |
| 23  | DB    | 2320 | U    |
| 23  | DB    | 2321 | U    |
| 23  | DB    | 2322 | A    |
| 23  | DB    | 2325 | G    |
| 23  | DB    | 2333 | A    |
| 23  | DB    | 2337 | G    |
| 23  | DB    | 2345 | G    |
| 23  | DB    | 2347 | C    |
| 23  | DB    | 2361 | G    |
| 23  | DB    | 2372 | U    |
| 23  | DB    | 2379 | G    |
| 23  | DB    | 2383 | G    |
| 23  | DB    | 2385 | C    |
| 23  | DB    | 2396 | G    |
| 23  | DB    | 2402 | U    |
| 23  | DB    | 2403 | C    |
| 23  | DB    | 2406 | A    |
| 23  | DB    | 2423 | U    |
| 23  | DB    | 2425 | A    |
| 23  | DB    | 2426 | A    |
| 23  | DB    | 2427 | C    |
| 23  | DB    | 2429 | G    |
| 23  | DB    | 2430 | A    |
| 23  | DB    | 2441 | U    |
| 23  | DB    | 2448 | A    |
| 23  | DB    | 2449 | U    |
| 23  | DB    | 2472 | G    |
| 23  | DB    | 2476 | A    |
| 23  | DB    | 2491 | U    |
| 23  | DB    | 2501 | C    |
| 23  | DB    | 2502 | G    |
| 23  | DB    | 2505 | G    |
| 23  | DB    | 2506 | U    |
| 23  | DB    | 2518 | A    |
| 23  | DB    | 2535 | G    |
| 23  | DB    | 2554 | U    |
| 23  | DB    | 2555 | U    |
| 23  | DB    | 2556 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 2566 | A    |
| 23  | DB    | 2567 | G    |
| 23  | DB    | 2572 | A    |
| 23  | DB    | 2582 | G    |
| 23  | DB    | 2586 | U    |
| 23  | DB    | 2602 | A    |
| 23  | DB    | 2609 | U    |
| 23  | DB    | 2611 | C    |
| 23  | DB    | 2613 | U    |
| 23  | DB    | 2619 | C    |
| 23  | DB    | 2629 | U    |
| 23  | DB    | 2630 | G    |
| 23  | DB    | 2634 | A    |
| 23  | DB    | 2646 | C    |
| 23  | DB    | 2654 | A    |
| 23  | DB    | 2682 | A    |
| 23  | DB    | 2689 | U    |
| 23  | DB    | 2690 | U    |
| 23  | DB    | 2714 | G    |
| 23  | DB    | 2739 | U    |
| 23  | DB    | 2744 | G    |
| 23  | DB    | 2748 | A    |
| 23  | DB    | 2757 | A    |
| 23  | DB    | 2765 | A    |
| 23  | DB    | 2778 | A    |
| 23  | DB    | 2798 | U    |
| 23  | DB    | 2799 | A    |
| 23  | DB    | 2800 | A    |
| 23  | DB    | 2802 | G    |
| 23  | DB    | 2808 | G    |
| 23  | DB    | 2820 | A    |
| 23  | DB    | 2821 | A    |
| 23  | DB    | 2823 | A    |
| 23  | DB    | 2831 | G    |
| 23  | DB    | 2836 | U    |
| 23  | DB    | 2850 | A    |
| 23  | DB    | 2866 | U    |
| 23  | DB    | 2867 | G    |
| 23  | DB    | 2872 | A    |
| 23  | DB    | 2873 | A    |
| 23  | DB    | 2883 | A    |
| 23  | DB    | 2894 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | DB    | 2903 | U    |

All (62) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 51   | A    |
| 1   | AA    | 239  | U    |
| 1   | AA    | 243  | A    |
| 1   | AA    | 279  | A    |
| 1   | AA    | 328  | C    |
| 1   | AA    | 366  | A    |
| 1   | AA    | 372  | C    |
| 1   | AA    | 428  | G    |
| 1   | AA    | 429  | U    |
| 1   | AA    | 960  | U    |
| 1   | AA    | 975  | A    |
| 1   | AA    | 1049 | U    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1302 | C    |
| 1   | AA    | 1397 | C    |
| 23  | BB    | 3    | U    |
| 23  | BB    | 162  | U    |
| 23  | BB    | 508  | A    |
| 23  | BB    | 546  | U    |
| 23  | BB    | 670  | A    |
| 23  | BB    | 1210 | G    |
| 23  | BB    | 1419 | A    |
| 23  | BB    | 1509 | A    |
| 23  | BB    | 2282 | G    |
| 23  | BB    | 2336 | A    |
| 23  | BB    | 2425 | A    |
| 23  | BB    | 2756 | U    |
| 23  | BB    | 2832 | U    |
| 23  | BB    | 2894 | G    |
| 1   | CA    | 51   | A    |
| 1   | CA    | 239  | U    |
| 1   | CA    | 243  | A    |
| 1   | CA    | 279  | A    |
| 1   | CA    | 328  | C    |
| 1   | CA    | 366  | A    |
| 1   | CA    | 372  | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 428  | G    |
| 1   | CA    | 429  | U    |
| 1   | CA    | 960  | U    |
| 1   | CA    | 975  | A    |
| 1   | CA    | 1049 | U    |
| 1   | CA    | 1065 | U    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1302 | C    |
| 1   | CA    | 1397 | C    |
| 23  | DB    | 139  | U    |
| 23  | DB    | 162  | U    |
| 23  | DB    | 508  | A    |
| 23  | DB    | 544  | C    |
| 23  | DB    | 546  | U    |
| 23  | DB    | 670  | A    |
| 23  | DB    | 1126 | A    |
| 23  | DB    | 1210 | G    |
| 23  | DB    | 1419 | A    |
| 23  | DB    | 1509 | A    |
| 23  | DB    | 2282 | G    |
| 23  | DB    | 2336 | A    |
| 23  | DB    | 2425 | A    |
| 23  | DB    | 2756 | U    |
| 23  | DB    | 2832 | U    |
| 23  | DB    | 2894 | G    |

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 55  | PAR  | AA    | 1661 | -    | 45,45,45     | 1.70 | 10 (22%) | 67,67,67    | 1.14 | 7 (10%)  |
| 55  | PAR  | BB    | 3111 | -    | 45,45,45     | 1.79 | 11 (24%) | 67,67,67    | 1.13 | 6 (8%)   |
| 55  | PAR  | CA    | 1662 | -    | 45,45,45     | 1.79 | 11 (24%) | 67,67,67    | 1.15 | 5 (7%)   |
| 55  | PAR  | DB    | 3112 | -    | 45,45,45     | 1.83 | 12 (26%) | 67,67,67    | 1.18 | 6 (8%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 55  | PAR  | AA    | 1661 | -    | -       | 0/18/94/94 | 0/4/4/4 |
| 55  | PAR  | BB    | 3111 | -    | -       | 0/18/94/94 | 0/4/4/4 |
| 55  | PAR  | CA    | 1662 | -    | -       | 0/18/94/94 | 0/4/4/4 |
| 55  | PAR  | DB    | 3112 | -    | -       | 0/18/94/94 | 0/4/4/4 |

All (44) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 55  | CA    | 1662 | PAR  | O54-C14 | 4.65 | 1.53        | 1.41     |
| 55  | BB    | 3111 | PAR  | O54-C14 | 4.52 | 1.53        | 1.41     |
| 55  | DB    | 3112 | PAR  | O54-C14 | 4.50 | 1.53        | 1.41     |
| 55  | AA    | 1661 | PAR  | O54-C14 | 4.42 | 1.53        | 1.41     |
| 55  | CA    | 1662 | PAR  | C31-C21 | 4.38 | 1.59        | 1.53     |
| 55  | BB    | 3111 | PAR  | C31-C21 | 4.36 | 1.59        | 1.53     |
| 55  | DB    | 3112 | PAR  | C31-C21 | 4.32 | 1.59        | 1.53     |
| 55  | AA    | 1661 | PAR  | C31-C21 | 4.02 | 1.59        | 1.53     |
| 55  | CA    | 1662 | PAR  | O51-C11 | 3.65 | 1.51        | 1.41     |
| 55  | AA    | 1661 | PAR  | O51-C11 | 3.58 | 1.51        | 1.41     |
| 55  | DB    | 3112 | PAR  | O51-C11 | 3.48 | 1.50        | 1.41     |
| 55  | BB    | 3111 | PAR  | O51-C11 | 3.43 | 1.50        | 1.41     |
| 55  | DB    | 3112 | PAR  | C64-C54 | 2.95 | 1.59        | 1.51     |
| 55  | BB    | 3111 | PAR  | C64-C54 | 2.95 | 1.59        | 1.51     |
| 55  | AA    | 1661 | PAR  | C64-C54 | 2.85 | 1.58        | 1.51     |
| 55  | CA    | 1662 | PAR  | C64-C54 | 2.81 | 1.58        | 1.51     |
| 55  | DB    | 3112 | PAR  | O54-C54 | 2.68 | 1.51        | 1.44     |
| 55  | DB    | 3112 | PAR  | C24-N24 | 2.61 | 1.51        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 55  | CA    | 1662 | PAR  | C24-N24 | 2.61 | 1.51        | 1.47     |
| 55  | CA    | 1662 | PAR  | O54-C54 | 2.56 | 1.50        | 1.44     |
| 55  | BB    | 3111 | PAR  | O54-C54 | 2.56 | 1.50        | 1.44     |
| 55  | BB    | 3111 | PAR  | C24-N24 | 2.45 | 1.51        | 1.47     |
| 55  | AA    | 1661 | PAR  | C24-N24 | 2.45 | 1.51        | 1.47     |
| 55  | AA    | 1661 | PAR  | O54-C54 | 2.35 | 1.50        | 1.44     |
| 55  | CA    | 1662 | PAR  | C23-C33 | 2.31 | 1.58        | 1.53     |
| 55  | DB    | 3112 | PAR  | O43-C13 | 2.31 | 1.45        | 1.41     |
| 55  | CA    | 1662 | PAR  | C62-C12 | 2.31 | 1.58        | 1.53     |
| 55  | CA    | 1662 | PAR  | O51-C51 | 2.28 | 1.50        | 1.44     |
| 55  | BB    | 3111 | PAR  | O51-C51 | 2.28 | 1.50        | 1.44     |
| 55  | AA    | 1661 | PAR  | O51-C51 | 2.27 | 1.50        | 1.44     |
| 55  | AA    | 1661 | PAR  | C62-C12 | 2.27 | 1.58        | 1.53     |
| 55  | DB    | 3112 | PAR  | C41-C51 | 2.26 | 1.58        | 1.53     |
| 55  | BB    | 3111 | PAR  | C41-C51 | 2.26 | 1.58        | 1.53     |
| 55  | BB    | 3111 | PAR  | C62-C12 | 2.26 | 1.58        | 1.53     |
| 55  | AA    | 1661 | PAR  | C23-C33 | 2.25 | 1.58        | 1.53     |
| 55  | DB    | 3112 | PAR  | O51-C51 | 2.24 | 1.50        | 1.44     |
| 55  | CA    | 1662 | PAR  | C41-C51 | 2.21 | 1.57        | 1.53     |
| 55  | DB    | 3112 | PAR  | C44-C34 | 2.18 | 1.58        | 1.52     |
| 55  | BB    | 3111 | PAR  | C44-C34 | 2.15 | 1.58        | 1.52     |
| 55  | AA    | 1661 | PAR  | C41-C51 | 2.13 | 1.57        | 1.53     |
| 55  | DB    | 3112 | PAR  | C62-C12 | 2.06 | 1.58        | 1.53     |
| 55  | BB    | 3111 | PAR  | C23-C33 | 2.04 | 1.57        | 1.53     |
| 55  | DB    | 3112 | PAR  | O33-C33 | 2.04 | 1.48        | 1.43     |
| 55  | CA    | 1662 | PAR  | C44-C34 | 2.03 | 1.57        | 1.52     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 55  | DB    | 3112 | PAR  | O52-C13-O43 | 3.58 | 115.04      | 111.57   |
| 55  | DB    | 3112 | PAR  | O33-C14-C24 | 3.25 | 114.50      | 108.08   |
| 55  | DB    | 3112 | PAR  | O54-C54-C64 | 3.18 | 112.02      | 105.97   |
| 55  | AA    | 1661 | PAR  | O54-C54-C64 | 3.17 | 112.00      | 105.97   |
| 55  | BB    | 3111 | PAR  | O33-C14-C24 | 3.11 | 114.23      | 108.08   |
| 55  | CA    | 1662 | PAR  | O54-C54-C64 | 3.07 | 111.81      | 105.97   |
| 55  | BB    | 3111 | PAR  | O54-C54-C64 | 3.07 | 111.81      | 105.97   |
| 55  | DB    | 3112 | PAR  | O52-C13-C23 | 2.96 | 112.79      | 107.50   |
| 55  | CA    | 1662 | PAR  | O33-C14-C24 | 2.92 | 113.85      | 108.08   |
| 55  | CA    | 1662 | PAR  | C14-O54-C54 | 2.84 | 119.22      | 113.73   |
| 55  | BB    | 3111 | PAR  | O52-C13-C23 | 2.79 | 112.48      | 107.50   |
| 55  | BB    | 3111 | PAR  | C14-O54-C54 | 2.78 | 119.12      | 113.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | AA    | 1661 | PAR  | C14-O54-C54 | 2.73  | 119.02      | 113.73   |
| 55  | AA    | 1661 | PAR  | O43-C13-C23 | 2.68  | 108.56      | 104.81   |
| 55  | DB    | 3112 | PAR  | C14-O54-C54 | 2.68  | 118.92      | 113.73   |
| 55  | AA    | 1661 | PAR  | O33-C14-C24 | 2.67  | 113.35      | 108.08   |
| 55  | DB    | 3112 | PAR  | O23-C23-C33 | 2.61  | 118.89      | 111.20   |
| 55  | CA    | 1662 | PAR  | O52-C13-C23 | 2.54  | 112.03      | 107.50   |
| 55  | CA    | 1662 | PAR  | O43-C13-C23 | 2.47  | 108.26      | 104.81   |
| 55  | BB    | 3111 | PAR  | O52-C13-O43 | 2.47  | 113.96      | 111.57   |
| 55  | BB    | 3111 | PAR  | O23-C23-C33 | 2.37  | 118.19      | 111.20   |
| 55  | AA    | 1661 | PAR  | O52-C13-C23 | 2.27  | 111.56      | 107.50   |
| 55  | AA    | 1661 | PAR  | O23-C23-C33 | 2.15  | 117.51      | 111.20   |
| 55  | AA    | 1661 | PAR  | O52-C13-O43 | -2.12 | 109.52      | 111.57   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 1530/1542 (99%) | -0.13  | 20 (1%) 74 60 | 8, 88, 162, 180       | 0     |
| 1   | CA    | 1530/1542 (99%) | -0.30  | 8 (0%) 88 79  | 5, 54, 146, 180       | 0     |
| 2   | AC    | 206/232 (88%)   | 0.78   | 26 (12%) 4 7  | 9, 89, 158, 180       | 0     |
| 2   | CC    | 206/232 (88%)   | 0.33   | 9 (4%) 33 29  | 9, 83, 141, 180       | 0     |
| 3   | AD    | 205/205 (100%)  | 0.65   | 22 (10%) 6 10 | 5, 97, 172, 180       | 0     |
| 3   | CD    | 205/205 (100%)  | 0.25   | 1 (0%) 88 79  | 5, 59, 151, 180       | 0     |
| 4   | AE    | 150/166 (90%)   | 0.47   | 7 (4%) 30 27  | 5, 85, 159, 180       | 0     |
| 4   | CE    | 150/166 (90%)   | 0.42   | 6 (4%) 36 32  | 5, 52, 137, 180       | 0     |
| 5   | AF    | 100/135 (74%)   | 0.41   | 5 (5%) 28 26  | 8, 73, 146, 172       | 0     |
| 5   | CF    | 100/135 (74%)   | 0.34   | 4 (4%) 36 32  | 5, 84, 153, 180       | 0     |
| 6   | AG    | 150/178 (84%)   | 0.57   | 13 (8%) 10 14 | 10, 110, 170, 180     | 0     |
| 6   | CG    | 152/178 (85%)   | 0.74   | 17 (11%) 6 10 | 28, 93, 162, 180      | 0     |
| 7   | AH    | 129/129 (100%)  | 0.82   | 13 (10%) 7 12 | 15, 85, 159, 180      | 0     |
| 7   | CH    | 129/129 (100%)  | 0.30   | 3 (2%) 57 45  | 5, 50, 128, 175       | 0     |
| 8   | AI    | 127/129 (98%)   | 1.18   | 28 (22%) 1 3  | 5, 98, 163, 180       | 0     |
| 8   | CI    | 127/129 (98%)   | 0.68   | 9 (7%) 16 18  | 5, 102, 180, 180      | 0     |
| 9   | AJ    | 98/103 (95%)    | 0.80   | 13 (13%) 4 7  | 5, 105, 174, 180      | 0     |
| 9   | CJ    | 98/103 (95%)    | 1.00   | 14 (14%) 3 6  | 10, 93, 158, 180      | 0     |
| 10  | AK    | 117/128 (91%)   | 0.47   | 5 (4%) 34 30  | 9, 67, 129, 146       | 0     |
| 10  | CK    | 117/128 (91%)   | 0.38   | 5 (4%) 34 30  | 5, 63, 134, 180       | 0     |
| 11  | AL    | 123/123 (100%)  | 0.76   | 9 (7%) 15 17  | 19, 84, 158, 180      | 0     |
| 11  | CL    | 123/123 (100%)  | 0.31   | 4 (3%) 44 37  | 5, 54, 113, 180       | 0     |
| 12  | AM    | 114/117 (97%)   | 0.89   | 16 (14%) 3 6  | 55, 122, 180, 180     | 0     |
| 12  | CM    | 113/117 (96%)   | 0.97   | 16 (14%) 3 6  | 31, 114, 180, 180     | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | AN    | 96/100 (96%)    | 1.16   | 20 (20%) 1 3  | 5, 108, 170, 180      | 0     |
| 13  | CN    | 96/100 (96%)    | 0.89   | 14 (14%) 3 6  | 6, 99, 162, 180       | 0     |
| 14  | AO    | 88/89 (98%)     | 0.41   | 5 (5%) 23 23  | 7, 86, 156, 180       | 0     |
| 14  | CO    | 88/89 (98%)     | 0.26   | 2 (2%) 57 45  | 5, 60, 132, 175       | 0     |
| 15  | AP    | 82/82 (100%)    | 1.40   | 17 (20%) 1 3  | 35, 106, 173, 180     | 0     |
| 15  | CP    | 80/82 (97%)     | 1.41   | 23 (28%) 1 3  | 5, 47, 142, 180       | 0     |
| 16  | AQ    | 80/83 (96%)     | 1.18   | 19 (23%) 1 3  | 48, 104, 180, 180     | 0     |
| 16  | CQ    | 81/83 (97%)     | 0.78   | 10 (12%) 5 8  | 5, 53, 140, 173       | 0     |
| 17  | AR    | 55/74 (74%)     | 0.60   | 2 (3%) 41 35  | 5, 65, 143, 180       | 0     |
| 17  | CR    | 55/74 (74%)     | 0.99   | 9 (16%) 2 5   | 13, 68, 130, 180      | 0     |
| 18  | AS    | 79/91 (86%)     | 1.70   | 30 (37%) 1 2  | 55, 129, 180, 180     | 0     |
| 18  | CS    | 80/91 (87%)     | 1.21   | 18 (22%) 1 3  | 46, 108, 180, 180     | 0     |
| 19  | AT    | 85/86 (98%)     | 1.19   | 20 (23%) 1 3  | 44, 105, 154, 180     | 0     |
| 19  | CT    | 85/86 (98%)     | 0.61   | 7 (8%) 12 15  | 5, 56, 117, 161       | 0     |
| 20  | AB    | 218/240 (90%)   | 0.51   | 11 (5%) 28 26 | 7, 105, 171, 180      | 0     |
| 20  | CB    | 218/240 (90%)   | 1.03   | 38 (17%) 2 4  | 23, 111, 172, 180     | 0     |
| 21  | AU    | 51/70 (72%)     | 0.91   | 9 (17%) 2 4   | 23, 104, 180, 180     | 0     |
| 21  | CU    | 51/70 (72%)     | 0.72   | 7 (13%) 4 6   | 24, 96, 173, 180      | 0     |
| 22  | BA    | 117/120 (97%)   | -0.36  | 1 (0%) 81 69  | 37, 82, 145, 178      | 0     |
| 22  | DA    | 117/120 (97%)   | -0.13  | 3 (2%) 53 43  | 18, 84, 143, 180      | 0     |
| 23  | BB    | 2841/2904 (97%) | -0.23  | 32 (1%) 77 63 | 6, 58, 150, 180       | 0     |
| 23  | DB    | 2841/2904 (97%) | -0.31  | 14 (0%) 88 79 | 5, 38, 149, 180       | 0     |
| 24  | BI    | 141/141 (100%)  | 2.04   | 60 (42%) 1 2  | 63, 161, 180, 180     | 0     |
| 24  | DI    | 141/141 (100%)  | 1.47   | 37 (26%) 1 3  | 65, 157, 180, 180     | 0     |
| 25  | BC    | 271/272 (99%)   | 0.45   | 9 (3%) 44 37  | 5, 48, 108, 166       | 0     |
| 25  | DC    | 271/272 (99%)   | 0.39   | 8 (2%) 48 39  | 5, 30, 102, 180       | 0     |
| 26  | BD    | 209/209 (100%)  | 0.70   | 16 (7%) 13 16 | 5, 79, 148, 180       | 0     |
| 26  | DD    | 209/209 (100%)  | 0.34   | 3 (1%) 72 58  | 5, 51, 123, 180       | 0     |
| 27  | BK    | 121/123 (98%)   | 0.91   | 15 (12%) 5 8  | 5, 74, 149, 180       | 0     |
| 27  | DK    | 121/123 (98%)   | 0.65   | 2 (1%) 67 54  | 5, 33, 106, 180       | 0     |
| 28  | BP    | 114/114 (100%)  | 0.74   | 14 (12%) 5 8  | 18, 89, 153, 180      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|-----|-----|-----------------------|-------|
| 28  | DP    | 114/114 (100%) | 0.51   | 3 (2%)   | 53  | 43  | 5, 48, 124, 180       | 0     |
| 29  | BE    | 201/201 (100%) | 0.50   | 9 (4%)   | 32  | 29  | 5, 67, 146, 180       | 0     |
| 29  | DE    | 201/201 (100%) | 0.38   | 6 (2%)   | 48  | 39  | 5, 67, 142, 177       | 0     |
| 30  | BY    | 58/58 (100%)   | 0.89   | 7 (12%)  | 5   | 8   | 18, 82, 151, 171      | 0     |
| 30  | DY    | 58/58 (100%)   | 0.66   | 3 (5%)   | 26  | 25  | 5, 68, 126, 162       | 0     |
| 31  | B0    | 56/56 (100%)   | 0.58   | 3 (5%)   | 25  | 23  | 5, 73, 153, 164       | 0     |
| 31  | D0    | 56/56 (100%)   | 0.53   | 6 (10%)  | 6   | 10  | 5, 56, 147, 180       | 0     |
| 32  | B4    | 38/38 (100%)   | 3.03   | 26 (68%) | 0   | 2   | 45, 115, 169, 180     | 0     |
| 32  | D4    | 38/38 (100%)   | 3.60   | 34 (89%) | 0   | 1   | 36, 110, 169, 180     | 0     |
| 33  | B1    | 50/54 (92%)    | 1.19   | 8 (16%)  | 3   | 5   | 22, 95, 157, 180      | 0     |
| 33  | D1    | 50/54 (92%)    | 1.32   | 12 (24%) | 1   | 3   | 19, 73, 122, 161      | 0     |
| 34  | B3    | 64/64 (100%)   | 0.81   | 5 (7%)   | 13  | 16  | 20, 63, 125, 145      | 0     |
| 34  | D3    | 64/64 (100%)   | 0.67   | 5 (7%)   | 13  | 16  | 5, 35, 88, 129        | 0     |
| 35  | BV    | 94/94 (100%)   | 0.61   | 6 (6%)   | 19  | 21  | 24, 96, 156, 180      | 0     |
| 35  | DV    | 94/94 (100%)   | 0.85   | 17 (18%) | 2   | 4   | 11, 93, 151, 180      | 0     |
| 36  | B2    | 46/46 (100%)   | 0.46   | 2 (4%)   | 34  | 30  | 5, 75, 137, 180       | 0     |
| 36  | D2    | 46/46 (100%)   | 0.40   | 0        | 100 | 100 | 5, 44, 101, 180       | 0     |
| 37  | BL    | 143/144 (99%)  | 0.61   | 6 (4%)   | 35  | 30  | 5, 71, 133, 180       | 0     |
| 37  | DL    | 143/144 (99%)  | 0.39   | 3 (2%)   | 60  | 48  | 5, 51, 116, 180       | 0     |
| 38  | BM    | 136/136 (100%) | 1.01   | 26 (19%) | 2   | 4   | 9, 70, 149, 180       | 0     |
| 38  | DM    | 136/136 (100%) | 0.68   | 6 (4%)   | 33  | 29  | 5, 50, 131, 176       | 0     |
| 39  | BX    | 63/63 (100%)   | 0.75   | 6 (9%)   | 8   | 13  | 7, 84, 165, 180       | 0     |
| 39  | DX    | 63/63 (100%)   | 0.53   | 3 (4%)   | 29  | 27  | 47, 108, 173, 180     | 0     |
| 40  | BH    | 149/149 (100%) | 0.94   | 17 (11%) | 6   | 9   | 5, 130, 180, 180      | 0     |
| 40  | DH    | 149/149 (100%) | 0.90   | 18 (12%) | 5   | 8   | 12, 97, 172, 180      | 0     |
| 41  | BJ    | 142/142 (100%) | 0.70   | 15 (10%) | 7   | 11  | 6, 81, 147, 180       | 0     |
| 41  | DJ    | 142/142 (100%) | 0.60   | 9 (6%)   | 19  | 21  | 5, 58, 135, 180       | 0     |
| 42  | BN    | 120/127 (94%)  | 0.55   | 7 (5%)   | 22  | 22  | 5, 68, 139, 178       | 0     |
| 42  | DN    | 120/127 (94%)  | 0.32   | 2 (1%)   | 67  | 54  | 5, 38, 101, 180       | 0     |
| 43  | BO    | 116/117 (99%)  | 1.21   | 29 (25%) | 1   | 3   | 21, 91, 147, 180      | 0     |
| 43  | DO    | 116/117 (99%)  | 1.16   | 25 (21%) | 1   | 3   | 8, 86, 164, 180       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | BQ    | 117/117 (100%)    | 0.39   | 5 (4%) 34 30    | 5, 66, 135, 176       | 0     |
| 44  | DQ    | 117/117 (100%)    | 0.36   | 3 (2%) 53 43    | 5, 48, 134, 180       | 0     |
| 45  | BS    | 110/110 (100%)    | 0.84   | 8 (7%) 15 17    | 6, 58, 139, 180       | 0     |
| 45  | DS    | 110/110 (100%)    | 0.50   | 2 (1%) 65 52    | 5, 50, 121, 180       | 0     |
| 46  | BU    | 102/103 (99%)     | 1.04   | 21 (20%) 1 3    | 5, 89, 144, 180       | 0     |
| 46  | DU    | 102/103 (99%)     | 0.97   | 15 (14%) 3 6    | 24, 99, 159, 180      | 0     |
| 47  | BF    | 178/178 (100%)    | 0.66   | 17 (9%) 8 12    | 36, 111, 174, 180     | 0     |
| 47  | DF    | 178/178 (100%)    | 0.68   | 15 (8%) 11 15   | 8, 103, 177, 180      | 0     |
| 48  | BG    | 176/176 (100%)    | 0.92   | 20 (11%) 6 9    | 9, 114, 179, 180      | 0     |
| 48  | DG    | 176/176 (100%)    | 1.03   | 24 (13%) 4 7    | 15, 91, 167, 180      | 0     |
| 49  | BR    | 103/103 (100%)    | 1.29   | 26 (25%) 1 3    | 16, 93, 157, 180      | 0     |
| 49  | DR    | 103/103 (100%)    | 0.96   | 12 (11%) 5 9    | 5, 88, 145, 180       | 0     |
| 50  | BT    | 93/100 (93%)      | 1.02   | 20 (21%) 1 3    | 5, 88, 180, 180       | 0     |
| 50  | DT    | 93/100 (93%)      | 1.01   | 16 (17%) 2 4    | 7, 90, 180, 180       | 0     |
| 51  | BZ    | 77/78 (98%)       | 0.77   | 6 (7%) 13 16    | 5, 52, 127, 154       | 0     |
| 51  | DZ    | 77/78 (98%)       | 0.89   | 7 (9%) 9 14     | 5, 43, 95, 135        | 0     |
| 52  | BW    | 79/84 (94%)       | 0.82   | 9 (11%) 6 9     | 10, 85, 145, 179      | 0     |
| 52  | DW    | 79/84 (94%)       | 0.96   | 6 (7%) 14 16    | 5, 66, 152, 180       | 0     |
| 53  | B6    | 185/185 (100%)    | 1.22   | 49 (26%) 1 3    | 5, 125, 180, 180      | 0     |
| 53  | D6    | 185/185 (100%)    | 0.70   | 22 (11%) 5 9    | 5, 90, 180, 180       | 0     |
| All | All   | 20787/21416 (97%) | 0.32   | 1375 (6%) 18 20 | 5, 70, 162, 180       | 0     |

All (1375) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 24  | BI    | 2    | LYS  | 10.9 |
| 24  | BI    | 5    | GLN  | 10.3 |
| 32  | D4    | 35   | GLN  | 9.4  |
| 24  | BI    | 1    | ALA  | 8.9  |
| 23  | BB    | 2147 | A    | 8.6  |
| 39  | DX    | 63   | ALA  | 8.6  |
| 24  | BI    | 6    | ALA  | 8.2  |
| 23  | BB    | 140  | C    | 8.0  |
| 52  | DW    | 84   | GLU  | 7.8  |
| 24  | BI    | 3    | LYS  | 7.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | B4    | 7    | VAL  | 7.1  |
| 32  | B4    | 24   | ARG  | 7.1  |
| 15  | AP    | 81   | ALA  | 6.9  |
| 24  | BI    | 4    | VAL  | 6.8  |
| 24  | DI    | 7    | TYR  | 6.7  |
| 24  | DI    | 52   | LEU  | 6.7  |
| 17  | CR    | 19   | GLU  | 6.6  |
| 18  | AS    | 29   | PRO  | 6.6  |
| 43  | BO    | 37   | ALA  | 6.5  |
| 15  | AP    | 82   | ALA  | 6.4  |
| 32  | B4    | 35   | GLN  | 6.1  |
| 24  | BI    | 7    | TYR  | 6.0  |
| 18  | AS    | 30   | LEU  | 6.0  |
| 38  | BM    | 103  | TYR  | 5.9  |
| 32  | D4    | 33   | HIS  | 5.8  |
| 32  | D4    | 25   | VAL  | 5.8  |
| 15  | AP    | 80   | LYS  | 5.8  |
| 51  | DZ    | 78   | TYR  | 5.7  |
| 33  | B1    | 52   | LYS  | 5.7  |
| 23  | BB    | 139  | U    | 5.7  |
| 17  | CR    | 31   | TYR  | 5.7  |
| 53  | D6    | 98   | ALA  | 5.6  |
| 23  | DB    | 2133 | G    | 5.6  |
| 24  | BI    | 58   | ILE  | 5.6  |
| 32  | B4    | 17   | VAL  | 5.5  |
| 23  | BB    | 2145 | C    | 5.5  |
| 20  | CB    | 216  | VAL  | 5.5  |
| 53  | B6    | 89   | GLY  | 5.5  |
| 48  | DG    | 88   | LEU  | 5.4  |
| 32  | D4    | 7    | VAL  | 5.4  |
| 43  | DO    | 37   | ALA  | 5.3  |
| 53  | D6    | 37   | LEU  | 5.3  |
| 18  | AS    | 65   | MET  | 5.3  |
| 8   | AI    | 16   | ALA  | 5.3  |
| 32  | D4    | 23   | ILE  | 5.3  |
| 32  | B4    | 23   | ILE  | 5.2  |
| 27  | BK    | 46   | ALA  | 5.2  |
| 40  | DH    | 149  | GLU  | 5.2  |
| 24  | DI    | 81   | LYS  | 5.1  |
| 23  | DB    | 1175 | A    | 5.1  |
| 53  | D6    | 46   | TYR  | 5.0  |
| 12  | CM    | 44   | ILE  | 5.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | CP    | 17   | TYR  | 5.0  |
| 24  | DI    | 6    | ALA  | 5.0  |
| 23  | BB    | 2146 | C    | 5.0  |
| 32  | B4    | 30   | GLU  | 5.0  |
| 18  | AS    | 39   | ILE  | 5.0  |
| 24  | BI    | 70   | THR  | 5.0  |
| 24  | BI    | 59   | THR  | 5.0  |
| 32  | B4    | 25   | VAL  | 4.9  |
| 32  | B4    | 36   | ARG  | 4.9  |
| 49  | BR    | 12   | HIS  | 4.9  |
| 1   | AA    | 86   | G    | 4.9  |
| 29  | BE    | 155  | GLU  | 4.9  |
| 24  | BI    | 54   | ILE  | 4.9  |
| 53  | B6    | 95   | LYS  | 4.9  |
| 32  | B4    | 31   | PRO  | 4.9  |
| 2   | CC    | 167  | TYR  | 4.8  |
| 24  | DI    | 53   | PRO  | 4.8  |
| 32  | D4    | 24   | ARG  | 4.8  |
| 7   | AH    | 126  | CYS  | 4.8  |
| 53  | B6    | 69   | GLN  | 4.7  |
| 53  | B6    | 84   | ARG  | 4.7  |
| 7   | AH    | 129  | ALA  | 4.7  |
| 43  | BO    | 28   | VAL  | 4.7  |
| 32  | D4    | 21   | GLY  | 4.7  |
| 53  | D6    | 38   | LEU  | 4.6  |
| 40  | BH    | 45   | GLU  | 4.6  |
| 49  | BR    | 13   | ARG  | 4.6  |
| 43  | BO    | 38   | GLN  | 4.6  |
| 23  | DB    | 139  | U    | 4.6  |
| 2   | CC    | 165  | GLU  | 4.6  |
| 32  | D4    | 17   | VAL  | 4.5  |
| 39  | BX    | 63   | ALA  | 4.5  |
| 32  | D4    | 36   | ARG  | 4.5  |
| 17  | AR    | 19   | GLU  | 4.5  |
| 24  | BI    | 115  | ASP  | 4.5  |
| 52  | BW    | 84   | GLU  | 4.4  |
| 13  | AN    | 30   | ILE  | 4.4  |
| 18  | AS    | 40   | PHE  | 4.4  |
| 11  | AL    | 123  | ALA  | 4.4  |
| 18  | CS    | 74   | ALA  | 4.3  |
| 1   | AA    | 121  | U    | 4.3  |
| 18  | AS    | 68   | HIS  | 4.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 20         | CB           | 212        | TYR         | 4.3         |
| 32         | D4           | 14         | CYS         | 4.3         |
| 53         | D6           | 95         | LYS         | 4.2         |
| 3          | AD           | 107        | GLY         | 4.2         |
| 43         | DO           | 38         | GLN         | 4.2         |
| 33         | B1           | 15         | GLY         | 4.2         |
| 6          | AG           | 78         | ARG         | 4.2         |
| 38         | BM           | 39         | GLY         | 4.2         |
| 51         | BZ           | 78         | TYR         | 4.2         |
| 48         | DG           | 41         | GLU         | 4.2         |
| 19         | AT           | 85         | LEU         | 4.2         |
| 53         | B6           | 35         | PRO         | 4.1         |
| 33         | B1           | 16         | THR         | 4.1         |
| 2          | AC           | 159        | ALA         | 4.1         |
| 39         | BX           | 62         | GLY         | 4.1         |
| 48         | DG           | 40         | VAL         | 4.1         |
| 39         | DX           | 1          | MET         | 4.1         |
| 6          | AG           | 79         | VAL         | 4.1         |
| 43         | DO           | 26         | LEU         | 4.1         |
| 2          | AC           | 167        | TYR         | 4.1         |
| 43         | BO           | 99         | TYR         | 4.1         |
| 53         | B6           | 87         | ASP         | 4.0         |
| 18         | AS           | 48         | ILE         | 4.0         |
| 24         | DI           | 49         | GLU         | 4.0         |
| 23         | BB           | 2139       | U           | 4.0         |
| 27         | BK           | 84         | CYS         | 4.0         |
| 53         | B6           | 88         | LEU         | 4.0         |
| 19         | AT           | 65         | LEU         | 4.0         |
| 20         | CB           | 163        | ILE         | 4.0         |
| 43         | BO           | 106        | LEU         | 3.9         |
| 32         | D4           | 22         | VAL         | 3.9         |
| 6          | AG           | 81         | GLY         | 3.9         |
| 32         | D4           | 11         | CYS         | 3.9         |
| 32         | B4           | 29         | ALA         | 3.9         |
| 43         | DO           | 28         | VAL         | 3.9         |
| 15         | CP           | 47         | GLU         | 3.9         |
| 15         | AP           | 17         | TYR         | 3.9         |
| 50         | BT           | 3          | ARG         | 3.9         |
| 52         | DW           | 65         | LYS         | 3.9         |
| 18         | AS           | 49         | ALA         | 3.9         |
| 32         | D4           | 37         | GLN         | 3.9         |
| 2          | AC           | 156        | LEU         | 3.9         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | CP    | 38   | PHE  | 3.9  |
| 32  | D4    | 27   | CYS  | 3.9  |
| 38  | DM    | 136  | MET  | 3.8  |
| 24  | BI    | 69   | VAL  | 3.8  |
| 1   | CA    | 1362 | A    | 3.8  |
| 32  | D4    | 9    | LYS  | 3.8  |
| 2   | AC    | 178  | ARG  | 3.8  |
| 43  | BO    | 107  | ALA  | 3.8  |
| 13  | AN    | 19   | TYR  | 3.8  |
| 40  | BH    | 27   | ARG  | 3.8  |
| 24  | BI    | 60   | VAL  | 3.8  |
| 24  | BI    | 8    | VAL  | 3.8  |
| 53  | B6    | 93   | SER  | 3.8  |
| 8   | AI    | 29   | ILE  | 3.8  |
| 16  | AQ    | 7    | LEU  | 3.8  |
| 40  | BH    | 1    | MET  | 3.8  |
| 43  | DO    | 59   | ALA  | 3.8  |
| 39  | BX    | 57   | LEU  | 3.8  |
| 15  | CP    | 52   | LEU  | 3.8  |
| 24  | DI    | 84   | GLY  | 3.7  |
| 23  | BB    | 2148 | G    | 3.7  |
| 33  | B1    | 51   | ALA  | 3.7  |
| 3   | AD    | 178  | GLU  | 3.7  |
| 29  | BE    | 143  | LEU  | 3.7  |
| 24  | DI    | 5    | GLN  | 3.7  |
| 12  | CM    | 42   | VAL  | 3.7  |
| 24  | BI    | 32   | VAL  | 3.7  |
| 32  | D4    | 16   | ILE  | 3.7  |
| 13  | CN    | 60   | ARG  | 3.7  |
| 32  | B4    | 27   | CYS  | 3.7  |
| 2   | AC    | 155  | ARG  | 3.7  |
| 9   | AJ    | 72   | ARG  | 3.7  |
| 38  | BM    | 33   | LEU  | 3.7  |
| 13  | CN    | 62   | ARG  | 3.7  |
| 46  | BU    | 93   | ARG  | 3.7  |
| 47  | DF    | 173  | ASP  | 3.7  |
| 13  | AN    | 54   | SER  | 3.7  |
| 18  | CS    | 31   | ARG  | 3.7  |
| 46  | BU    | 61   | GLU  | 3.7  |
| 47  | BF    | 103  | ILE  | 3.7  |
| 21  | AU    | 35   | GLU  | 3.7  |
| 24  | BI    | 57   | VAL  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 53  | B6    | 34  | ASN  | 3.7  |
| 51  | BZ    | 76  | GLU  | 3.6  |
| 53  | B6    | 36  | ALA  | 3.6  |
| 24  | BI    | 17  | ALA  | 3.6  |
| 41  | BJ    | 83  | GLY  | 3.6  |
| 19  | AT    | 66  | ILE  | 3.6  |
| 15  | CP    | 80  | LYS  | 3.6  |
| 32  | B4    | 38  | GLY  | 3.6  |
| 26  | BD    | 186 | LEU  | 3.6  |
| 32  | D4    | 18  | LYS  | 3.6  |
| 7   | CH    | 120 | LEU  | 3.6  |
| 23  | DB    | 846 | U    | 3.6  |
| 3   | AD    | 3   | TYR  | 3.6  |
| 33  | D1    | 20  | TYR  | 3.6  |
| 20  | CB    | 56  | LEU  | 3.6  |
| 24  | BI    | 71  | LYS  | 3.6  |
| 8   | CI    | 40  | ARG  | 3.6  |
| 19  | AT    | 86  | ALA  | 3.6  |
| 30  | DY    | 1   | ALA  | 3.6  |
| 43  | DO    | 53  | THR  | 3.6  |
| 9   | AJ    | 10  | LEU  | 3.5  |
| 32  | D4    | 19  | ARG  | 3.5  |
| 39  | BX    | 5   | GLU  | 3.5  |
| 5   | CF    | 90  | MET  | 3.5  |
| 30  | DY    | 28  | LEU  | 3.5  |
| 18  | AS    | 60  | PHE  | 3.5  |
| 43  | DO    | 61  | GLN  | 3.5  |
| 38  | BM    | 105 | MET  | 3.5  |
| 18  | CS    | 39  | ILE  | 3.5  |
| 40  | DH    | 122 | LEU  | 3.5  |
| 43  | BO    | 115 | LEU  | 3.5  |
| 32  | B4    | 22  | VAL  | 3.5  |
| 20  | CB    | 184 | ALA  | 3.5  |
| 48  | BG    | 120 | ILE  | 3.5  |
| 32  | D4    | 30  | GLU  | 3.5  |
| 50  | BT    | 65  | GLY  | 3.5  |
| 10  | AK    | 126 | ARG  | 3.5  |
| 19  | AT    | 38  | ILE  | 3.5  |
| 24  | BI    | 52  | LEU  | 3.5  |
| 43  | DO    | 60  | GLU  | 3.5  |
| 46  | BU    | 59  | GLU  | 3.5  |
| 33  | B1    | 14  | ALA  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 43  | BO    | 92   | PHE  | 3.5  |
| 32  | D4    | 8    | LYS  | 3.5  |
| 12  | AM    | 91   | ARG  | 3.5  |
| 48  | BG    | 8    | VAL  | 3.5  |
| 24  | DI    | 62   | ALA  | 3.5  |
| 53  | B6    | 98   | ALA  | 3.5  |
| 19  | CT    | 66   | ILE  | 3.5  |
| 23  | DB    | 140  | C    | 3.4  |
| 11  | CL    | 89   | LEU  | 3.4  |
| 24  | DI    | 9    | LYS  | 3.4  |
| 8   | AI    | 8    | THR  | 3.4  |
| 40  | BH    | 85   | GLY  | 3.4  |
| 32  | D4    | 1    | MET  | 3.4  |
| 43  | BO    | 29   | HIS  | 3.4  |
| 8   | AI    | 78   | ILE  | 3.4  |
| 50  | DT    | 11   | LEU  | 3.4  |
| 52  | BW    | 43   | LYS  | 3.4  |
| 53  | B6    | 41   | LEU  | 3.4  |
| 19  | AT    | 35   | TYR  | 3.4  |
| 31  | D0    | 47   | TYR  | 3.4  |
| 15  | AP    | 6    | LEU  | 3.4  |
| 15  | CP    | 9    | HIS  | 3.4  |
| 9   | CJ    | 35   | GLN  | 3.4  |
| 50  | BT    | 82   | LYS  | 3.4  |
| 7   | AH    | 128  | VAL  | 3.4  |
| 20  | AB    | 100  | LEU  | 3.4  |
| 23  | BB    | 1175 | A    | 3.4  |
| 32  | D4    | 34   | LYS  | 3.4  |
| 40  | DH    | 83   | LYS  | 3.4  |
| 53  | B6    | 48   | ALA  | 3.4  |
| 7   | AH    | 102  | VAL  | 3.4  |
| 43  | DO    | 27   | VAL  | 3.4  |
| 20  | CB    | 130  | LYS  | 3.4  |
| 19  | AT    | 71   | ALA  | 3.4  |
| 23  | BB    | 2140 | G    | 3.4  |
| 16  | AQ    | 6    | THR  | 3.4  |
| 8   | AI    | 21   | LYS  | 3.4  |
| 53  | B6    | 100  | TYR  | 3.4  |
| 53  | B6    | 38   | LEU  | 3.4  |
| 6   | CG    | 84   | TYR  | 3.4  |
| 32  | B4    | 8    | LYS  | 3.4  |
| 44  | DQ    | 117  | ALA  | 3.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 13         | AN           | 52         | ARG         | 3.4         |
| 51         | DZ           | 6          | GLN         | 3.4         |
| 53         | D6           | 66         | LEU         | 3.4         |
| 52         | BW           | 39         | GLN         | 3.4         |
| 41         | DJ           | 74         | TYR         | 3.4         |
| 53         | B6           | 67         | VAL         | 3.4         |
| 5          | AF           | 62         | MET         | 3.4         |
| 35         | DV           | 91         | PHE         | 3.4         |
| 12         | AM           | 92         | ARG         | 3.4         |
| 19         | CT           | 60         | GLN         | 3.4         |
| 38         | BM           | 32         | GLY         | 3.3         |
| 50         | DT           | 14         | PRO         | 3.3         |
| 40         | DH           | 80         | ILE         | 3.3         |
| 24         | BI           | 72         | THR         | 3.3         |
| 46         | BU           | 52         | ASN         | 3.3         |
| 35         | BV           | 82         | TYR         | 3.3         |
| 48         | BG           | 42         | VAL         | 3.3         |
| 18         | AS           | 42         | ASN         | 3.3         |
| 47         | BF           | 129        | MET         | 3.3         |
| 13         | AN           | 51         | PRO         | 3.3         |
| 48         | DG           | 160        | GLY         | 3.3         |
| 50         | BT           | 83         | ALA         | 3.3         |
| 15         | CP           | 15         | PRO         | 3.3         |
| 26         | BD           | 188        | LEU         | 3.3         |
| 50         | DT           | 12         | ARG         | 3.3         |
| 2          | AC           | 158        | GLY         | 3.3         |
| 40         | DH           | 82         | SER         | 3.3         |
| 48         | DG           | 116        | LEU         | 3.3         |
| 50         | BT           | 11         | LEU         | 3.3         |
| 42         | BN           | 20         | MET         | 3.3         |
| 12         | AM           | 4          | ALA         | 3.3         |
| 24         | BI           | 34         | ILE         | 3.3         |
| 6          | CG           | 74         | VAL         | 3.3         |
| 26         | BD           | 4          | LEU         | 3.3         |
| 15         | CP           | 7          | ALA         | 3.3         |
| 20         | CB           | 67         | LEU         | 3.3         |
| 43         | BO           | 93         | ASP         | 3.3         |
| 53         | D6           | 41         | LEU         | 3.3         |
| 41         | DJ           | 52         | ASP         | 3.3         |
| 48         | DG           | 114        | HIS         | 3.3         |
| 6          | CG           | 85         | GLN         | 3.3         |
| 38         | BM           | 67         | VAL         | 3.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 46  | DU    | 63   | ALA  | 3.2  |
| 35  | DV    | 74   | ALA  | 3.2  |
| 1   | CA    | 1534 | A    | 3.2  |
| 25  | DC    | 33   | LEU  | 3.2  |
| 40  | DH    | 81   | ALA  | 3.2  |
| 16  | AQ    | 74   | LEU  | 3.2  |
| 9   | CJ    | 65   | TYR  | 3.2  |
| 32  | B4    | 37   | GLN  | 3.2  |
| 29  | BE    | 148  | ILE  | 3.2  |
| 53  | B6    | 90   | LEU  | 3.2  |
| 20  | CB    | 79   | VAL  | 3.2  |
| 53  | D6    | 45   | TYR  | 3.2  |
| 24  | DI    | 83   | ALA  | 3.2  |
| 28  | BP    | 70   | GLU  | 3.2  |
| 6   | AG    | 80   | GLY  | 3.2  |
| 40  | DH    | 94   | ILE  | 3.2  |
| 24  | DI    | 82   | ALA  | 3.2  |
| 43  | BO    | 88   | LYS  | 3.2  |
| 18  | AS    | 73   | PHE  | 3.2  |
| 53  | B6    | 47   | GLY  | 3.2  |
| 49  | BR    | 22   | LEU  | 3.2  |
| 24  | BI    | 18   | ASN  | 3.2  |
| 24  | BI    | 19   | PRO  | 3.2  |
| 24  | BI    | 116  | MET  | 3.2  |
| 23  | BB    | 1176 | U    | 3.2  |
| 39  | DX    | 62   | GLY  | 3.2  |
| 49  | BR    | 3    | ALA  | 3.2  |
| 24  | BI    | 56   | VAL  | 3.2  |
| 46  | BU    | 14   | THR  | 3.2  |
| 48  | DG    | 161  | VAL  | 3.2  |
| 21  | CU    | 34   | ARG  | 3.2  |
| 15  | AP    | 5    | ARG  | 3.2  |
| 24  | BI    | 31   | GLY  | 3.2  |
| 32  | B4    | 33   | HIS  | 3.2  |
| 23  | DB    | 141  | G    | 3.2  |
| 8   | CI    | 34   | LEU  | 3.2  |
| 24  | BI    | 11   | GLN  | 3.2  |
| 23  | BB    | 2141 | G    | 3.1  |
| 53  | B6    | 49   | HIS  | 3.1  |
| 23  | DB    | 613  | A    | 3.1  |
| 43  | BO    | 102  | ARG  | 3.1  |
| 53  | D6    | 79   | ILE  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | D6    | 99   | LEU  | 3.1  |
| 50  | DT    | 53   | VAL  | 3.1  |
| 15  | CP    | 37   | GLY  | 3.1  |
| 43  | DO    | 92   | PHE  | 3.1  |
| 48  | DG    | 176  | LYS  | 3.1  |
| 18  | AS    | 43   | MET  | 3.1  |
| 12  | AM    | 90   | HIS  | 3.1  |
| 32  | B4    | 9    | LYS  | 3.1  |
| 22  | DA    | 88   | C    | 3.1  |
| 23  | DB    | 143  | C    | 3.1  |
| 53  | B6    | 110  | ARG  | 3.1  |
| 20  | AB    | 192  | PRO  | 3.1  |
| 20  | CB    | 68   | PHE  | 3.1  |
| 24  | DI    | 99   | LYS  | 3.1  |
| 19  | CT    | 65   | LEU  | 3.1  |
| 23  | BB    | 141  | G    | 3.1  |
| 38  | BM    | 40   | ARG  | 3.1  |
| 13  | AN    | 58   | ARG  | 3.1  |
| 51  | DZ    | 49   | LEU  | 3.1  |
| 53  | B6    | 75   | ALA  | 3.1  |
| 15  | CP    | 6    | LEU  | 3.0  |
| 25  | DC    | 5    | CYS  | 3.1  |
| 13  | AN    | 20   | PHE  | 3.0  |
| 2   | AC    | 102  | ILE  | 3.0  |
| 24  | DI    | 79   | LEU  | 3.0  |
| 44  | DQ    | 90   | ASP  | 3.0  |
| 47  | BF    | 153  | ILE  | 3.0  |
| 1   | AA    | 1150 | A    | 3.0  |
| 26  | BD    | 27   | ILE  | 3.0  |
| 8   | AI    | 20   | ILE  | 3.0  |
| 20  | CB    | 150  | ILE  | 3.0  |
| 24  | DI    | 80   | LYS  | 3.0  |
| 23  | BB    | 846  | U    | 3.0  |
| 32  | D4    | 31   | PRO  | 3.0  |
| 30  | BY    | 8    | GLN  | 3.0  |
| 48  | BG    | 132  | LEU  | 3.0  |
| 26  | BD    | 111  | GLY  | 3.0  |
| 38  | DM    | 1    | MET  | 3.0  |
| 47  | BF    | 127  | TYR  | 3.0  |
| 1   | AA    | 407  | U    | 3.0  |
| 3   | AD    | 2    | ARG  | 3.0  |
| 21  | AU    | 34   | ARG  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | BE    | 1    | MET  | 3.0  |
| 10  | AK    | 92   | ARG  | 3.0  |
| 13  | AN    | 23   | ARG  | 3.0  |
| 20  | AB    | 193  | ASP  | 3.0  |
| 43  | BO    | 35   | ILE  | 3.0  |
| 21  | CU    | 35   | GLU  | 3.0  |
| 48  | DG    | 150  | TYR  | 3.0  |
| 32  | D4    | 2    | LYS  | 3.0  |
| 3   | AD    | 108  | ALA  | 3.0  |
| 24  | DI    | 85   | ILE  | 3.0  |
| 24  | BI    | 27   | LEU  | 3.0  |
| 53  | B6    | 40   | HIS  | 3.0  |
| 8   | AI    | 65   | THR  | 3.0  |
| 24  | BI    | 68   | PHE  | 3.0  |
| 3   | AD    | 22   | SER  | 3.0  |
| 33  | D1    | 52   | LYS  | 3.0  |
| 43  | DO    | 36   | TYR  | 3.0  |
| 32  | D4    | 26   | ILE  | 3.0  |
| 26  | BD    | 187  | LEU  | 3.0  |
| 47  | DF    | 111  | ARG  | 3.0  |
| 38  | BM    | 128  | THR  | 3.0  |
| 53  | B6    | 59   | THR  | 3.0  |
| 4   | CE    | 50   | GLY  | 3.0  |
| 53  | D6    | 94   | ASN  | 3.0  |
| 2   | CC    | 166  | TRP  | 3.0  |
| 17  | CR    | 22   | TYR  | 3.0  |
| 50  | DT    | 42   | GLU  | 3.0  |
| 19  | AT    | 41   | GLY  | 3.0  |
| 35  | DV    | 79   | ARG  | 3.0  |
| 7   | AH    | 125  | ILE  | 3.0  |
| 23  | DB    | 2402 | U    | 3.0  |
| 34  | B3    | 60   | CYS  | 3.0  |
| 6   | CG    | 108  | ARG  | 3.0  |
| 53  | B6    | 37   | LEU  | 3.0  |
| 2   | AC    | 179  | ALA  | 3.0  |
| 8   | AI    | 47   | VAL  | 2.9  |
| 9   | AJ    | 42   | LEU  | 2.9  |
| 18  | AS    | 75   | PRO  | 2.9  |
| 33  | D1    | 18   | HIS  | 2.9  |
| 17  | CR    | 66   | LEU  | 2.9  |
| 38  | BM    | 102  | LEU  | 2.9  |
| 1   | CA    | 1001 | C    | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 12  | CM    | 92  | ARG  | 2.9  |
| 13  | AN    | 62  | ARG  | 2.9  |
| 53  | B6    | 96  | GLY  | 2.9  |
| 6   | AG    | 150 | PHE  | 2.9  |
| 15  | AP    | 38  | PHE  | 2.9  |
| 18  | CS    | 75  | PRO  | 2.9  |
| 13  | CN    | 42  | ASN  | 2.9  |
| 29  | BE    | 124 | PHE  | 2.9  |
| 2   | CC    | 151 | GLU  | 2.9  |
| 35  | DV    | 31  | TYR  | 2.9  |
| 18  | AS    | 74  | ALA  | 2.9  |
| 47  | DF    | 174 | PHE  | 2.9  |
| 18  | AS    | 70  | LEU  | 2.9  |
| 48  | DG    | 172 | GLU  | 2.9  |
| 24  | BI    | 80  | LYS  | 2.9  |
| 3   | AD    | 121 | ALA  | 2.9  |
| 20  | CB    | 215 | ALA  | 2.9  |
| 48  | DG    | 89  | VAL  | 2.9  |
| 21  | CU    | 36  | PHE  | 2.9  |
| 24  | BI    | 73  | PRO  | 2.9  |
| 43  | DO    | 97  | PHE  | 2.9  |
| 53  | B6    | 62  | ASP  | 2.9  |
| 15  | AP    | 52  | LEU  | 2.9  |
| 46  | DU    | 4   | ILE  | 2.9  |
| 2   | AC    | 48  | LYS  | 2.9  |
| 30  | BY    | 55  | LYS  | 2.9  |
| 40  | DH    | 110 | VAL  | 2.9  |
| 49  | BR    | 14  | VAL  | 2.9  |
| 7   | AH    | 100 | ILE  | 2.9  |
| 24  | DI    | 44  | LYS  | 2.9  |
| 38  | BM    | 129 | THR  | 2.9  |
| 47  | DF    | 178 | LYS  | 2.9  |
| 15  | CP    | 18  | GLN  | 2.9  |
| 24  | DI    | 8   | VAL  | 2.9  |
| 32  | D4    | 10  | LEU  | 2.9  |
| 48  | BG    | 116 | LEU  | 2.9  |
| 35  | DV    | 29  | ILE  | 2.9  |
| 43  | DO    | 62  | LEU  | 2.9  |
| 13  | AN    | 77  | GLY  | 2.9  |
| 8   | AI    | 63  | TYR  | 2.9  |
| 12  | AM    | 18  | LEU  | 2.9  |
| 2   | AC    | 205 | GLU  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | BG    | 114  | HIS  | 2.9  |
| 49  | DR    | 66   | HIS  | 2.9  |
| 24  | DI    | 29   | GLN  | 2.9  |
| 29  | DE    | 105  | LEU  | 2.9  |
| 38  | BM    | 65   | ILE  | 2.9  |
| 50  | BT    | 84   | TYR  | 2.9  |
| 53  | B6    | 63   | PRO  | 2.9  |
| 3   | AD    | 203  | TYR  | 2.9  |
| 20  | CB    | 52   | ALA  | 2.9  |
| 2   | AC    | 171  | ARG  | 2.9  |
| 19  | AT    | 45   | ALA  | 2.9  |
| 18  | AS    | 64   | GLU  | 2.8  |
| 33  | D1    | 10   | LEU  | 2.8  |
| 24  | BI    | 14   | ALA  | 2.8  |
| 20  | CB    | 91   | VAL  | 2.8  |
| 43  | BO    | 103  | VAL  | 2.8  |
| 53  | D6    | 100  | TYR  | 2.8  |
| 15  | CP    | 39   | PHE  | 2.8  |
| 20  | AB    | 8    | MET  | 2.8  |
| 52  | BW    | 42   | THR  | 2.8  |
| 32  | D4    | 4    | ARG  | 2.8  |
| 35  | DV    | 42   | LEU  | 2.8  |
| 53  | B6    | 91   | ASN  | 2.8  |
| 38  | BM    | 93   | VAL  | 2.8  |
| 15  | CP    | 14   | ARG  | 2.8  |
| 43  | BO    | 26   | LEU  | 2.8  |
| 2   | CC    | 55   | VAL  | 2.8  |
| 23  | BB    | 1095 | A    | 2.8  |
| 23  | DB    | 2148 | G    | 2.8  |
| 13  | AN    | 53   | ASP  | 2.8  |
| 29  | BE    | 144  | GLU  | 2.8  |
| 31  | D0    | 35   | GLU  | 2.8  |
| 39  | BX    | 60   | LYS  | 2.8  |
| 18  | AS    | 47   | THR  | 2.8  |
| 24  | BI    | 79   | LEU  | 2.8  |
| 27  | BK    | 8    | LEU  | 2.8  |
| 35  | BV    | 86   | LEU  | 2.8  |
| 32  | D4    | 5    | ALA  | 2.8  |
| 24  | BI    | 86   | LYS  | 2.8  |
| 24  | DI    | 54   | ILE  | 2.8  |
| 50  | BT    | 58   | VAL  | 2.8  |
| 53  | B6    | 80   | GLU  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 15  | CP    | 10  | GLY  | 2.8  |
| 21  | AU    | 3   | ILE  | 2.8  |
| 20  | CB    | 38  | HIS  | 2.8  |
| 41  | BJ    | 122 | LEU  | 2.8  |
| 23  | BB    | 715 | A    | 2.8  |
| 43  | BO    | 51  | ALA  | 2.8  |
| 27  | BK    | 45  | GLU  | 2.8  |
| 40  | BH    | 18  | GLN  | 2.8  |
| 49  | DR    | 12  | HIS  | 2.8  |
| 49  | BR    | 20  | VAL  | 2.8  |
| 20  | AB    | 212 | TYR  | 2.8  |
| 22  | DA    | 52  | A    | 2.8  |
| 45  | BS    | 94  | ASP  | 2.8  |
| 24  | BI    | 81  | LYS  | 2.8  |
| 41  | BJ    | 82  | GLY  | 2.8  |
| 16  | CQ    | 6   | THR  | 2.8  |
| 20  | CB    | 213 | LEU  | 2.8  |
| 35  | DV    | 50  | MET  | 2.8  |
| 33  | D1    | 8   | ILE  | 2.8  |
| 24  | BI    | 78  | LEU  | 2.8  |
| 53  | B6    | 86  | SER  | 2.8  |
| 46  | DU    | 61  | GLU  | 2.8  |
| 8   | AI    | 18  | VAL  | 2.8  |
| 21  | CU    | 32  | ARG  | 2.8  |
| 8   | CI    | 31  | GLN  | 2.8  |
| 45  | BS    | 74  | ILE  | 2.8  |
| 16  | AQ    | 35  | LYS  | 2.8  |
| 41  | BJ    | 123 | LYS  | 2.8  |
| 12  | CM    | 91  | ARG  | 2.8  |
| 15  | AP    | 22  | ALA  | 2.8  |
| 8   | AI    | 97  | LEU  | 2.8  |
| 20  | AB    | 216 | VAL  | 2.8  |
| 18  | AS    | 58  | PRO  | 2.8  |
| 8   | AI    | 102 | PHE  | 2.8  |
| 37  | BL    | 112 | LEU  | 2.8  |
| 47  | DF    | 169 | LEU  | 2.8  |
| 2   | AC    | 71  | ARG  | 2.8  |
| 9   | CJ    | 25  | ILE  | 2.8  |
| 26  | DD    | 2   | ILE  | 2.8  |
| 40  | DH    | 72  | ILE  | 2.8  |
| 7   | CH    | 122 | GLY  | 2.7  |
| 8   | AI    | 9   | GLY  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | BP    | 96   | LEU  | 2.7  |
| 49  | BR    | 93   | PHE  | 2.7  |
| 28  | BP    | 61   | ARG  | 2.7  |
| 49  | BR    | 21   | ARG  | 2.7  |
| 7   | AH    | 83   | ARG  | 2.7  |
| 53  | D6    | 43   | VAL  | 2.7  |
| 32  | D4    | 15   | LYS  | 2.7  |
| 13  | CN    | 93   | PRO  | 2.7  |
| 1   | AA    | 85   | U    | 2.7  |
| 43  | BO    | 27   | VAL  | 2.7  |
| 40  | BH    | 12   | LEU  | 2.7  |
| 12  | CM    | 3    | ILE  | 2.7  |
| 46  | DU    | 62   | ALA  | 2.7  |
| 8   | AI    | 66   | VAL  | 2.7  |
| 18  | AS    | 59   | VAL  | 2.7  |
| 23  | BB    | 2138 | G    | 2.7  |
| 38  | DM    | 60   | GLN  | 2.7  |
| 12  | AM    | 21   | ILE  | 2.7  |
| 50  | DT    | 90   | GLY  | 2.7  |
| 12  | AM    | 86   | ARG  | 2.7  |
| 49  | BR    | 72   | VAL  | 2.7  |
| 1   | AA    | 65   | A    | 2.7  |
| 18  | AS    | 38   | THR  | 2.7  |
| 47  | BF    | 156  | THR  | 2.7  |
| 8   | AI    | 15   | ALA  | 2.7  |
| 31  | D0    | 45   | ASP  | 2.7  |
| 49  | BR    | 40   | MET  | 2.7  |
| 22  | DA    | 25   | U    | 2.7  |
| 50  | BT    | 42   | GLU  | 2.7  |
| 16  | CQ    | 44   | HIS  | 2.7  |
| 51  | BZ    | 77   | LYS  | 2.7  |
| 8   | AI    | 19   | PHE  | 2.7  |
| 15  | CP    | 36   | VAL  | 2.7  |
| 38  | BM    | 95   | LEU  | 2.7  |
| 41  | BJ    | 84   | ILE  | 2.7  |
| 1   | CA    | 121  | U    | 2.7  |
| 20  | CB    | 129  | THR  | 2.7  |
| 25  | DC    | 61   | TYR  | 2.7  |
| 34  | D3    | 19   | GLY  | 2.7  |
| 3   | AD    | 1    | ALA  | 2.7  |
| 19  | AT    | 39   | GLU  | 2.7  |
| 33  | B1    | 10   | LEU  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | DG    | 147  | LEU  | 2.7  |
| 30  | BY    | 56   | VAL  | 2.7  |
| 43  | BO    | 81   | ARG  | 2.7  |
| 12  | AM    | 38   | ILE  | 2.7  |
| 12  | AM    | 55   | LEU  | 2.7  |
| 24  | DI    | 78   | LEU  | 2.7  |
| 31  | D0    | 56   | LYS  | 2.7  |
| 20  | CB    | 69   | VAL  | 2.7  |
| 47  | BF    | 30   | VAL  | 2.7  |
| 6   | CG    | 100  | MET  | 2.7  |
| 47  | BF    | 155  | ILE  | 2.7  |
| 49  | BR    | 2    | TYR  | 2.7  |
| 20  | AB    | 24   | PRO  | 2.7  |
| 12  | CM    | 90   | HIS  | 2.7  |
| 23  | BB    | 1537 | G    | 2.7  |
| 43  | BO    | 110  | ALA  | 2.7  |
| 51  | DZ    | 77   | LYS  | 2.7  |
| 23  | BB    | 2402 | U    | 2.7  |
| 24  | DI    | 125  | THR  | 2.7  |
| 27  | BK    | 110  | GLU  | 2.7  |
| 40  | BH    | 25   | TYR  | 2.7  |
| 46  | DU    | 3    | LYS  | 2.7  |
| 52  | DW    | 83   | ALA  | 2.7  |
| 3   | AD    | 129  | VAL  | 2.6  |
| 19  | CT    | 57   | VAL  | 2.6  |
| 23  | BB    | 2155 | U    | 2.6  |
| 14  | AO    | 17   | ARG  | 2.6  |
| 30  | BY    | 15   | ARG  | 2.6  |
| 3   | AD    | 4    | LEU  | 2.6  |
| 5   | AF    | 6    | ILE  | 2.6  |
| 41  | BJ    | 54   | ILE  | 2.6  |
| 43  | DO    | 25   | ARG  | 2.6  |
| 48  | BG    | 49   | LEU  | 2.6  |
| 52  | BW    | 77   | LYS  | 2.6  |
| 2   | AC    | 161  | ILE  | 2.6  |
| 45  | BS    | 103  | ILE  | 2.6  |
| 50  | BT    | 81   | LYS  | 2.6  |
| 1   | AA    | 972  | C    | 2.6  |
| 43  | DO    | 29   | HIS  | 2.6  |
| 49  | DR    | 27   | ILE  | 2.6  |
| 18  | CS    | 70   | LEU  | 2.6  |
| 19  | CT    | 71   | ALA  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 50  | BT    | 32   | LEU  | 2.6  |
| 53  | D6    | 42   | LYS  | 2.6  |
| 8   | AI    | 30   | ASN  | 2.6  |
| 10  | CK    | 12   | ARG  | 2.6  |
| 17  | CR    | 60   | ARG  | 2.6  |
| 9   | AJ    | 73   | LEU  | 2.6  |
| 27  | BK    | 21   | CYS  | 2.6  |
| 38  | BM    | 96   | ILE  | 2.6  |
| 23  | DB    | 645  | C    | 2.6  |
| 43  | BO    | 95   | SER  | 2.6  |
| 12  | CM    | 78   | ARG  | 2.6  |
| 53  | D6    | 32   | ARG  | 2.6  |
| 9   | CJ    | 36   | VAL  | 2.6  |
| 26  | BD    | 25   | THR  | 2.6  |
| 13  | CN    | 46   | LYS  | 2.6  |
| 24  | BI    | 117  | THR  | 2.6  |
| 47  | BF    | 99   | PHE  | 2.6  |
| 6   | AG    | 29   | LEU  | 2.6  |
| 16  | AQ    | 43   | LEU  | 2.6  |
| 50  | DT    | 72   | GLN  | 2.6  |
| 53  | B6    | 104  | PRO  | 2.6  |
| 15  | AP    | 7    | ALA  | 2.6  |
| 53  | B6    | 85   | ASP  | 2.6  |
| 46  | DU    | 24   | VAL  | 2.6  |
| 15  | CP    | 8    | ARG  | 2.6  |
| 41  | DJ    | 64   | VAL  | 2.6  |
| 3   | AD    | 177  | MET  | 2.6  |
| 42  | BN    | 1    | MET  | 2.6  |
| 25  | DC    | 62   | ARG  | 2.6  |
| 46  | DU    | 34   | ILE  | 2.6  |
| 18  | AS    | 50   | VAL  | 2.6  |
| 21  | AU    | 36   | PHE  | 2.6  |
| 46  | BU    | 17   | ASP  | 2.6  |
| 2   | CC    | 156  | LEU  | 2.6  |
| 1   | AA    | 1240 | U    | 2.6  |
| 9   | AJ    | 9    | ARG  | 2.6  |
| 48  | DG    | 54   | ARG  | 2.6  |
| 49  | DR    | 50   | GLY  | 2.6  |
| 20  | CB    | 99   | MET  | 2.6  |
| 31  | D0    | 36   | LYS  | 2.6  |
| 31  | B0    | 42   | ILE  | 2.6  |
| 35  | DV    | 30   | ILE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 38  | BM    | 17  | ASN  | 2.6  |
| 40  | BH    | 105 | ALA  | 2.6  |
| 50  | DT    | 91  | GLN  | 2.6  |
| 2   | CC    | 133 | MET  | 2.6  |
| 20  | CB    | 36  | LYS  | 2.6  |
| 6   | CG    | 29  | LEU  | 2.6  |
| 35  | BV    | 83  | LYS  | 2.6  |
| 37  | BL    | 45  | GLY  | 2.6  |
| 48  | DG    | 55  | ASP  | 2.6  |
| 2   | AC    | 162 | ALA  | 2.6  |
| 26  | BD    | 3   | GLY  | 2.6  |
| 48  | DG    | 90  | GLY  | 2.6  |
| 53  | B6    | 99  | LEU  | 2.6  |
| 24  | DI    | 21  | PRO  | 2.6  |
| 26  | BD    | 75  | ALA  | 2.6  |
| 46  | DU    | 59  | GLU  | 2.6  |
| 4   | AE    | 158 | LYS  | 2.6  |
| 15  | AP    | 23  | ASP  | 2.6  |
| 32  | D4    | 3   | VAL  | 2.6  |
| 40  | BH    | 19  | VAL  | 2.5  |
| 13  | AN    | 16  | ALA  | 2.5  |
| 50  | BT    | 5   | GLU  | 2.5  |
| 13  | CN    | 95  | LEU  | 2.5  |
| 24  | DI    | 115 | ASP  | 2.5  |
| 33  | D1    | 35  | LEU  | 2.5  |
| 41  | BJ    | 74  | TYR  | 2.5  |
| 8   | AI    | 64  | ILE  | 2.5  |
| 15  | AP    | 4   | ILE  | 2.5  |
| 38  | BM    | 19  | GLY  | 2.5  |
| 2   | AC    | 150 | VAL  | 2.5  |
| 1   | AA    | 971 | G    | 2.5  |
| 48  | BG    | 117 | PRO  | 2.5  |
| 44  | BQ    | 90  | ASP  | 2.5  |
| 10  | CK    | 55  | ARG  | 2.5  |
| 18  | AS    | 10  | ILE  | 2.5  |
| 49  | BR    | 88  | GLY  | 2.5  |
| 25  | BC    | 1   | ALA  | 2.5  |
| 25  | BC    | 34  | GLU  | 2.5  |
| 44  | BQ    | 94  | LEU  | 2.5  |
| 53  | B6    | 184 | LEU  | 2.5  |
| 7   | AH    | 110 | MET  | 2.5  |
| 8   | AI    | 10  | ARG  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 12  | CM    | 43  | LYS  | 2.5  |
| 20  | CB    | 127 | LYS  | 2.5  |
| 49  | BR    | 85  | LYS  | 2.5  |
| 47  | BF    | 31  | GLU  | 2.5  |
| 53  | D6    | 96  | GLY  | 2.5  |
| 2   | AC    | 75  | VAL  | 2.5  |
| 47  | DF    | 30  | VAL  | 2.5  |
| 16  | AQ    | 46  | HIS  | 2.5  |
| 19  | AT    | 42  | ASP  | 2.5  |
| 34  | B3    | 19  | GLY  | 2.5  |
| 47  | BF    | 35  | LEU  | 2.5  |
| 49  | DR    | 101 | ILE  | 2.5  |
| 3   | AD    | 153 | ARG  | 2.5  |
| 20  | CB    | 195 | VAL  | 2.5  |
| 15  | AP    | 1   | MET  | 2.5  |
| 3   | AD    | 106 | PHE  | 2.5  |
| 4   | CE    | 32  | PHE  | 2.5  |
| 24  | DI    | 98  | GLY  | 2.5  |
| 9   | CJ    | 40  | ILE  | 2.5  |
| 28  | BP    | 54  | LEU  | 2.5  |
| 43  | BO    | 114 | GLY  | 2.5  |
| 23  | BB    | 645 | C    | 2.5  |
| 24  | DI    | 116 | MET  | 2.5  |
| 42  | DN    | 112 | TYR  | 2.5  |
| 49  | BR    | 11  | GLN  | 2.5  |
| 6   | AG    | 58  | LEU  | 2.5  |
| 24  | BI    | 97  | VAL  | 2.5  |
| 13  | CN    | 59  | GLN  | 2.5  |
| 41  | DJ    | 87  | ALA  | 2.5  |
| 20  | CB    | 157 | PRO  | 2.5  |
| 43  | DO    | 40  | ILE  | 2.5  |
| 50  | DT    | 34  | VAL  | 2.5  |
| 50  | DT    | 55  | VAL  | 2.5  |
| 53  | B6    | 92  | PRO  | 2.5  |
| 7   | AH    | 74  | ILE  | 2.5  |
| 18  | AS    | 14  | LEU  | 2.5  |
| 2   | AC    | 165 | GLU  | 2.5  |
| 20  | AB    | 99  | MET  | 2.5  |
| 12  | AM    | 87  | GLY  | 2.5  |
| 13  | CN    | 9   | GLU  | 2.5  |
| 38  | BM    | 66  | ARG  | 2.5  |
| 10  | AK    | 88  | PRO  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | CM    | 47   | LEU  | 2.5  |
| 41  | DJ    | 86   | GLN  | 2.5  |
| 47  | DF    | 82   | TYR  | 2.5  |
| 11  | AL    | 122  | LYS  | 2.5  |
| 12  | AM    | 84   | CYS  | 2.5  |
| 16  | AQ    | 38   | LYS  | 2.5  |
| 32  | B4    | 18   | LYS  | 2.5  |
| 38  | BM    | 1    | MET  | 2.5  |
| 28  | BP    | 47   | ILE  | 2.5  |
| 43  | DO    | 55   | GLU  | 2.5  |
| 26  | BD    | 72   | GLY  | 2.5  |
| 16  | AQ    | 36   | PHE  | 2.5  |
| 27  | DK    | 33   | ALA  | 2.5  |
| 38  | BM    | 71   | LYS  | 2.5  |
| 47  | BF    | 131  | VAL  | 2.5  |
| 50  | DT    | 70   | HIS  | 2.5  |
| 53  | B6    | 44   | GLU  | 2.5  |
| 1   | AA    | 134  | G    | 2.5  |
| 11  | AL    | 52   | CYS  | 2.5  |
| 5   | AF    | 8    | PHE  | 2.5  |
| 38  | BM    | 136  | MET  | 2.5  |
| 41  | BJ    | 1    | MET  | 2.5  |
| 18  | CS    | 30   | LEU  | 2.5  |
| 16  | AQ    | 52   | CYS  | 2.5  |
| 46  | DU    | 69   | VAL  | 2.5  |
| 53  | B6    | 78   | ALA  | 2.5  |
| 49  | BR    | 67   | GLY  | 2.5  |
| 5   | CF    | 88   | MET  | 2.5  |
| 21  | AU    | 44   | ARG  | 2.5  |
| 1   | AA    | 1363 | A    | 2.5  |
| 11  | AL    | 63   | THR  | 2.5  |
| 3   | CD    | 129  | VAL  | 2.5  |
| 11  | CL    | 86   | VAL  | 2.5  |
| 23  | BB    | 561  | G    | 2.5  |
| 6   | CG    | 4    | ARG  | 2.5  |
| 33  | B1    | 8    | ILE  | 2.5  |
| 49  | BR    | 46   | GLU  | 2.4  |
| 16  | CQ    | 8    | GLN  | 2.4  |
| 46  | DU    | 33   | VAL  | 2.4  |
| 17  | CR    | 20   | ILE  | 2.4  |
| 50  | BT    | 12   | ARG  | 2.4  |
| 51  | BZ    | 72   | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | AC    | 151  | GLU  | 2.4  |
| 28  | BP    | 76   | HIS  | 2.4  |
| 30  | BY    | 54   | VAL  | 2.4  |
| 24  | BI    | 82   | ALA  | 2.4  |
| 40  | BH    | 35   | LYS  | 2.4  |
| 8   | CI    | 20   | ILE  | 2.4  |
| 16  | AQ    | 60   | ILE  | 2.4  |
| 15  | CP    | 34   | GLU  | 2.4  |
| 9   | CJ    | 34   | ALA  | 2.4  |
| 41  | BJ    | 80   | HIS  | 2.4  |
| 43  | DO    | 117  | PHE  | 2.4  |
| 13  | AN    | 55   | SER  | 2.4  |
| 47  | BF    | 152  | ASP  | 2.4  |
| 49  | BR    | 5    | PHE  | 2.4  |
| 10  | CK    | 13   | LYS  | 2.4  |
| 16  | AQ    | 58   | VAL  | 2.4  |
| 26  | BD    | 165  | MET  | 2.4  |
| 44  | BQ    | 14   | LYS  | 2.4  |
| 25  | BC    | 102  | TYR  | 2.4  |
| 46  | BU    | 13   | LEU  | 2.4  |
| 23  | BB    | 2154 | A    | 2.4  |
| 38  | BM    | 94   | ALA  | 2.4  |
| 53  | B6    | 33   | ALA  | 2.4  |
| 38  | BM    | 73   | ILE  | 2.4  |
| 13  | AN    | 50   | LEU  | 2.4  |
| 35  | DV    | 86   | LEU  | 2.4  |
| 18  | CS    | 64   | GLU  | 2.4  |
| 38  | DM    | 37   | GLY  | 2.4  |
| 29  | DE    | 188  | MET  | 2.4  |
| 51  | BZ    | 47   | VAL  | 2.4  |
| 52  | BW    | 76   | ARG  | 2.4  |
| 50  | BT    | 35   | ALA  | 2.4  |
| 1   | AA    | 209  | U    | 2.4  |
| 3   | AD    | 83   | GLY  | 2.4  |
| 21  | AU    | 4    | LYS  | 2.4  |
| 32  | D4    | 32   | LYS  | 2.4  |
| 11  | CL    | 92   | VAL  | 2.4  |
| 25  | BC    | 3    | VAL  | 2.4  |
| 29  | BE    | 196  | VAL  | 2.4  |
| 40  | BH    | 30   | LEU  | 2.4  |
| 46  | DU    | 27   | VAL  | 2.4  |
| 48  | DG    | 117  | PRO  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 49  | BR    | 68   | ARG  | 2.4  |
| 2   | AC    | 134  | LYS  | 2.4  |
| 2   | CC    | 56   | ILE  | 2.4  |
| 40  | DH    | 141  | LYS  | 2.4  |
| 53  | B6    | 83   | ILE  | 2.4  |
| 53  | B6    | 97   | ASP  | 2.4  |
| 26  | BD    | 26   | VAL  | 2.4  |
| 6   | CG    | 78   | ARG  | 2.4  |
| 24  | DI    | 105  | LEU  | 2.4  |
| 47  | DF    | 175  | PRO  | 2.4  |
| 47  | DF    | 177  | ARG  | 2.4  |
| 53  | D6    | 29   | ARG  | 2.4  |
| 2   | AC    | 169  | GLU  | 2.4  |
| 9   | AJ    | 37   | ARG  | 2.4  |
| 16  | CQ    | 7    | LEU  | 2.4  |
| 23  | BB    | 1536 | C    | 2.4  |
| 23  | BB    | 2157 | G    | 2.4  |
| 24  | DI    | 48   | ILE  | 2.4  |
| 34  | D3    | 14   | LYS  | 2.4  |
| 35  | BV    | 91   | PHE  | 2.4  |
| 6   | CG    | 70   | PRO  | 2.4  |
| 46  | BU    | 51   | LEU  | 2.4  |
| 53  | B6    | 39   | LEU  | 2.4  |
| 20  | CB    | 220  | VAL  | 2.4  |
| 42  | BN    | 16   | HIS  | 2.4  |
| 45  | DS    | 24   | ILE  | 2.4  |
| 1   | AA    | 54   | C    | 2.4  |
| 12  | CM    | 82   | LEU  | 2.4  |
| 15  | CP    | 41   | PRO  | 2.4  |
| 16  | AQ    | 9    | GLY  | 2.4  |
| 24  | DI    | 106  | GLN  | 2.4  |
| 49  | DR    | 76   | LYS  | 2.4  |
| 33  | D1    | 22   | THR  | 2.4  |
| 38  | BM    | 41   | LEU  | 2.4  |
| 47  | BF    | 174  | PHE  | 2.4  |
| 5   | AF    | 59   | TYR  | 2.4  |
| 16  | CQ    | 82   | VAL  | 2.4  |
| 18  | AS    | 66   | VAL  | 2.4  |
| 25  | BC    | 5    | CYS  | 2.4  |
| 49  | DR    | 13   | ARG  | 2.4  |
| 13  | AN    | 46   | LYS  | 2.4  |
| 27  | BK    | 103  | VAL  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | B6    | 58   | VAL  | 2.4  |
| 26  | DD    | 4    | LEU  | 2.4  |
| 48  | DG    | 42   | VAL  | 2.4  |
| 8   | CI    | 48   | ARG  | 2.4  |
| 27  | BK    | 102  | PRO  | 2.4  |
| 44  | DQ    | 116  | LEU  | 2.4  |
| 20  | AB    | 195  | VAL  | 2.4  |
| 23  | BB    | 436  | C    | 2.4  |
| 23  | BB    | 2144 | G    | 2.4  |
| 25  | BC    | 17   | LYS  | 2.4  |
| 32  | D4    | 38   | GLY  | 2.4  |
| 19  | AT    | 40   | ALA  | 2.4  |
| 24  | BI    | 85   | ILE  | 2.4  |
| 51  | DZ    | 4    | VAL  | 2.4  |
| 4   | CE    | 13   | LYS  | 2.4  |
| 45  | BS    | 12   | SER  | 2.3  |
| 49  | BR    | 25   | LEU  | 2.3  |
| 24  | BI    | 35   | MET  | 2.3  |
| 37  | DL    | 2    | ARG  | 2.3  |
| 40  | BH    | 88   | GLY  | 2.3  |
| 24  | DI    | 27   | LEU  | 2.3  |
| 35  | DV    | 47   | VAL  | 2.3  |
| 49  | BR    | 82   | HIS  | 2.3  |
| 18  | AS    | 32   | THR  | 2.3  |
| 19  | CT    | 58   | ASP  | 2.3  |
| 23  | BB    | 1057 | A    | 2.3  |
| 42  | BN    | 21   | PHE  | 2.3  |
| 48  | DG    | 95   | ALA  | 2.3  |
| 53  | B6    | 60   | ALA  | 2.3  |
| 5   | CF    | 86   | ARG  | 2.3  |
| 18  | AS    | 18   | VAL  | 2.3  |
| 40  | DH    | 87   | GLU  | 2.3  |
| 21  | CU    | 28   | LEU  | 2.3  |
| 30  | DY    | 53   | MET  | 2.3  |
| 43  | DO    | 115  | LEU  | 2.3  |
| 18  | CS    | 1    | PRO  | 2.3  |
| 20  | CB    | 162  | VAL  | 2.3  |
| 40  | BH    | 89   | LYS  | 2.3  |
| 47  | BF    | 116  | LEU  | 2.3  |
| 18  | CS    | 8    | PRO  | 2.3  |
| 49  | BR    | 74   | ILE  | 2.3  |
| 29  | DE    | 124  | PHE  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 48  | BG    | 51  | PHE  | 2.3  |
| 51  | DZ    | 11  | ARG  | 2.3  |
| 1   | AA    | 78  | A    | 2.3  |
| 42  | BN    | 40  | LYS  | 2.3  |
| 50  | BT    | 66  | LYS  | 2.3  |
| 8   | CI    | 47  | VAL  | 2.3  |
| 43  | BO    | 7   | ARG  | 2.3  |
| 20  | CB    | 151 | LYS  | 2.3  |
| 7   | AH    | 60  | LEU  | 2.3  |
| 9   | AJ    | 8   | ILE  | 2.3  |
| 28  | DP    | 109 | ILE  | 2.3  |
| 41  | DJ    | 20  | ALA  | 2.3  |
| 49  | DR    | 65  | ALA  | 2.3  |
| 27  | BK    | 17  | ARG  | 2.3  |
| 3   | AD    | 176 | LYS  | 2.3  |
| 48  | DG    | 137 | LYS  | 2.3  |
| 7   | AH    | 101 | ALA  | 2.3  |
| 30  | BY    | 12  | ALA  | 2.3  |
| 32  | D4    | 29  | ALA  | 2.3  |
| 34  | D3    | 28  | LEU  | 2.3  |
| 40  | BH    | 5   | LEU  | 2.3  |
| 49  | BR    | 89  | HIS  | 2.3  |
| 29  | DE    | 96  | VAL  | 2.3  |
| 46  | BU    | 21  | ARG  | 2.3  |
| 46  | BU    | 92  | VAL  | 2.3  |
| 50  | BT    | 64  | LYS  | 2.3  |
| 11  | CL    | 81  | ILE  | 2.3  |
| 18  | CS    | 73  | PHE  | 2.3  |
| 15  | AP    | 18  | GLN  | 2.3  |
| 24  | BI    | 24  | GLY  | 2.3  |
| 2   | AC    | 133 | MET  | 2.3  |
| 8   | AI    | 31  | GLN  | 2.3  |
| 15  | CP    | 19  | VAL  | 2.3  |
| 16  | AQ    | 45  | VAL  | 2.3  |
| 26  | BD    | 11  | MET  | 2.3  |
| 40  | BH    | 46  | PHE  | 2.3  |
| 49  | BR    | 94  | THR  | 2.3  |
| 15  | AP    | 48  | GLU  | 2.3  |
| 24  | BI    | 13  | ALA  | 2.3  |
| 24  | DI    | 57  | VAL  | 2.3  |
| 28  | BP    | 58  | PHE  | 2.3  |
| 35  | BV    | 57  | TYR  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | AQ    | 72   | TRP  | 2.3  |
| 36  | B2    | 16   | HIS  | 2.3  |
| 16  | AQ    | 20   | ILE  | 2.3  |
| 27  | BK    | 53   | LYS  | 2.3  |
| 50  | BT    | 2    | ILE  | 2.3  |
| 23  | BB    | 2149 | U    | 2.3  |
| 3   | AD    | 173  | ASP  | 2.3  |
| 6   | AG    | 73   | GLU  | 2.3  |
| 8   | AI    | 56   | MET  | 2.3  |
| 22  | BA    | 52   | A    | 2.3  |
| 9   | AJ    | 43   | PRO  | 2.3  |
| 11  | AL    | 68   | GLY  | 2.3  |
| 46  | BU    | 33   | VAL  | 2.3  |
| 46  | BU    | 69   | VAL  | 2.3  |
| 48  | DG    | 52   | GLY  | 2.3  |
| 23  | BB    | 901  | C    | 2.3  |
| 45  | BS    | 7    | HIS  | 2.3  |
| 2   | AC    | 160  | GLU  | 2.3  |
| 6   | AG    | 86   | VAL  | 2.3  |
| 20  | CB    | 186  | VAL  | 2.3  |
| 35  | DV    | 63   | ILE  | 2.3  |
| 35  | DV    | 75   | GLN  | 2.3  |
| 41  | DJ    | 44   | TYR  | 2.3  |
| 48  | BG    | 150  | TYR  | 2.3  |
| 31  | D0    | 54   | ILE  | 2.3  |
| 40  | DH    | 116  | ARG  | 2.3  |
| 42  | BN    | 100  | CYS  | 2.3  |
| 9   | AJ    | 71   | LEU  | 2.3  |
| 16  | CQ    | 72   | TRP  | 2.3  |
| 26  | BD    | 10   | GLY  | 2.3  |
| 1   | CA    | 1032 | G    | 2.2  |
| 8   | CI    | 129  | ARG  | 2.2  |
| 24  | BI    | 114  | ALA  | 2.2  |
| 28  | BP    | 71   | ARG  | 2.2  |
| 4   | CE    | 51   | LYS  | 2.2  |
| 5   | CF    | 59   | TYR  | 2.2  |
| 1   | AA    | 5    | U    | 2.2  |
| 13  | AN    | 28   | ALA  | 2.2  |
| 19  | AT    | 46   | ALA  | 2.2  |
| 41  | BJ    | 121  | LYS  | 2.2  |
| 46  | BU    | 60   | LYS  | 2.2  |
| 46  | DU    | 23   | LYS  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | DF    | 116  | LEU  | 2.2  |
| 53  | D6    | 75   | ALA  | 2.2  |
| 43  | BO    | 100  | HIS  | 2.2  |
| 3   | AD    | 171  | GLU  | 2.2  |
| 6   | AG    | 84   | TYR  | 2.2  |
| 19  | CT    | 53   | MET  | 2.2  |
| 20  | CB    | 34   | ARG  | 2.2  |
| 20  | CB    | 131  | LYS  | 2.2  |
| 8   | CI    | 8    | THR  | 2.2  |
| 10  | AK    | 128  | VAL  | 2.2  |
| 16  | AQ    | 37   | ILE  | 2.2  |
| 46  | DU    | 84   | PHE  | 2.2  |
| 14  | AO    | 59   | MET  | 2.2  |
| 18  | CS    | 65   | MET  | 2.2  |
| 24  | BI    | 119  | ALA  | 2.2  |
| 48  | BG    | 163  | TYR  | 2.2  |
| 50  | BT    | 34   | VAL  | 2.2  |
| 7   | CH    | 91   | LEU  | 2.2  |
| 9   | AJ    | 89   | ARG  | 2.2  |
| 19  | AT    | 36   | ALA  | 2.2  |
| 25  | DC    | 92   | LEU  | 2.2  |
| 33  | D1    | 48   | TYR  | 2.2  |
| 46  | BU    | 12   | VAL  | 2.2  |
| 8   | AI    | 27   | ILE  | 2.2  |
| 38  | BM    | 99   | GLY  | 2.2  |
| 16  | CQ    | 26   | ARG  | 2.2  |
| 25  | BC    | 62   | ARG  | 2.2  |
| 28  | BP    | 48   | ALA  | 2.2  |
| 6   | CG    | 153  | TYR  | 2.2  |
| 9   | CJ    | 71   | LEU  | 2.2  |
| 10  | CK    | 81   | LEU  | 2.2  |
| 12  | AM    | 79   | LEU  | 2.2  |
| 4   | AE    | 35   | LEU  | 2.2  |
| 29  | DE    | 155  | GLU  | 2.2  |
| 50  | DT    | 54   | GLU  | 2.2  |
| 19  | AT    | 82   | ILE  | 2.2  |
| 23  | DB    | 2147 | A    | 2.2  |
| 6   | CG    | 5    | VAL  | 2.2  |
| 19  | AT    | 34   | VAL  | 2.2  |
| 49  | DR    | 96   | VAL  | 2.2  |
| 18  | CS    | 78   | THR  | 2.2  |
| 48  | BG    | 93   | TYR  | 2.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 46         | BU           | 84         | PHE         | 2.2         |
| 34         | B3           | 12         | ARG         | 2.2         |
| 42         | DN           | 98         | LEU         | 2.2         |
| 48         | BG           | 147        | LEU         | 2.2         |
| 9          | AJ           | 74         | VAL         | 2.2         |
| 17         | CR           | 63         | TYR         | 2.2         |
| 32         | B4           | 6          | SER         | 2.2         |
| 35         | DV           | 38         | LEU         | 2.2         |
| 14         | AO           | 60         | VAL         | 2.2         |
| 44         | BQ           | 88         | GLU         | 2.2         |
| 20         | AB           | 66         | ILE         | 2.2         |
| 24         | BI           | 53         | PRO         | 2.2         |
| 38         | DM           | 98         | PRO         | 2.2         |
| 12         | CM           | 12         | LYS         | 2.2         |
| 12         | CM           | 55         | LEU         | 2.2         |
| 34         | B3           | 20         | GLY         | 2.2         |
| 29         | DE           | 65         | THR         | 2.2         |
| 41         | DJ           | 54         | ILE         | 2.2         |
| 6          | CG           | 119        | LEU         | 2.2         |
| 17         | CR           | 67         | LEU         | 2.2         |
| 24         | BI           | 38         | CYS         | 2.2         |
| 37         | DL           | 123        | ARG         | 2.2         |
| 43         | BO           | 30         | ARG         | 2.2         |
| 53         | B6           | 68         | VAL         | 2.2         |
| 23         | DB           | 2146       | C           | 2.2         |
| 27         | DK           | 103        | VAL         | 2.2         |
| 37         | BL           | 58         | TYR         | 2.2         |
| 52         | DW           | 44         | PHE         | 2.2         |
| 20         | CB           | 70         | GLY         | 2.2         |
| 53         | B6           | 74         | ASN         | 2.2         |
| 6          | CG           | 25         | PHE         | 2.2         |
| 49         | BR           | 91         | GLN         | 2.2         |
| 13         | AN           | 15         | LEU         | 2.2         |
| 4          | AE           | 33         | THR         | 2.2         |
| 13         | AN           | 42         | ASN         | 2.2         |
| 27         | BK           | 104        | THR         | 2.2         |
| 18         | CS           | 29         | PRO         | 2.2         |
| 43         | DO           | 39         | VAL         | 2.2         |
| 53         | D6           | 104        | PRO         | 2.2         |
| 44         | BQ           | 116        | LEU         | 2.2         |
| 15         | AP           | 37         | GLY         | 2.2         |
| 32         | B4           | 19         | ARG         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | D1    | 4    | ILE  | 2.2  |
| 33  | D1    | 21   | THR  | 2.2  |
| 40  | DH    | 142  | VAL  | 2.2  |
| 53  | D6    | 44   | GLU  | 2.2  |
| 49  | DR    | 28   | ALA  | 2.2  |
| 20  | CB    | 72   | LYS  | 2.2  |
| 41  | DJ    | 75   | TYR  | 2.2  |
| 49  | BR    | 83   | TYR  | 2.2  |
| 25  | DC    | 101  | ARG  | 2.2  |
| 32  | B4    | 26   | ILE  | 2.2  |
| 43  | DO    | 35   | ILE  | 2.2  |
| 9   | CJ    | 81   | GLU  | 2.2  |
| 12  | CM    | 14   | ALA  | 2.2  |
| 19  | AT    | 37   | ALA  | 2.2  |
| 24  | DI    | 25   | PRO  | 2.2  |
| 28  | BP    | 67   | GLU  | 2.2  |
| 48  | BG    | 7    | PRO  | 2.2  |
| 52  | BW    | 64   | GLY  | 2.2  |
| 53  | B6    | 42   | LYS  | 2.2  |
| 53  | D6    | 83   | ILE  | 2.2  |
| 1   | CA    | 1497 | G    | 2.2  |
| 15  | CP    | 45   | GLU  | 2.2  |
| 13  | CN    | 76   | PHE  | 2.2  |
| 20  | CB    | 209  | VAL  | 2.2  |
| 2   | AC    | 74   | ILE  | 2.2  |
| 24  | BI    | 112  | LYS  | 2.2  |
| 52  | DW    | 61   | LYS  | 2.2  |
| 11  | AL    | 109  | ARG  | 2.2  |
| 15  | AP    | 51   | ARG  | 2.2  |
| 15  | CP    | 4    | ILE  | 2.2  |
| 53  | B6    | 64   | ARG  | 2.2  |
| 24  | DI    | 30   | GLN  | 2.1  |
| 48  | BG    | 160  | GLY  | 2.1  |
| 40  | BH    | 124  | THR  | 2.1  |
| 53  | D6    | 49   | HIS  | 2.1  |
| 9   | CJ    | 74   | VAL  | 2.1  |
| 10  | CK    | 51   | PHE  | 2.1  |
| 40  | DH    | 140  | ALA  | 2.1  |
| 14  | AO    | 87   | LEU  | 2.1  |
| 24  | BI    | 10   | LEU  | 2.1  |
| 3   | AD    | 145  | ARG  | 2.1  |
| 9   | CJ    | 26   | VAL  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 24  | BI    | 37   | PHE  | 2.1  |
| 28  | BP    | 69   | VAL  | 2.1  |
| 32  | D4    | 6    | SER  | 2.1  |
| 21  | AU    | 43   | GLU  | 2.1  |
| 50  | BT    | 4    | GLU  | 2.1  |
| 24  | BI    | 9    | LYS  | 2.1  |
| 24  | BI    | 67   | THR  | 2.1  |
| 33  | D1    | 16   | THR  | 2.1  |
| 33  | D1    | 37   | LYS  | 2.1  |
| 46  | DU    | 71   | ILE  | 2.1  |
| 17  | AR    | 22   | TYR  | 2.1  |
| 18  | CS    | 50   | VAL  | 2.1  |
| 24  | BI    | 77   | VAL  | 2.1  |
| 23  | BB    | 138  | U    | 2.1  |
| 24  | DI    | 73   | PRO  | 2.1  |
| 20  | CB    | 128  | LEU  | 2.1  |
| 50  | DT    | 87   | LEU  | 2.1  |
| 6   | CG    | 79   | VAL  | 2.1  |
| 46  | DU    | 35   | VAL  | 2.1  |
| 12  | AM    | 85   | TYR  | 2.1  |
| 9   | AJ    | 100  | ILE  | 2.1  |
| 9   | CJ    | 18   | ILE  | 2.1  |
| 20  | CB    | 183  | PHE  | 2.1  |
| 28  | DP    | 19   | PHE  | 2.1  |
| 37  | BL    | 101  | ILE  | 2.1  |
| 47  | BF    | 102  | LEU  | 2.1  |
| 47  | DF    | 157  | THR  | 2.1  |
| 49  | DR    | 59   | ILE  | 2.1  |
| 50  | BT    | 10   | VAL  | 2.1  |
| 52  | BW    | 78   | PHE  | 2.1  |
| 6   | AG    | 82   | SER  | 2.1  |
| 8   | CI    | 120  | ALA  | 2.1  |
| 1   | AA    | 1362 | A    | 2.1  |
| 1   | AA    | 1492 | A    | 2.1  |
| 28  | BP    | 73   | PHE  | 2.1  |
| 1   | AA    | 79   | G    | 2.1  |
| 12  | AM    | 3    | ILE  | 2.1  |
| 32  | B4    | 2    | LYS  | 2.1  |
| 40  | DH    | 58   | LEU  | 2.1  |
| 50  | DT    | 82   | LYS  | 2.1  |
| 11  | AL    | 26   | CYS  | 2.1  |
| 1   | AA    | 87   | C    | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | AI    | 80  | HIS  | 2.1  |
| 11  | AL    | 121 | PRO  | 2.1  |
| 38  | BM    | 117 | PHE  | 2.1  |
| 43  | BO    | 50  | ALA  | 2.1  |
| 2   | AC    | 195 | ILE  | 2.1  |
| 6   | CG    | 22  | LEU  | 2.1  |
| 9   | CJ    | 42  | LEU  | 2.1  |
| 13  | AN    | 45  | LEU  | 2.1  |
| 4   | CE    | 12  | GLU  | 2.1  |
| 14  | AO    | 25  | THR  | 2.1  |
| 14  | CO    | 56  | LEU  | 2.1  |
| 41  | BJ    | 85  | LYS  | 2.1  |
| 12  | AM    | 89  | ARG  | 2.1  |
| 16  | AQ    | 61  | ARG  | 2.1  |
| 40  | BH    | 86  | ASP  | 2.1  |
| 4   | AE    | 91  | SER  | 2.1  |
| 4   | AE    | 110 | MET  | 2.1  |
| 31  | B0    | 54  | ILE  | 2.1  |
| 32  | B4    | 21  | GLY  | 2.1  |
| 23  | BB    | 930 | G    | 2.1  |
| 16  | AQ    | 5   | ARG  | 2.1  |
| 27  | BK    | 10  | VAL  | 2.1  |
| 29  | BE    | 170 | ARG  | 2.1  |
| 13  | CN    | 77  | GLY  | 2.1  |
| 16  | CQ    | 43  | LEU  | 2.1  |
| 41  | BJ    | 75  | TYR  | 2.1  |
| 46  | BU    | 32  | LYS  | 2.1  |
| 4   | AE    | 34  | ALA  | 2.1  |
| 43  | DO    | 52  | SER  | 2.1  |
| 51  | DZ    | 50  | ARG  | 2.1  |
| 3   | AD    | 122 | ILE  | 2.1  |
| 8   | AI    | 50  | PRO  | 2.1  |
| 27  | BK    | 15  | GLY  | 2.1  |
| 46  | BU    | 31  | GLY  | 2.1  |
| 6   | AG    | 61  | PHE  | 2.1  |
| 7   | AH    | 127 | TYR  | 2.1  |
| 8   | AI    | 34  | LEU  | 2.1  |
| 28  | BP    | 75  | THR  | 2.1  |
| 45  | BS    | 48  | LYS  | 2.1  |
| 45  | BS    | 71  | VAL  | 2.1  |
| 13  | CN    | 91  | GLU  | 2.1  |
| 48  | BG    | 37  | ASN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 24  | DI    | 11  | GLN  | 2.1  |
| 32  | B4    | 5   | ALA  | 2.1  |
| 40  | DH    | 137 | GLU  | 2.1  |
| 20  | CB    | 100 | LEU  | 2.1  |
| 20  | CB    | 161 | PHE  | 2.1  |
| 27  | BK    | 43  | ILE  | 2.1  |
| 28  | DP    | 69  | VAL  | 2.1  |
| 34  | D3    | 21  | PHE  | 2.1  |
| 37  | DL    | 142 | ILE  | 2.1  |
| 48  | DG    | 104 | LEU  | 2.1  |
| 26  | BD    | 134 | HIS  | 2.1  |
| 9   | CJ    | 95  | GLY  | 2.1  |
| 25  | BC    | 234 | GLY  | 2.1  |
| 47  | BF    | 118 | ALA  | 2.1  |
| 18  | AS    | 61  | VAL  | 2.1  |
| 47  | BF    | 157 | THR  | 2.1  |
| 18  | AS    | 28  | LYS  | 2.1  |
| 43  | BO    | 36  | TYR  | 2.1  |
| 15  | CP    | 16  | PHE  | 2.1  |
| 18  | CS    | 40  | PHE  | 2.1  |
| 21  | AU    | 23  | GLU  | 2.1  |
| 25  | BC    | 60  | ALA  | 2.1  |
| 40  | DH    | 120 | GLY  | 2.1  |
| 6   | AG    | 6   | ILE  | 2.1  |
| 46  | BU    | 41  | VAL  | 2.1  |
| 47  | DF    | 172 | PHE  | 2.1  |
| 48  | BG    | 102 | ILE  | 2.1  |
| 35  | DV    | 61  | LEU  | 2.1  |
| 8   | AI    | 103 | VAL  | 2.1  |
| 46  | BU    | 83  | GLY  | 2.1  |
| 52  | DW    | 43  | LYS  | 2.1  |
| 14  | CO    | 88  | ARG  | 2.1  |
| 25  | DC    | 79  | ARG  | 2.1  |
| 26  | DD    | 27  | ILE  | 2.1  |
| 47  | DF    | 18  | GLU  | 2.1  |
| 48  | BG    | 9   | VAL  | 2.1  |
| 8   | AI    | 51  | LEU  | 2.1  |
| 13  | AN    | 31  | SER  | 2.1  |
| 20  | CB    | 147 | LEU  | 2.1  |
| 24  | BI    | 30  | GLN  | 2.1  |
| 20  | CB    | 90  | PHE  | 2.1  |
| 48  | DG    | 57  | TYR  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | AS    | 41   | PRO  | 2.1  |
| 1   | AA    | 135  | C    | 2.1  |
| 12  | CM    | 18   | LEU  | 2.1  |
| 21  | CU    | 24   | LYS  | 2.1  |
| 23  | DB    | 2903 | U    | 2.1  |
| 49  | DR    | 48   | LYS  | 2.1  |
| 2   | AC    | 100  | ILE  | 2.1  |
| 18  | CS    | 23   | GLU  | 2.1  |
| 24  | BI    | 55   | PRO  | 2.1  |
| 43  | DO    | 7    | ARG  | 2.1  |
| 4   | AE    | 86   | GLY  | 2.1  |
| 24  | DI    | 124  | MET  | 2.1  |
| 6   | CG    | 113  | LYS  | 2.1  |
| 35  | DV    | 92   | VAL  | 2.1  |
| 43  | DO    | 56   | LYS  | 2.1  |
| 43  | DO    | 90   | VAL  | 2.1  |
| 31  | B0    | 1    | ALA  | 2.1  |
| 15  | CP    | 35   | ARG  | 2.1  |
| 32  | B4    | 4    | ARG  | 2.1  |
| 4   | CE    | 95   | MET  | 2.1  |
| 43  | BO    | 116  | GLN  | 2.1  |
| 12  | CM    | 38   | ILE  | 2.1  |
| 24  | BI    | 51   | GLY  | 2.1  |
| 35  | BV    | 84   | PRO  | 2.1  |
| 37  | BL    | 2    | ARG  | 2.1  |
| 25  | DC    | 32   | LEU  | 2.1  |
| 3   | AD    | 151  | GLN  | 2.0  |
| 37  | BL    | 73   | ILE  | 2.0  |
| 8   | AI    | 93   | LEU  | 2.0  |
| 23  | BB    | 2133 | G    | 2.0  |
| 24  | DI    | 10   | LEU  | 2.0  |
| 36  | B2    | 31   | LEU  | 2.0  |
| 38  | BM    | 98   | PRO  | 2.0  |
| 30  | BY    | 19   | HIS  | 2.0  |
| 51  | BZ    | 49   | LEU  | 2.0  |
| 9   | AJ    | 76   | ILE  | 2.0  |
| 43  | BO    | 49   | VAL  | 2.0  |
| 45  | BS    | 96   | ILE  | 2.0  |
| 10  | AK    | 41   | LEU  | 2.0  |
| 16  | AQ    | 26   | ARG  | 2.0  |
| 38  | DM    | 103  | TYR  | 2.0  |
| 49  | BR    | 95   | ASP  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | AB    | 161  | PHE  | 2.0  |
| 34  | D3    | 13   | PHE  | 2.0  |
| 1   | CA    | 1492 | A    | 2.0  |
| 18  | CS    | 10   | ILE  | 2.0  |
| 18  | CS    | 43   | MET  | 2.0  |
| 19  | AT    | 44   | ALA  | 2.0  |
| 24  | BI    | 76   | ALA  | 2.0  |
| 32  | B4    | 14   | CYS  | 2.0  |
| 40  | DH    | 84   | ALA  | 2.0  |
| 46  | BU    | 20   | LYS  | 2.0  |
| 50  | DT    | 81   | LYS  | 2.0  |
| 13  | CN    | 45   | LEU  | 2.0  |
| 26  | BD    | 35   | THR  | 2.0  |
| 3   | AD    | 154  | VAL  | 2.0  |
| 11  | AL    | 106  | VAL  | 2.0  |
| 35  | DV    | 56   | PHE  | 2.0  |
| 41  | BJ    | 44   | TYR  | 2.0  |
| 47  | DF    | 21   | TYR  | 2.0  |
| 6   | CG    | 152  | HIS  | 2.0  |
| 19  | AT    | 43   | LYS  | 2.0  |
| 48  | DG    | 23   | ILE  | 2.0  |
| 48  | DG    | 45   | ALA  | 2.0  |
| 2   | CC    | 152  | VAL  | 2.0  |
| 7   | AH    | 71   | VAL  | 2.0  |
| 12  | AM    | 82   | LEU  | 2.0  |
| 21  | CU    | 33   | ARG  | 2.0  |
| 39  | BX    | 23   | ARG  | 2.0  |
| 45  | DS    | 104  | THR  | 2.0  |
| 24  | BI    | 28   | GLY  | 2.0  |
| 13  | CN    | 92   | ILE  | 2.0  |
| 20  | CB    | 30   | ILE  | 2.0  |
| 50  | DT    | 33   | LYS  | 2.0  |
| 52  | BW    | 65   | LYS  | 2.0  |
| 33  | B1    | 22   | THR  | 2.0  |
| 9   | CJ    | 102  | LEU  | 2.0  |
| 16  | CQ    | 83   | LEU  | 2.0  |
| 18  | AS    | 46   | LEU  | 2.0  |
| 50  | BT    | 80   | TRP  | 2.0  |
| 27  | BK    | 11   | ALA  | 2.0  |
| 35  | DV    | 40   | ILE  | 2.0  |
| 41  | BJ    | 72   | LYS  | 2.0  |
| 48  | BG    | 23   | ILE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | AC    | 176 | THR  | 2.0  |
| 41  | BJ    | 76  | HIS  | 2.0  |
| 43  | BO    | 90  | VAL  | 2.0  |
| 13  | CN    | 94  | GLY  | 2.0  |
| 17  | CR    | 64  | LEU  | 2.0  |
| 29  | BE    | 188 | MET  | 2.0  |
| 53  | B6    | 61  | PRO  | 2.0  |
| 16  | CQ    | 24  | ILE  | 2.0  |
| 21  | AU    | 24  | LYS  | 2.0  |
| 19  | AT    | 12  | GLN  | 2.0  |
| 24  | BI    | 12  | VAL  | 2.0  |
| 28  | BP    | 99  | LEU  | 2.0  |
| 1   | CA    | 85  | U    | 2.0  |
| 46  | BU    | 42  | LYS  | 2.0  |
| 47  | DF    | 71  | LYS  | 2.0  |
| 48  | BG    | 121 | THR  | 2.0  |
| 34  | B3    | 62  | PRO  | 2.0  |
| 42  | BN    | 10  | LEU  | 2.0  |
| 53  | B6    | 51  | PRO  | 2.0  |
| 12  | CM    | 52  | ILE  | 2.0  |
| 5   | AF    | 5   | GLU  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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 | RSR  | LLDF   | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|----------------------------|-------|
| 54  | MG   | CA    | 1623 | 1/1   | 0.61 | 108.00 | 180,180,180,180            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 54  | MG   | AA    | 1657 | 1/1   | 1.39 | 61.65 | 155,155,155,155            | 0     |
| 54  | MG   | AA    | 1626 | 1/1   | 0.81 | 45.62 | 28,28,28,28                | 1     |
| 54  | MG   | BB    | 3057 | 1/1   | 0.47 | 43.00 | 65,65,65,65                | 0     |
| 54  | MG   | AA    | 1619 | 1/1   | 1.30 | 33.94 | 180,180,180,180            | 0     |
| 54  | MG   | CA    | 1657 | 1/1   | 0.48 | 31.19 | 97,97,97,97                | 0     |
| 54  | MG   | AA    | 1658 | 1/1   | 0.19 | 29.67 | 97,97,97,97                | 0     |
| 54  | MG   | AA    | 1647 | 1/1   | 0.92 | 27.19 | 180,180,180,180            | 0     |
| 54  | MG   | AA    | 1637 | 1/1   | 1.05 | 22.34 | 146,146,146,146            | 0     |
| 54  | MG   | CE    | 201  | 1/1   | 0.80 | 17.42 | 145,145,145,145            | 0     |
| 54  | MG   | DB    | 3036 | 1/1   | 0.45 | 14.83 | 51,51,51,51                | 0     |
| 54  | MG   | AA    | 1623 | 1/1   | 0.67 | 14.63 | 33,33,33,33                | 1     |
| 54  | MG   | CA    | 1615 | 1/1   | 0.26 | 14.22 | 180,180,180,180            | 0     |
| 54  | MG   | CA    | 1658 | 1/1   | 0.34 | 11.40 | 70,70,70,70                | 0     |
| 54  | MG   | CA    | 1628 | 1/1   | 0.32 | 10.92 | 82,82,82,82                | 0     |
| 54  | MG   | CA    | 1608 | 1/1   | 0.53 | 10.71 | 178,178,178,178            | 0     |
| 54  | MG   | CA    | 1627 | 1/1   | 0.36 | 10.42 | 35,35,35,35                | 1     |
| 54  | MG   | CA    | 1641 | 1/1   | 0.27 | 9.47  | 76,76,76,76                | 0     |
| 54  | MG   | DB    | 3083 | 1/1   | 0.38 | 9.21  | 72,72,72,72                | 0     |
| 54  | MG   | DB    | 3086 | 1/1   | 0.23 | 8.82  | 25,25,25,25                | 0     |
| 54  | MG   | AA    | 1621 | 1/1   | 0.31 | 8.71  | 27,27,27,27                | 0     |
| 54  | MG   | DB    | 3058 | 1/1   | 0.50 | 8.12  | 157,157,157,157            | 0     |
| 54  | MG   | DB    | 3028 | 1/1   | 0.28 | 7.54  | 33,33,33,33                | 0     |
| 54  | MG   | BB    | 3108 | 1/1   | 0.33 | 6.81  | 88,88,88,88                | 0     |
| 54  | MG   | AA    | 1639 | 1/1   | 2.26 | 6.72  | 126,126,126,126            | 0     |
| 54  | MG   | DB    | 3065 | 1/1   | 0.21 | 6.37  | 68,68,68,68                | 0     |
| 55  | PAR  | BB    | 3111 | 42/42 | 0.40 | 6.27  | 100,100,100,100            | 42    |
| 54  | MG   | BB    | 3047 | 1/1   | 0.24 | 5.97  | 92,92,92,92                | 0     |
| 54  | MG   | AA    | 1633 | 1/1   | 0.42 | 5.85  | 56,56,56,56                | 0     |
| 54  | MG   | AA    | 1608 | 1/1   | 0.43 | 5.85  | 136,136,136,136            | 0     |
| 54  | MG   | BB    | 3036 | 1/1   | 0.30 | 5.77  | 68,68,68,68                | 0     |
| 54  | MG   | CA    | 1620 | 1/1   | 0.23 | 5.73  | 104,104,104,104            | 0     |
| 54  | MG   | DB    | 3052 | 1/1   | 0.28 | 5.70  | 166,166,166,166            | 0     |
| 55  | PAR  | DB    | 3112 | 42/42 | 0.39 | 5.57  | 55,55,55,55                | 42    |
| 54  | MG   | AA    | 1632 | 1/1   | 0.45 | 5.57  | 80,80,80,80                | 0     |
| 54  | MG   | AA    | 1617 | 1/1   | 0.25 | 5.34  | 138,138,138,138            | 0     |
| 54  | MG   | BB    | 3020 | 1/1   | 0.37 | 5.31  | 23,23,23,23                | 0     |
| 54  | MG   | BB    | 3064 | 1/1   | 0.24 | 5.10  | 78,78,78,78                | 0     |
| 54  | MG   | BB    | 3097 | 1/1   | 0.24 | 5.08  | 95,95,95,95                | 0     |
| 54  | MG   | BB    | 3080 | 1/1   | 0.32 | 4.89  | 131,131,131,131            | 0     |
| 54  | MG   | CA    | 1621 | 1/1   | 0.34 | 4.66  | 67,67,67,67                | 0     |
| 54  | MG   | AA    | 1627 | 1/1   | 0.22 | 4.10  | 46,46,46,46                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | AA    | 1622 | 1/1   | 0.27 | 4.09 | 111,111,111,111            | 0     |
| 54  | MG   | AA    | 1659 | 1/1   | 0.59 | 3.93 | 127,127,127,127            | 0     |
| 54  | MG   | DB    | 3030 | 1/1   | 0.25 | 3.91 | 30,30,30,30                | 0     |
| 54  | MG   | AA    | 1652 | 1/1   | 0.25 | 3.79 | 126,126,126,126            | 0     |
| 54  | MG   | AA    | 1656 | 1/1   | 0.23 | 3.71 | 50,50,50,50                | 0     |
| 54  | MG   | BB    | 3051 | 1/1   | 0.26 | 3.54 | 75,75,75,75                | 0     |
| 54  | MG   | BB    | 3033 | 1/1   | 0.18 | 3.50 | 125,125,125,125            | 0     |
| 54  | MG   | BB    | 3093 | 1/1   | 0.31 | 3.39 | 98,98,98,98                | 0     |
| 54  | MG   | BB    | 3028 | 1/1   | 0.24 | 3.19 | 95,95,95,95                | 0     |
| 54  | MG   | BB    | 3018 | 1/1   | 0.26 | 2.99 | 32,32,32,32                | 0     |
| 54  | MG   | BB    | 3078 | 1/1   | 0.26 | 2.96 | 92,92,92,92                | 0     |
| 54  | MG   | DB    | 3108 | 1/1   | 0.33 | 2.84 | 13,13,13,13                | 0     |
| 54  | MG   | AA    | 1651 | 1/1   | 0.22 | 2.79 | 55,55,55,55                | 0     |
| 54  | MG   | DB    | 3068 | 1/1   | 0.26 | 2.70 | 16,16,16,16                | 0     |
| 54  | MG   | BB    | 3055 | 1/1   | 0.25 | 2.67 | 78,78,78,78                | 0     |
| 54  | MG   | AA    | 1624 | 1/1   | 0.30 | 2.57 | 76,76,76,76                | 0     |
| 54  | MG   | DB    | 3101 | 1/1   | 0.28 | 2.46 | 7,7,7,7                    | 0     |
| 54  | MG   | CA    | 1626 | 1/1   | 0.22 | 2.41 | 23,23,23,23                | 1     |
| 54  | MG   | CA    | 1646 | 1/1   | 0.23 | 2.32 | 78,78,78,78                | 0     |
| 54  | MG   | AA    | 1614 | 1/1   | 0.24 | 2.31 | 131,131,131,131            | 0     |
| 54  | MG   | AA    | 1625 | 1/1   | 0.20 | 2.29 | 144,144,144,144            | 1     |
| 54  | MG   | CA    | 1625 | 1/1   | 0.18 | 2.25 | 46,46,46,46                | 0     |
| 54  | MG   | BB    | 3017 | 1/1   | 0.20 | 2.25 | 46,46,46,46                | 0     |
| 54  | MG   | BB    | 3100 | 1/1   | 0.21 | 2.03 | 109,109,109,109            | 0     |
| 54  | MG   | DB    | 3111 | 1/1   | 0.26 | 2.01 | 68,68,68,68                | 0     |
| 54  | MG   | BB    | 3059 | 1/1   | 0.26 | 2.01 | 39,39,39,39                | 0     |
| 54  | MG   | CA    | 1629 | 1/1   | 0.28 | 1.96 | 96,96,96,96                | 1     |
| 54  | MG   | AA    | 1650 | 1/1   | 0.16 | 1.92 | 116,116,116,116            | 0     |
| 54  | MG   | CA    | 1632 | 1/1   | 0.23 | 1.82 | 34,34,34,34                | 0     |
| 54  | MG   | CA    | 1636 | 1/1   | 0.33 | 1.64 | 90,90,90,90                | 0     |
| 54  | MG   | DB    | 3066 | 1/1   | 0.13 | 1.60 | 123,123,123,123            | 0     |
| 54  | MG   | DB    | 3013 | 1/1   | 0.21 | 1.56 | 35,35,35,35                | 0     |
| 54  | MG   | DB    | 3004 | 1/1   | 0.25 | 1.51 | 40,40,40,40                | 0     |
| 54  | MG   | BB    | 3075 | 1/1   | 0.21 | 1.49 | 55,55,55,55                | 0     |
| 54  | MG   | BB    | 3082 | 1/1   | 0.31 | 1.44 | 22,22,22,22                | 0     |
| 54  | MG   | BB    | 3013 | 1/1   | 0.19 | 1.40 | 86,86,86,86                | 0     |
| 54  | MG   | DB    | 3061 | 1/1   | 0.16 | 1.37 | 95,95,95,95                | 0     |
| 54  | MG   | AA    | 1610 | 1/1   | 0.29 | 1.34 | 82,82,82,82                | 0     |
| 54  | MG   | AA    | 1612 | 1/1   | 0.20 | 1.28 | 96,96,96,96                | 0     |
| 54  | MG   | CA    | 1649 | 1/1   | 0.33 | 1.20 | 134,134,134,134            | 0     |
| 54  | MG   | BB    | 3048 | 1/1   | 0.28 | 1.17 | 8,8,8,8                    | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 54  | MG   | DB    | 3089 | 1/1   | 0.23 | 1.15  | 75,75,75,75                 | 0     |
| 55  | PAR  | AA    | 1661 | 42/42 | 0.29 | 1.12  | 62,62,62,62                 | 0     |
| 54  | MG   | BB    | 3003 | 1/1   | 0.16 | 0.87  | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1652 | 1/1   | 0.26 | 0.83  | 58,58,58,58                 | 0     |
| 54  | MG   | BB    | 3011 | 1/1   | 0.20 | 0.77  | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1651 | 1/1   | 0.17 | 0.64  | 37,37,37,37                 | 0     |
| 54  | MG   | AA    | 1615 | 1/1   | 0.36 | 0.57  | 171,171,171,171             | 0     |
| 54  | MG   | CA    | 1624 | 1/1   | 0.13 | 0.54  | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1634 | 1/1   | 0.15 | 0.53  | 30,30,30,30                 | 0     |
| 54  | MG   | DB    | 3011 | 1/1   | 0.16 | 0.52  | 22,22,22,22                 | 0     |
| 54  | MG   | BB    | 3037 | 1/1   | 0.19 | 0.37  | 63,63,63,63                 | 0     |
| 54  | MG   | DB    | 3046 | 1/1   | 0.15 | 0.36  | 38,38,38,38                 | 0     |
| 54  | MG   | CA    | 1614 | 1/1   | 0.32 | 0.36  | 85,85,85,85                 | 0     |
| 54  | MG   | BB    | 3038 | 1/1   | 0.14 | 0.32  | 157,157,157,157             | 0     |
| 54  | MG   | DB    | 3032 | 1/1   | 0.18 | 0.28  | 21,21,21,21                 | 0     |
| 54  | MG   | AA    | 1636 | 1/1   | 0.18 | 0.27  | 38,38,38,38                 | 0     |
| 54  | MG   | DB    | 3085 | 1/1   | 0.21 | 0.26  | 49,49,49,49                 | 0     |
| 54  | MG   | AA    | 1635 | 1/1   | 0.19 | 0.21  | 120,120,120,120             | 0     |
| 54  | MG   | CA    | 1603 | 1/1   | 0.17 | 0.18  | 37,37,37,37                 | 0     |
| 54  | MG   | DB    | 3096 | 1/1   | 0.16 | 0.16  | 37,37,37,37                 | 0     |
| 54  | MG   | BB    | 3019 | 1/1   | 0.17 | 0.16  | 56,56,56,56                 | 0     |
| 54  | MG   | BB    | 3014 | 1/1   | 0.15 | 0.16  | 46,46,46,46                 | 0     |
| 55  | PAR  | CA    | 1662 | 42/42 | 0.21 | 0.12  | 45,45,45,45                 | 0     |
| 54  | MG   | CA    | 1633 | 1/1   | 0.19 | 0.11  | 106,106,106,106             | 0     |
| 54  | MG   | BB    | 3071 | 1/1   | 0.19 | 0.09  | 63,63,63,63                 | 0     |
| 54  | MG   | BB    | 3012 | 1/1   | 0.20 | 0.08  | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1613 | 1/1   | 0.18 | 0.02  | 24,24,24,24                 | 0     |
| 54  | MG   | DB    | 3048 | 1/1   | 0.14 | -0.00 | 8,8,8,8                     | 0     |
| 54  | MG   | DB    | 3074 | 1/1   | 0.17 | -0.01 | 17,17,17,17                 | 0     |
| 54  | MG   | BB    | 3101 | 1/1   | 0.23 | -0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | DB    | 3087 | 1/1   | 0.18 | -0.08 | 67,67,67,67                 | 0     |
| 54  | MG   | DB    | 3022 | 1/1   | 0.15 | -0.09 | 85,85,85,85                 | 0     |
| 54  | MG   | DB    | 3027 | 1/1   | 0.20 | -0.09 | 11,11,11,11                 | 0     |
| 54  | MG   | BB    | 3087 | 1/1   | 0.18 | -0.14 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1616 | 1/1   | 0.27 | -0.16 | 94,94,94,94                 | 0     |
| 54  | MG   | DB    | 3090 | 1/1   | 0.20 | -0.19 | 35,35,35,35                 | 0     |
| 54  | MG   | BB    | 3098 | 1/1   | 0.15 | -0.19 | 10,10,10,10                 | 0     |
| 54  | MG   | CA    | 1605 | 1/1   | 0.20 | -0.26 | 5,5,5,5                     | 0     |
| 54  | MG   | DB    | 3037 | 1/1   | 0.12 | -0.29 | 45,45,45,45                 | 0     |
| 54  | MG   | AA    | 1607 | 1/1   | 0.23 | -0.30 | 35,35,35,35                 | 0     |
| 54  | MG   | DB    | 3008 | 1/1   | 0.19 | -0.33 | 11,11,11,11                 | 0     |
| 54  | MG   | CA    | 1619 | 1/1   | 0.21 | -0.34 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 54  | MG   | DB    | 3003 | 1/1   | 0.19 | -0.36 | 5,5,5,5                    | 0     |
| 54  | MG   | CA    | 1654 | 1/1   | 0.14 | -0.37 | 72,72,72,72                | 0     |
| 54  | MG   | DB    | 3018 | 1/1   | 0.17 | -0.40 | 17,17,17,17                | 0     |
| 54  | MG   | BB    | 3105 | 1/1   | 0.15 | -0.42 | 21,21,21,21                | 0     |
| 54  | MG   | CA    | 1647 | 1/1   | 0.14 | -0.42 | 58,58,58,58                | 0     |
| 54  | MG   | DB    | 3014 | 1/1   | 0.18 | -0.42 | 39,39,39,39                | 0     |
| 54  | MG   | DB    | 3099 | 1/1   | 0.17 | -0.43 | 21,21,21,21                | 0     |
| 54  | MG   | BB    | 3049 | 1/1   | 0.17 | -0.44 | 25,25,25,25                | 0     |
| 54  | MG   | DB    | 3102 | 1/1   | 0.21 | -0.46 | 20,20,20,20                | 0     |
| 54  | MG   | DB    | 3059 | 1/1   | 0.13 | -0.46 | 152,152,152,152            | 0     |
| 54  | MG   | DB    | 3049 | 1/1   | 0.16 | -0.49 | 11,11,11,11                | 0     |
| 54  | MG   | CA    | 1661 | 1/1   | 0.11 | -0.49 | 40,40,40,40                | 0     |
| 54  | MG   | DB    | 3060 | 1/1   | 0.13 | -0.50 | 160,160,160,160            | 0     |
| 54  | MG   | BB    | 3027 | 1/1   | 0.14 | -0.51 | 83,83,83,83                | 0     |
| 54  | MG   | CA    | 1622 | 1/1   | 0.14 | -0.52 | 38,38,38,38                | 0     |
| 54  | MG   | AA    | 1628 | 1/1   | 0.18 | -0.53 | 49,49,49,49                | 0     |
| 54  | MG   | CA    | 1659 | 1/1   | 0.11 | -0.55 | 70,70,70,70                | 0     |
| 54  | MG   | AA    | 1655 | 1/1   | 0.20 | -0.59 | 83,83,83,83                | 0     |
| 54  | MG   | BB    | 3041 | 1/1   | 0.14 | -0.62 | 15,15,15,15                | 0     |
| 54  | MG   | DB    | 3094 | 1/1   | 0.11 | -0.62 | 81,81,81,81                | 0     |
| 54  | MG   | BB    | 3021 | 1/1   | 0.11 | -0.66 | 62,62,62,62                | 0     |
| 54  | MG   | BB    | 3077 | 1/1   | 0.17 | -0.68 | 64,64,64,64                | 0     |
| 54  | MG   | CA    | 1639 | 1/1   | 0.16 | -0.69 | 5,5,5,5                    | 0     |
| 54  | MG   | DB    | 3110 | 1/1   | 0.14 | -0.70 | 44,44,44,44                | 0     |
| 54  | MG   | AA    | 1640 | 1/1   | 0.10 | -0.71 | 77,77,77,77                | 0     |
| 54  | MG   | BB    | 3009 | 1/1   | 0.11 | -0.72 | 76,76,76,76                | 0     |
| 54  | MG   | DB    | 3075 | 1/1   | 0.14 | -0.72 | 10,10,10,10                | 0     |
| 54  | MG   | DB    | 3026 | 1/1   | 0.19 | -0.72 | 54,54,54,54                | 0     |
| 54  | MG   | BB    | 3043 | 1/1   | 0.15 | -0.75 | 97,97,97,97                | 0     |
| 54  | MG   | AA    | 1642 | 1/1   | 0.15 | -0.75 | 63,63,63,63                | 0     |
| 54  | MG   | DB    | 3073 | 1/1   | 0.13 | -0.76 | 25,25,25,25                | 0     |
| 54  | MG   | AA    | 1649 | 1/1   | 0.11 | -0.78 | 93,93,93,93                | 0     |
| 54  | MG   | DB    | 3079 | 1/1   | 0.15 | -0.79 | 30,30,30,30                | 0     |
| 54  | MG   | DB    | 3109 | 1/1   | 0.17 | -0.79 | 27,27,27,27                | 0     |
| 54  | MG   | AA    | 1602 | 1/1   | 0.17 | -0.80 | 105,105,105,105            | 0     |
| 54  | MG   | DB    | 3050 | 1/1   | 0.12 | -0.83 | 118,118,118,118            | 0     |
| 54  | MG   | DB    | 3023 | 1/1   | 0.10 | -0.85 | 35,35,35,35                | 0     |
| 54  | MG   | DB    | 3100 | 1/1   | 0.16 | -0.86 | 22,22,22,22                | 0     |
| 54  | MG   | BB    | 3083 | 1/1   | 0.17 | -0.89 | 51,51,51,51                | 0     |
| 54  | MG   | CA    | 1637 | 1/1   | 0.13 | -0.90 | 116,116,116,116            | 0     |
| 54  | MG   | DB    | 3007 | 1/1   | 0.16 | -0.91 | 27,27,27,27                | 0     |
| 54  | MG   | CA    | 1642 | 1/1   | 0.09 | -0.92 | 85,85,85,85                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 54  | MG   | BB    | 3026 | 1/1   | 0.14 | -0.93 | 44,44,44,44                 | 0     |
| 54  | MG   | BB    | 3023 | 1/1   | 0.13 | -0.94 | 6,6,6,6                     | 0     |
| 54  | MG   | CA    | 1612 | 1/1   | 0.12 | -0.96 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1613 | 1/1   | 0.19 | -0.96 | 82,82,82,82                 | 0     |
| 54  | MG   | BB    | 3029 | 1/1   | 0.11 | -0.96 | 12,12,12,12                 | 0     |
| 54  | MG   | CA    | 1606 | 1/1   | 0.19 | -1.04 | 103,103,103,103             | 0     |
| 54  | MG   | BB    | 3104 | 1/1   | 0.16 | -1.04 | 43,43,43,43                 | 0     |
| 54  | MG   | BB    | 3034 | 1/1   | 0.14 | -1.05 | 41,41,41,41                 | 0     |
| 54  | MG   | BB    | 3092 | 1/1   | 0.08 | -1.05 | 60,60,60,60                 | 0     |
| 54  | MG   | DB    | 3051 | 1/1   | 0.14 | -1.06 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3015 | 1/1   | 0.10 | -1.07 | 39,39,39,39                 | 0     |
| 54  | MG   | BB    | 3001 | 1/1   | 0.10 | -1.07 | 14,14,14,14                 | 0     |
| 54  | MG   | DB    | 3045 | 1/1   | 0.12 | -1.10 | 108,108,108,108             | 0     |
| 54  | MG   | BB    | 3099 | 1/1   | 0.10 | -1.11 | 40,40,40,40                 | 0     |
| 54  | MG   | CA    | 1653 | 1/1   | 0.05 | -1.13 | 43,43,43,43                 | 0     |
| 54  | MG   | BB    | 3062 | 1/1   | 0.16 | -1.13 | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3065 | 1/1   | 0.14 | -1.13 | 30,30,30,30                 | 0     |
| 54  | MG   | CA    | 1660 | 1/1   | 0.12 | -1.16 | 58,58,58,58                 | 0     |
| 54  | MG   | BB    | 3046 | 1/1   | 0.20 | -1.19 | 64,64,64,64                 | 0     |
| 54  | MG   | BB    | 3006 | 1/1   | 0.08 | -1.19 | 37,37,37,37                 | 0     |
| 54  | MG   | CA    | 1602 | 1/1   | 0.17 | -1.23 | 16,16,16,16                 | 0     |
| 54  | MG   | BB    | 3109 | 1/1   | 0.11 | -1.23 | 49,49,49,49                 | 0     |
| 54  | MG   | AA    | 1603 | 1/1   | 0.17 | -1.23 | 38,38,38,38                 | 0     |
| 54  | MG   | BB    | 3040 | 1/1   | 0.12 | -1.23 | 47,47,47,47                 | 0     |
| 54  | MG   | BB    | 3106 | 1/1   | 0.13 | -1.24 | 45,45,45,45                 | 0     |
| 54  | MG   | BB    | 3039 | 1/1   | 0.12 | -1.25 | 12,12,12,12                 | 0     |
| 54  | MG   | BB    | 3096 | 1/1   | 0.16 | -1.28 | 69,69,69,69                 | 0     |
| 54  | MG   | DB    | 3097 | 1/1   | 0.15 | -1.28 | 32,32,32,32                 | 0     |
| 54  | MG   | DB    | 3024 | 1/1   | 0.18 | -1.29 | 47,47,47,47                 | 0     |
| 54  | MG   | DB    | 3010 | 1/1   | 0.15 | -1.29 | 5,5,5,5                     | 0     |
| 54  | MG   | DB    | 3019 | 1/1   | 0.15 | -1.29 | 8,8,8,8                     | 0     |
| 54  | MG   | BB    | 3090 | 1/1   | 0.13 | -1.33 | 115,115,115,115             | 0     |
| 54  | MG   | CA    | 1617 | 1/1   | 0.10 | -1.33 | 12,12,12,12                 | 0     |
| 54  | MG   | BB    | 3067 | 1/1   | 0.11 | -1.34 | 25,25,25,25                 | 0     |
| 54  | MG   | DB    | 3025 | 1/1   | 0.10 | -1.34 | 18,18,18,18                 | 0     |
| 54  | MG   | AA    | 1648 | 1/1   | 0.10 | -1.36 | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3005 | 1/1   | 0.11 | -1.44 | 9,9,9,9                     | 0     |
| 54  | MG   | DB    | 3035 | 1/1   | 0.13 | -1.45 | 52,52,52,52                 | 0     |
| 54  | MG   | BB    | 3079 | 1/1   | 0.17 | -1.48 | 43,43,43,43                 | 0     |
| 54  | MG   | AA    | 1660 | 1/1   | 0.12 | -1.48 | 75,75,75,75                 | 0     |
| 54  | MG   | BB    | 3025 | 1/1   | 0.11 | -1.49 | 22,22,22,22                 | 0     |
| 54  | MG   | DB    | 3078 | 1/1   | 0.08 | -1.51 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 54  | MG   | DB    | 3106 | 1/1   | 0.12 | -1.53 | 17,17,17,17                 | 0     |
| 54  | MG   | BB    | 3060 | 1/1   | 0.15 | -1.53 | 43,43,43,43                 | 0     |
| 54  | MG   | BB    | 3053 | 1/1   | 0.11 | -1.53 | 38,38,38,38                 | 0     |
| 54  | MG   | DB    | 3069 | 1/1   | 0.18 | -1.54 | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3094 | 1/1   | 0.12 | -1.55 | 55,55,55,55                 | 0     |
| 54  | MG   | BB    | 3008 | 1/1   | 0.16 | -1.56 | 81,81,81,81                 | 0     |
| 54  | MG   | DB    | 3064 | 1/1   | 0.12 | -1.56 | 23,23,23,23                 | 0     |
| 54  | MG   | CA    | 1643 | 1/1   | 0.13 | -1.57 | 11,11,11,11                 | 0     |
| 54  | MG   | BB    | 3042 | 1/1   | 0.07 | -1.59 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1618 | 1/1   | 0.12 | -1.66 | 23,23,23,23                 | 0     |
| 54  | MG   | DB    | 3088 | 1/1   | 0.14 | -1.67 | 31,31,31,31                 | 0     |
| 54  | MG   | AA    | 1645 | 1/1   | 0.12 | -1.69 | 138,138,138,138             | 0     |
| 54  | MG   | DB    | 3055 | 1/1   | 0.14 | -1.71 | 26,26,26,26                 | 0     |
| 54  | MG   | BB    | 3007 | 1/1   | 0.15 | -1.73 | 103,103,103,103             | 0     |
| 54  | MG   | BB    | 3110 | 1/1   | 0.15 | -1.73 | 41,41,41,41                 | 0     |
| 54  | MG   | AA    | 1611 | 1/1   | 0.09 | -1.78 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1650 | 1/1   | 0.05 | -1.86 | 5,5,5,5                     | 0     |
| 54  | MG   | AA    | 1638 | 1/1   | 0.15 | -1.87 | 45,45,45,45                 | 0     |
| 54  | MG   | DB    | 3095 | 1/1   | 0.13 | -1.89 | 62,62,62,62                 | 0     |
| 56  | ZN   | B4    | 101  | 1/1   | 0.23 | -1.91 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1644 | 1/1   | 0.12 | -1.92 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1604 | 1/1   | 0.10 | -1.93 | 11,11,11,11                 | 0     |
| 54  | MG   | CA    | 1630 | 1/1   | 0.12 | -1.93 | 65,65,65,65                 | 0     |
| 54  | MG   | BB    | 3010 | 1/1   | 0.11 | -1.95 | 38,38,38,38                 | 0     |
| 54  | MG   | DB    | 3084 | 1/1   | 0.16 | -1.95 | 14,14,14,14                 | 0     |
| 54  | MG   | BB    | 3086 | 1/1   | 0.11 | -1.96 | 5,5,5,5                     | 0     |
| 54  | MG   | DB    | 3047 | 1/1   | 0.16 | -1.96 | 31,31,31,31                 | 0     |
| 54  | MG   | AA    | 1618 | 1/1   | 0.06 | -1.96 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1638 | 1/1   | 0.10 | -1.99 | 56,56,56,56                 | 0     |
| 54  | MG   | BB    | 3052 | 1/1   | 0.10 | -2.04 | 59,59,59,59                 | 0     |
| 54  | MG   | BB    | 3004 | 1/1   | 0.19 | -2.06 | 44,44,44,44                 | 0     |
| 54  | MG   | BB    | 3024 | 1/1   | 0.07 | -2.07 | 76,76,76,76                 | 0     |
| 54  | MG   | BB    | 3002 | 1/1   | 0.10 | -2.09 | 18,18,18,18                 | 0     |
| 54  | MG   | CA    | 1607 | 1/1   | 0.05 | -2.10 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3063 | 1/1   | 0.08 | -2.10 | 23,23,23,23                 | 0     |
| 54  | MG   | DB    | 3005 | 1/1   | 0.12 | -2.11 | 52,52,52,52                 | 0     |
| 54  | MG   | BB    | 3045 | 1/1   | 0.09 | -2.12 | 32,32,32,32                 | 0     |
| 54  | MG   | BB    | 3091 | 1/1   | 0.10 | -2.14 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1634 | 1/1   | 0.11 | -2.17 | 79,79,79,79                 | 0     |
| 56  | ZN   | D4    | 101  | 1/1   | 0.44 | -2.17 | 96,96,96,96                 | 0     |
| 54  | MG   | DB    | 3057 | 1/1   | 0.05 | -2.20 | 17,17,17,17                 | 0     |
| 54  | MG   | AA    | 1644 | 1/1   | 0.09 | -2.20 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 54  | MG   | DB    | 3040 | 1/1   | 0.12 | -2.34 | 5,5,5,5                     | 0     |
| 54  | MG   | DB    | 3098 | 1/1   | 0.11 | -2.36 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1610 | 1/1   | 0.09 | -2.38 | 65,65,65,65                 | 0     |
| 54  | MG   | DB    | 3033 | 1/1   | 0.22 | -2.39 | 20,20,20,20                 | 0     |
| 54  | MG   | AA    | 1653 | 1/1   | 0.08 | -2.39 | 51,51,51,51                 | 0     |
| 54  | MG   | DB    | 3104 | 1/1   | 0.13 | -2.41 | 21,21,21,21                 | 0     |
| 54  | MG   | BB    | 3031 | 1/1   | 0.14 | -2.41 | 44,44,44,44                 | 0     |
| 54  | MG   | DB    | 3043 | 1/1   | 0.12 | -2.45 | 7,7,7,7                     | 0     |
| 54  | MG   | AA    | 1601 | 1/1   | 0.12 | -2.45 | 10,10,10,10                 | 0     |
| 54  | MG   | DB    | 3105 | 1/1   | 0.07 | -2.45 | 24,24,24,24                 | 0     |
| 54  | MG   | DB    | 3092 | 1/1   | 0.10 | -2.45 | 60,60,60,60                 | 0     |
| 54  | MG   | BB    | 3068 | 1/1   | 0.16 | -2.48 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1630 | 1/1   | 0.11 | -2.49 | 118,118,118,118             | 0     |
| 54  | MG   | CA    | 1601 | 1/1   | 0.13 | -2.52 | 9,9,9,9                     | 0     |
| 54  | MG   | AA    | 1654 | 1/1   | 0.08 | -2.53 | 52,52,52,52                 | 0     |
| 54  | MG   | BB    | 3072 | 1/1   | 0.12 | -2.53 | 64,64,64,64                 | 0     |
| 54  | MG   | DB    | 3093 | 1/1   | 0.14 | -2.53 | 9,9,9,9                     | 0     |
| 54  | MG   | DB    | 3076 | 1/1   | 0.12 | -2.61 | 27,27,27,27                 | 0     |
| 54  | MG   | BB    | 3081 | 1/1   | 0.15 | -2.61 | 31,31,31,31                 | 0     |
| 54  | MG   | AA    | 1609 | 1/1   | 0.08 | -2.63 | 11,11,11,11                 | 0     |
| 54  | MG   | BB    | 3073 | 1/1   | 0.12 | -2.68 | 70,70,70,70                 | 0     |
| 54  | MG   | BB    | 3107 | 1/1   | 0.06 | -2.68 | 13,13,13,13                 | 0     |
| 54  | MG   | DB    | 3012 | 1/1   | 0.13 | -2.68 | 8,8,8,8                     | 0     |
| 54  | MG   | AA    | 1616 | 1/1   | 0.08 | -2.75 | 15,15,15,15                 | 0     |
| 54  | MG   | DB    | 3053 | 1/1   | 0.11 | -2.77 | 65,65,65,65                 | 0     |
| 54  | MG   | DB    | 3067 | 1/1   | 0.14 | -2.78 | 13,13,13,13                 | 0     |
| 54  | MG   | CA    | 1656 | 1/1   | 0.05 | -2.83 | 7,7,7,7                     | 0     |
| 54  | MG   | BB    | 3070 | 1/1   | 0.12 | -2.86 | 40,40,40,40                 | 0     |
| 54  | MG   | DB    | 3002 | 1/1   | 0.10 | -2.88 | 14,14,14,14                 | 0     |
| 54  | MG   | BB    | 3016 | 1/1   | 0.10 | -2.89 | 94,94,94,94                 | 0     |
| 54  | MG   | DB    | 3001 | 1/1   | 0.10 | -2.92 | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3054 | 1/1   | 0.08 | -2.95 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1631 | 1/1   | 0.07 | -2.98 | 61,61,61,61                 | 0     |
| 54  | MG   | DB    | 3091 | 1/1   | 0.10 | -3.01 | 11,11,11,11                 | 0     |
| 54  | MG   | BB    | 3061 | 1/1   | 0.09 | -3.02 | 46,46,46,46                 | 0     |
| 54  | MG   | DB    | 3016 | 1/1   | 0.11 | -3.03 | 5,5,5,5                     | 0     |
| 54  | MG   | DB    | 3103 | 1/1   | 0.09 | -3.04 | 37,37,37,37                 | 0     |
| 54  | MG   | BB    | 3085 | 1/1   | 0.11 | -3.05 | 76,76,76,76                 | 0     |
| 54  | MG   | BB    | 3088 | 1/1   | 0.06 | -3.05 | 11,11,11,11                 | 0     |
| 54  | MG   | DB    | 3021 | 1/1   | 0.14 | -3.09 | 18,18,18,18                 | 0     |
| 54  | MG   | BB    | 3035 | 1/1   | 0.15 | -3.10 | 60,60,60,60                 | 0     |
| 54  | MG   | DB    | 3070 | 1/1   | 0.09 | -3.12 | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 54  | MG   | DB    | 3042 | 1/1   | 0.07 | -3.16 | 36,36,36,36                 | 0     |
| 54  | MG   | DB    | 3031 | 1/1   | 0.10 | -3.16 | 29,29,29,29                 | 0     |
| 54  | MG   | AA    | 1620 | 1/1   | 0.05 | -3.17 | 95,95,95,95                 | 0     |
| 54  | MG   | DB    | 3017 | 1/1   | 0.13 | -3.23 | 23,23,23,23                 | 0     |
| 54  | MG   | AA    | 1606 | 1/1   | 0.05 | -3.29 | 73,73,73,73                 | 0     |
| 54  | MG   | BB    | 3066 | 1/1   | 0.06 | -3.30 | 34,34,34,34                 | 0     |
| 54  | MG   | DB    | 3077 | 1/1   | 0.10 | -3.30 | 17,17,17,17                 | 0     |
| 54  | MG   | DB    | 3044 | 1/1   | 0.11 | -3.32 | 16,16,16,16                 | 0     |
| 54  | MG   | DB    | 3039 | 1/1   | 0.07 | -3.34 | 34,34,34,34                 | 0     |
| 54  | MG   | CA    | 1640 | 1/1   | 0.14 | -3.38 | 35,35,35,35                 | 0     |
| 54  | MG   | CA    | 1648 | 1/1   | 0.14 | -3.40 | 17,17,17,17                 | 0     |
| 54  | MG   | BB    | 3032 | 1/1   | 0.11 | -3.58 | 31,31,31,31                 | 0     |
| 54  | MG   | BB    | 3050 | 1/1   | 0.09 | -3.60 | 16,16,16,16                 | 0     |
| 54  | MG   | AA    | 1641 | 1/1   | 0.05 | -3.60 | 32,32,32,32                 | 0     |
| 54  | MG   | BB    | 3076 | 1/1   | 0.08 | -3.65 | 48,48,48,48                 | 0     |
| 54  | MG   | DB    | 3071 | 1/1   | 0.09 | -3.70 | 41,41,41,41                 | 0     |
| 54  | MG   | CA    | 1611 | 1/1   | 0.09 | -3.73 | 114,114,114,114             | 0     |
| 54  | MG   | DB    | 3080 | 1/1   | 0.12 | -3.92 | 13,13,13,13                 | 0     |
| 54  | MG   | AA    | 1646 | 1/1   | 0.09 | -3.92 | 98,98,98,98                 | 0     |
| 54  | MG   | DB    | 3020 | 1/1   | 0.10 | -3.93 | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3074 | 1/1   | 0.07 | -3.96 | 7,7,7,7                     | 0     |
| 54  | MG   | AA    | 1629 | 1/1   | 0.12 | -3.99 | 44,44,44,44                 | 0     |
| 54  | MG   | CA    | 1635 | 1/1   | 0.09 | -4.00 | 105,105,105,105             | 0     |
| 54  | MG   | BB    | 3103 | 1/1   | 0.09 | -4.17 | 20,20,20,20                 | 0     |
| 54  | MG   | BB    | 3056 | 1/1   | 0.06 | -4.21 | 61,61,61,61                 | 0     |
| 54  | MG   | BB    | 3058 | 1/1   | 0.08 | -4.29 | 17,17,17,17                 | 0     |
| 54  | MG   | DB    | 3081 | 1/1   | 0.08 | -4.33 | 20,20,20,20                 | 0     |
| 54  | MG   | DB    | 3041 | 1/1   | 0.09 | -4.34 | 9,9,9,9                     | 0     |
| 54  | MG   | BB    | 3102 | 1/1   | 0.12 | -4.42 | 76,76,76,76                 | 0     |
| 54  | MG   | DB    | 3056 | 1/1   | 0.15 | -4.45 | 16,16,16,16                 | 0     |
| 54  | MG   | BB    | 3022 | 1/1   | 0.05 | -4.46 | 34,34,34,34                 | 0     |
| 54  | MG   | AA    | 1643 | 1/1   | 0.09 | -4.59 | 118,118,118,118             | 0     |
| 54  | MG   | BB    | 3044 | 1/1   | 0.06 | -4.69 | 29,29,29,29                 | 0     |
| 54  | MG   | BB    | 3084 | 1/1   | 0.09 | -4.69 | 60,60,60,60                 | 0     |
| 54  | MG   | DB    | 3072 | 1/1   | 0.07 | -4.76 | 48,48,48,48                 | 0     |
| 54  | MG   | DB    | 3006 | 1/1   | 0.07 | -4.76 | 15,15,15,15                 | 0     |
| 54  | MG   | BB    | 3030 | 1/1   | 0.05 | -4.87 | 83,83,83,83                 | 0     |
| 54  | MG   | BB    | 3069 | 1/1   | 0.07 | -4.94 | 5,5,5,5                     | 0     |
| 54  | MG   | CA    | 1655 | 1/1   | 0.08 | -5.01 | 22,22,22,22                 | 0     |
| 54  | MG   | AA    | 1604 | 1/1   | 0.10 | -5.30 | 37,37,37,37                 | 0     |
| 54  | MG   | BB    | 3089 | 1/1   | 0.06 | -5.43 | 30,30,30,30                 | 0     |
| 54  | MG   | DB    | 3038 | 1/1   | 0.11 | -5.54 | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|-----------------------------|-------|
| 54  | MG   | AA    | 1605 | 1/1   | 0.11 | -5.55  | 54,54,54,54                 | 0     |
| 54  | MG   | BB    | 3095 | 1/1   | 0.11 | -5.61  | 65,65,65,65                 | 0     |
| 54  | MG   | DB    | 3009 | 1/1   | 0.09 | -5.97  | 22,22,22,22                 | 0     |
| 54  | MG   | DB    | 3034 | 1/1   | 0.11 | -6.08  | 52,52,52,52                 | 0     |
| 54  | MG   | DB    | 3062 | 1/1   | 0.06 | -6.57  | 44,44,44,44                 | 0     |
| 54  | MG   | CA    | 1609 | 1/1   | 0.13 | -6.73  | 81,81,81,81                 | 0     |
| 54  | MG   | BB    | 3063 | 1/1   | 0.09 | -7.12  | 5,5,5,5                     | 0     |
| 54  | MG   | BB    | 3015 | 1/1   | 0.08 | -8.97  | 9,9,9,9                     | 0     |
| 54  | MG   | DB    | 3082 | 1/1   | 0.07 | -9.09  | 37,37,37,37                 | 0     |
| 54  | MG   | CA    | 1631 | 1/1   | 0.10 | -9.82  | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1645 | 1/1   | 0.07 | -10.22 | 82,82,82,82                 | 0     |
| 54  | MG   | DB    | 3107 | 1/1   | 0.08 | -14.40 | 51,51,51,51                 | 0     |
| 54  | MG   | DB    | 3054 | 1/1   | 0.13 | -33.00 | 69,69,69,69                 | 0     |
| 54  | MG   | DB    | 3029 | 1/1   | 0.18 | -      | 70,70,70,70                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.