



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:55 am BST

PDB ID : 4V64
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with hygromycin B.
Authors : Borovinskaya, M.A.; Shoji, S.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2008-06-11
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

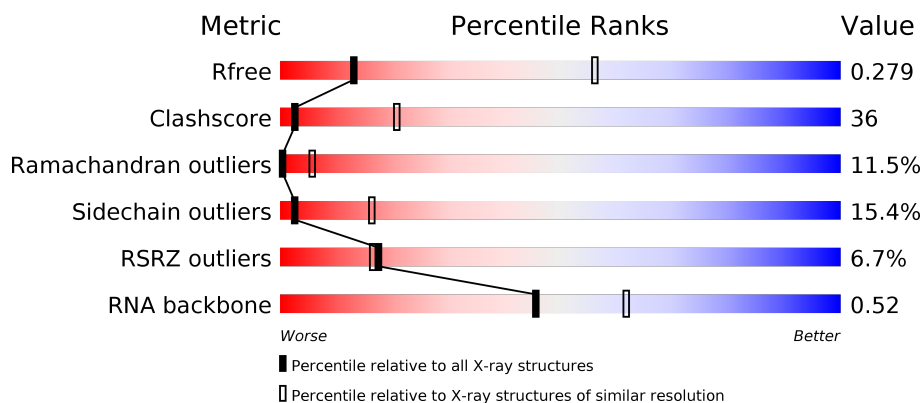
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



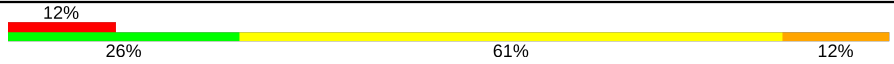

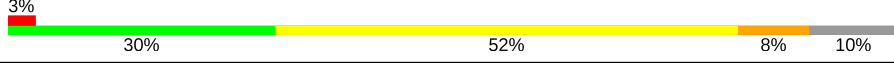
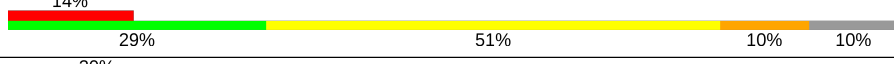
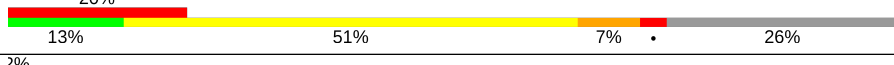
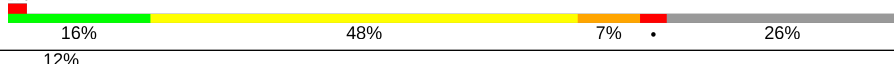
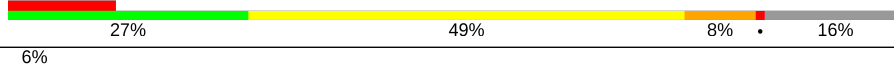
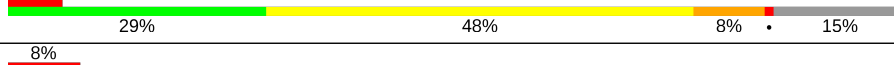
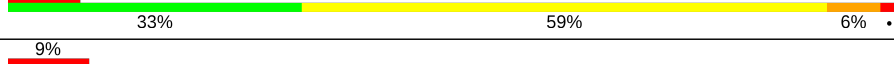
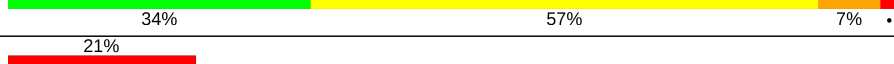

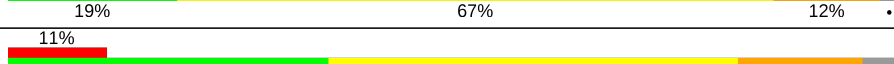
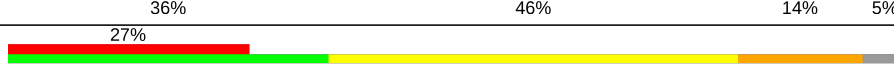
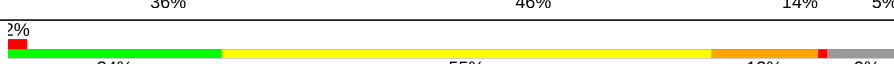
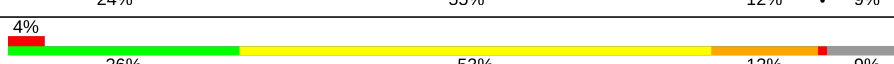
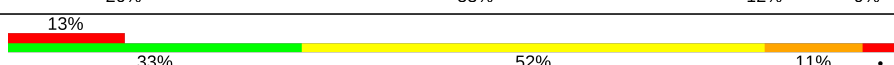
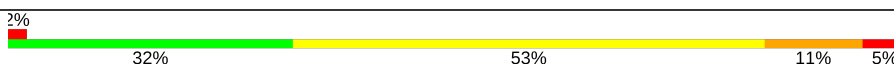
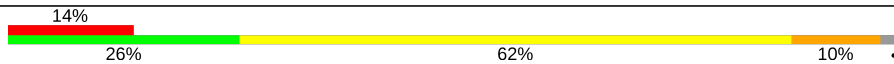
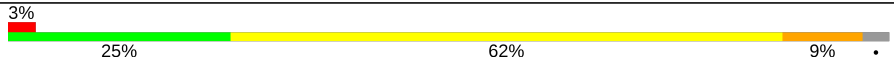
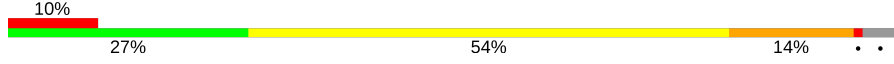

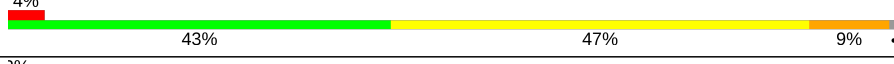



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1659 (3.60-3.40) |
| Clashscore | 141614 | 1036 (3.58-3.42) |
| Ramachandran outliers | 138981 | 1005 (3.58-3.42) |
| Sidechain outliers | 138945 | 1006 (3.58-3.42) |
| RSRZ outliers | 127900 | 1559 (3.60-3.40) |
| RNA backbone | 3102 | 1002 (4.00-3.00) |

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------|
| 1 | AA | 1542 | 22% 63% 14% .. |
| 1 | CA | 1542 | 21% 65% 13% .. |
| 2 | AC | 232 | 13% 31% 43% 13% • 11% |
| 2 | CC | 232 | 7% 31% 44% 13% • 11% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | AD | 205 |  |
| 3 | CD | 205 |  |
| 4 | AE | 166 |  |
| 4 | CE | 166 |  |
| 5 | AF | 135 |  |
| 5 | CF | 135 |  |
| 6 | AG | 178 |  |
| 6 | CG | 178 |  |
| 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 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | 71 | |
| 21 | CU | 71 | |
| 22 | BA | 120 | |
| 22 | DA | 120 | |
| 23 | BB | 2904 | |
| 23 | DB | 2904 | |
| 24 | BV | 94 | |
| 24 | DV | 94 | |
| 25 | BC | 273 | |
| 25 | DC | 273 | |
| 26 | BD | 209 | |
| 26 | DD | 209 | |
| 27 | BE | 201 | |
| 27 | DE | 201 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | BF | 178 | |
| 28 | DF | 178 | |
| 29 | BG | 176 | |
| 29 | DG | 176 | |
| 30 | BH | 149 | |
| 30 | DH | 149 | |
| 31 | BJ | 142 | |
| 31 | DJ | 142 | |
| 32 | BK | 123 | |
| 32 | DK | 123 | |
| 33 | BL | 144 | |
| 33 | DL | 144 | |
| 34 | BM | 136 | |
| 34 | DM | 136 | |
| 35 | BN | 127 | |
| 35 | DN | 127 | |
| 36 | BO | 117 | |
| 36 | DO | 117 | |
| 37 | BP | 114 | |
| 37 | DP | 114 | |
| 38 | BQ | 117 | |
| 38 | DQ | 117 | |
| 39 | BR | 103 | |
| 39 | DR | 103 | |
| 40 | BS | 110 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | DS | 110 | |
| 41 | BT | 100 | |
| 41 | DT | 100 | |
| 42 | BU | 103 | |
| 42 | DU | 103 | |
| 43 | BW | 84 | |
| 43 | DW | 84 | |
| 44 | BX | 63 | |
| 44 | DX | 63 | |
| 45 | BY | 58 | |
| 45 | DY | 58 | |
| 46 | BZ | 78 | |
| 46 | DZ | 78 | |
| 47 | B0 | 56 | |
| 47 | D0 | 56 | |
| 48 | B1 | 54 | |
| 48 | D1 | 54 | |
| 49 | B2 | 46 | |
| 49 | D2 | 46 | |
| 50 | B3 | 64 | |
| 50 | D3 | 64 | |
| 51 | B4 | 38 | |
| 51 | D4 | 38 | |
| 52 | BI | 141 | |
| 52 | DI | 141 | |

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 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 |
| | | | 715 | 440 | 146 | 128 | 1 | | | |
| 14 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 715 | 440 | 146 | 128 | 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 |
| | | | 656 | 417 | 122 | 114 | 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 ribosomal RNA.

| 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 ribosomal RNA.

| 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 L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | BV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 24 | DV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- 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 L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | BE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 27 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |
| 28 | DF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 29 | DG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |
| 30 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |
| 32 | DK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |
| 35 | DN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |
| 41 | DT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BU | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42 | DU | 102 | Total | C | N | O | | | |
| | | | 779 | 492 | 146 | 141 | 0 | 0 | 0 |

- Molecule 43 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BW | 79 | Total | C | N | O | S | | | |
| | | | 596 | 367 | 120 | 108 | 1 | 0 | 0 | 0 |
| 43 | DW | 79 | Total | C | N | O | S | | | |
| | | | 596 | 367 | 120 | 108 | 1 | 0 | 0 | 0 |

- Molecule 44 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 44 | BX | 63 | Total | C | N | O | S | | | |
| | | | 509 | 313 | 99 | 95 | 2 | 0 | 0 | 0 |
| 44 | DX | 63 | Total | C | N | O | S | | | |
| | | | 509 | 313 | 99 | 95 | 2 | 0 | 0 | 0 |

- Molecule 45 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 45 | BY | 58 | Total | C | N | O | S | | | |
| | | | 449 | 281 | 87 | 79 | 2 | 0 | 0 | 0 |
| 45 | DY | 58 | Total | C | N | O | S | | | |
| | | | 449 | 281 | 87 | 79 | 2 | 0 | 0 | 0 |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BZ | 77 | Total | C | N | O | S | | | |
| | | | 625 | 388 | 129 | 106 | 2 | 0 | 0 | 0 |
| 46 | DZ | 77 | Total | C | N | O | S | | | |
| | | | 625 | 388 | 129 | 106 | 2 | 0 | 0 | 0 |

- Molecule 47 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 47 | B0 | 56 | Total | C | N | O | S | | | |
| | | | 444 | 269 | 94 | 80 | 1 | 0 | 0 | 0 |
| 47 | D0 | 56 | Total | C | N | O | S | | | |
| | | | 444 | 269 | 94 | 80 | 1 | 0 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 48 | B1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |
| 48 | D1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49 | B2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 49 | D2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 50 | B3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 50 | D3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | B4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 51 | D4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

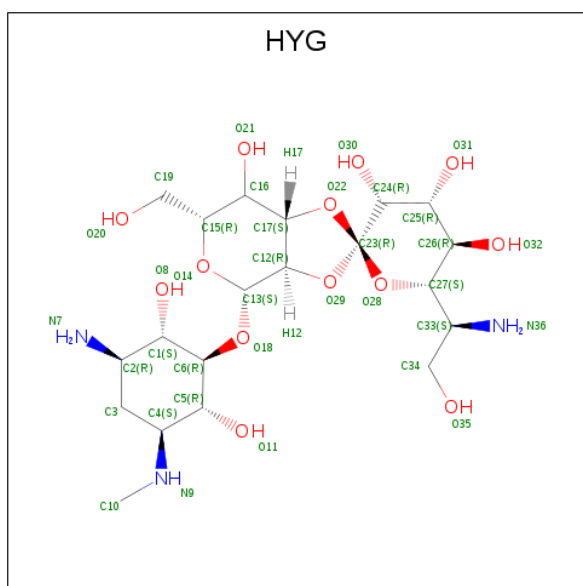
- Molecule 52 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | BI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 52 | DI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 53 | BB | 110 | Total | Mg | 0 | 0 |
| | | | 110 | 110 | | |
| 53 | CA | 61 | Total | Mg | 0 | 0 |
| | | | 61 | 61 | | |
| 53 | AE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 53 | AA | 58 | Total | Mg | 0 | 0 |
| | | | 58 | 58 | | |
| 53 | AN | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 53 | CE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 53 | DB | 111 | Total | Mg | 0 | 0 |
| | | | 111 | 111 | | |

- Molecule 54 is HYGROMYCIN B (three-letter code: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 55 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 56 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | AA | 282 | Total | O | 0 | 0 |
| | | | 282 | 282 | | |
| 56 | AE | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | AK | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | AL | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | AN | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | AT | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | BB | 492 | Total | O | 0 | 0 |
| | | | 492 | 492 | | |
| 56 | BC | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |
| 56 | BD | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | BE | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | BH | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | BL | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | B2 | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | CA | 294 | Total | O | 0 | 0 |
| | | | 294 | 294 | | |
| 56 | CE | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | CI | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | CK | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | CL | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |

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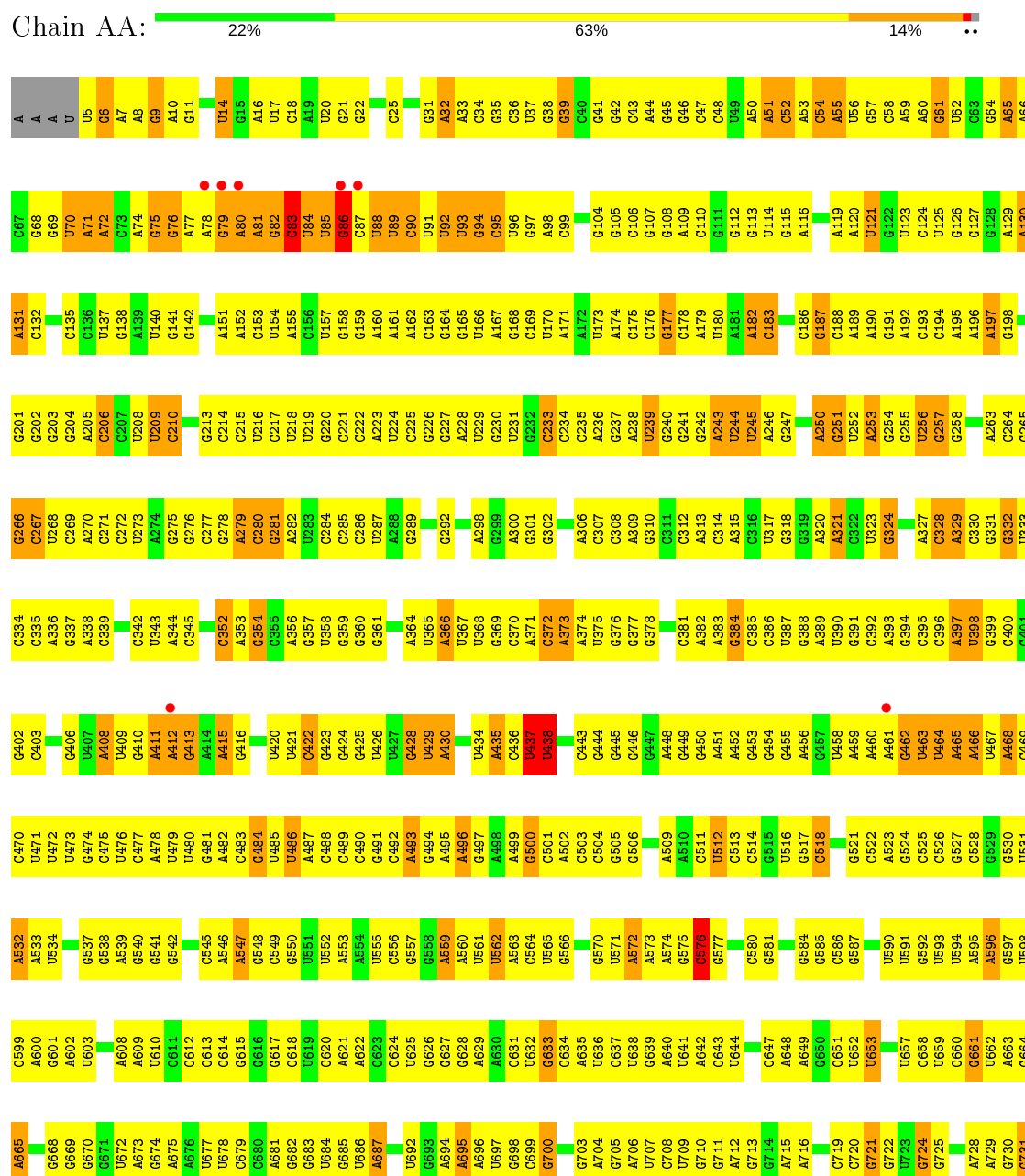
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 56 | CN | 3 | Total 3 | O 3 | 0 | 0 |
| 56 | CT | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | DB | 499 | Total 499 | O 499 | 0 | 0 |
| 56 | DC | 5 | Total 5 | O 5 | 0 | 0 |
| 56 | DD | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | DE | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | DL | 5 | Total 5 | O 5 | 0 | 0 |
| 56 | DP | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | D2 | 1 | Total 1 | O 1 | 0 | 0 |

3 Residue-property plots

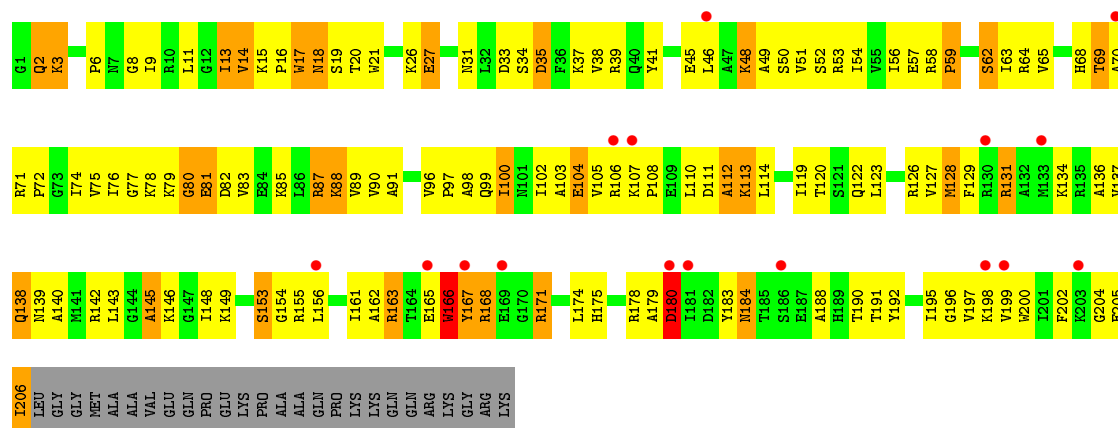
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 16S ribosomal RNA

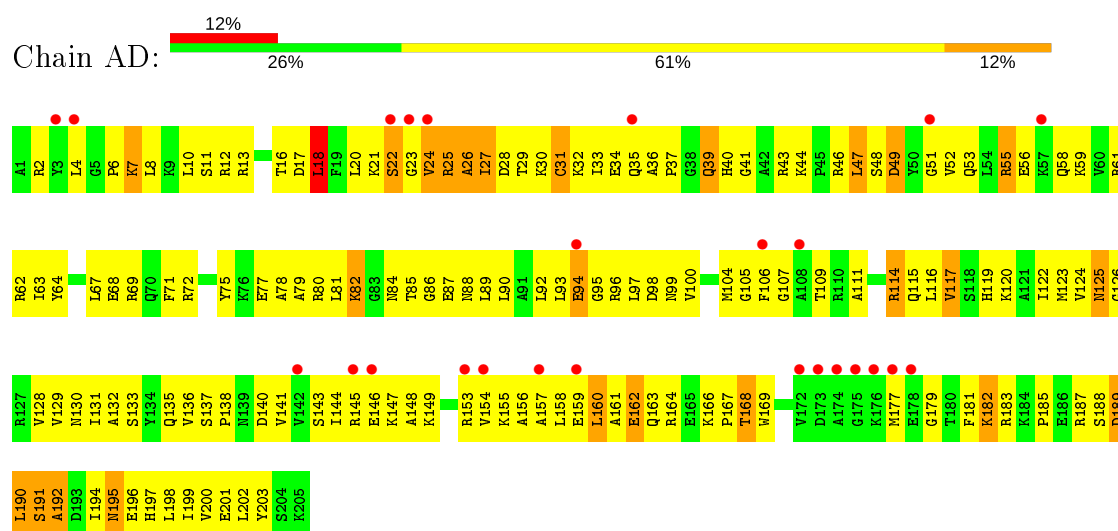


| | | | | | | | | | | | | | | | |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A996 | U997 | C931 | A860 | U793 | G724 | C660 | A595 | G539 | U464 | A397 | G332 | A263 | G201 | C135 | G69 |
| C998 | C998 | C934 | G861 | A794 | G725 | G661 | A596 | G530 | A465 | U998 | U333 | C264 | G202 | C136 | U70 |
| C999 | A935 | A935 | U862 | C795 | A728 | U662 | G597 | U531 | A466 | C399 | C394 | G265 | G203 | G137 | A71 |
| A1000 | A864 | A936 | G863 | C796 | A729 | A663 | U598 | A532 | U467 | C400 | C335 | G266 | G204 | G138 | A72 |
| C1001 | A937 | A937 | A865 | C797 | A730 | A664 | C599 | A533 | A468 | G401 | A336 | C267 | A205 | C267 | C73 |
| G1002 | A938 | A938 | C866 | U798 | G731 | A665 | A600 | U534 | C469 | C403 | A338 | U268 | C206 | G141 | |
| G1003 | G939 | G939 | G867 | | | | G601 | G537 | C470 | C403 | A339 | C269 | C207 | G142 | A77 |
| A1004 | C940 | C940 | C868 | A802 | G734 | G668 | A602 | G538 | U471 | G406 | C399 | A270 | U208 | A143 | A78 |
| G1005 | G941 | G941 | G869 | G803 | C735 | G669 | U603 | A539 | U472 | U407 | U340 | C271 | U209 | G144 | G79 |
| A1006 | | | G870 | U804 | C736 | G670 | | G540 | U473 | A408 | C342 | U272 | C210 | G145 | A80 |
| U1007 | G945 | G945 | U875 | C805 | A737 | G671 | A607 | G541 | U474 | U409 | U343 | U273 | | | A81 |
| A946 | A946 | A946 | C876 | C806 | C737 | U672 | A608 | G542 | C475 | U409 | U344 | A274 | G213 | A149 | G82 |
| G947 | G947 | G947 | G877 | A807 | C738 | A673 | A609 | G543 | U476 | G410 | U345 | G275 | C214 | U150 | C83 |
| U1009 | | | A878 | C808 | C739 | G674 | U610 | U543 | C477 | A411 | C346 | G276 | C215 | A151 | U84 |
| U1010 | | | A879 | G809 | | | G611 | G544 | U478 | A412 | C352 | | | | |
| C948 | C948 | C948 | C879 | C810 | G742 | A675 | C612 | G545 | U479 | A413 | A353 | C277 | U216 | A152 | G86 |
| A949 | G950 | G950 | C880 | C811 | A743 | U677 | G613 | A546 | U480 | A414 | A354 | A279 | C217 | C153 | G87 |
| G951 | G951 | G951 | G881 | G812 | C744 | U678 | G614 | A547 | A481 | A415 | A355 | C280 | U218 | U154 | U88 |
| A1014 | U952 | U952 | C882 | U813 | G745 | C679 | G615 | G548 | A482 | G416 | C356 | G281 | U219 | A155 | U89 |
| G953 | G953 | G953 | C883 | A814 | A746 | G680 | G616 | G549 | C483 | | A356 | A282 | G220 | C156 | U90 |
| G954 | G954 | G954 | U884 | A815 | A747 | A681 | G617 | G550 | A484 | U420 | A357 | A283 | C221 | U157 | C90 |
| A1016 | G955 | G955 | G885 | A816 | C748 | U682 | G618 | U551 | U485 | U421 | U358 | A284 | C222 | G158 | U91 |
| U1017 | U956 | U956 | G886 | G817 | A749 | G683 | U619 | U552 | U486 | C422 | C359 | C285 | A223 | G159 | U92 |
| G1018 | G957 | G957 | | C817 | G750 | U684 | C620 | A553 | A487 | G423 | G360 | C286 | U224 | A160 | U93 |
| A1019 | U957 | U957 | | G818 | U751 | U685 | A621 | A554 | C488 | G424 | G361 | U287 | C225 | A161 | G94 |
| A958 | A958 | A958 | A889 | A819 | | U686 | A622 | U555 | C489 | G425 | G362 | A288 | G226 | A162 | C95 |
| A959 | A959 | A959 | C893 | U820 | | | A623 | G556 | C490 | U426 | A363 | G289 | G227 | C163 | U96 |
| U960 | U960 | U960 | G894 | G821 | C754 | A687 | C624 | C556 | A491 | U427 | A364 | G290 | A228 | G164 | G97 |
| U1022 | U1022 | U1022 | G894 | U822 | G755 | G688 | C625 | | C492 | G428 | U365 | G292 | U229 | G165 | A98 |
| G1024 | | | | C923 | | | U625 | A559 | C493 | U429 | U366 | G293 | U230 | U166 | C99 |
| U1025 | A964 | A964 | G898 | G824 | U762 | U692 | G626 | A560 | A494 | A430 | A366 | A298 | U231 | A167 | G100 |
| G1026 | U965 | U965 | C899 | A825 | G763 | G693 | G627 | U561 | C495 | A431 | U367 | C299 | G232 | G168 | A101 |
| C1027 | G966 | G966 | A900 | C826 | C764 | A694 | G628 | U562 | A496 | | U368 | G300 | C233 | C169 | |
| C1028 | C967 | C967 | A901 | U827 | A765 | A695 | A629 | A563 | A497 | U434 | G369 | A300 | C234 | U170 | G104 |
| U1029 | A968 | A968 | G902 | U828 | A766 | A696 | G630 | C564 | G497 | U435 | C370 | G301 | C235 | G105 | C106 |
| U1030 | A969 | A969 | G903 | G829 | A767 | U697 | G631 | U565 | A498 | C436 | A371 | G302 | A236 | G107 | G108 |
| G1031 | C970 | C970 | U904 | G830 | G775 | G705 | U632 | G566 | A499 | G437 | C372 | G237 | G237 | C175 | A109 |
| G971 | G971 | G971 | U905 | G832 | G776 | A706 | G633 | G576 | G500 | U437 | A373 | A306 | A238 | C176 | |
| C972 | C972 | C972 | A906 | G833 | C770 | G707 | C634 | G570 | C501 | U438 | A374 | C307 | U239 | C177 | G110 |
| G973 | G973 | G973 | U916 | U842 | G778 | U708 | A635 | U571 | A502 | | U375 | C308 | G240 | G177 | |
| A1035 | A974 | A974 | G917 | U843 | U772 | U709 | G636 | A572 | C503 | C443 | G376 | A309 | G241 | C178 | G111 |
| A1036 | A975 | A975 | A918 | G844 | G773 | G703 | C637 | A573 | C504 | G444 | G377 | G310 | G242 | A179 | G112 |
| C1037 | G976 | G976 | A919 | A845 | G774 | A704 | U638 | A574 | G505 | G445 | G378 | A243 | G243 | U180 | G113 |
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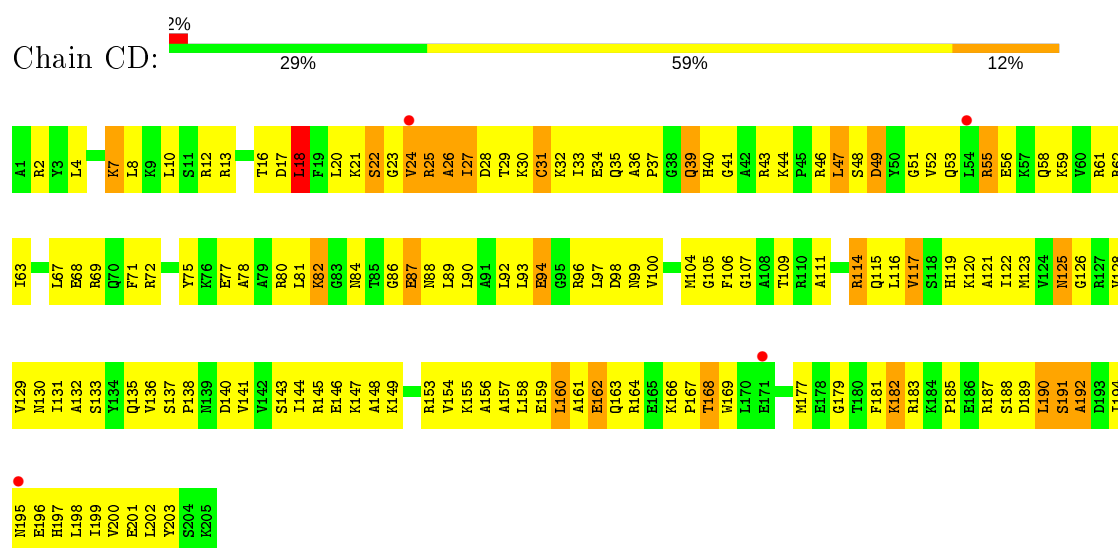




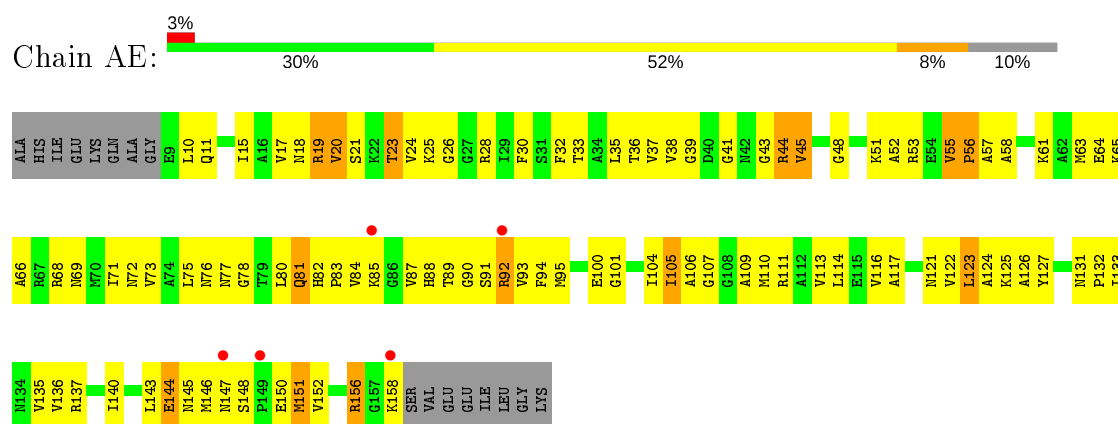
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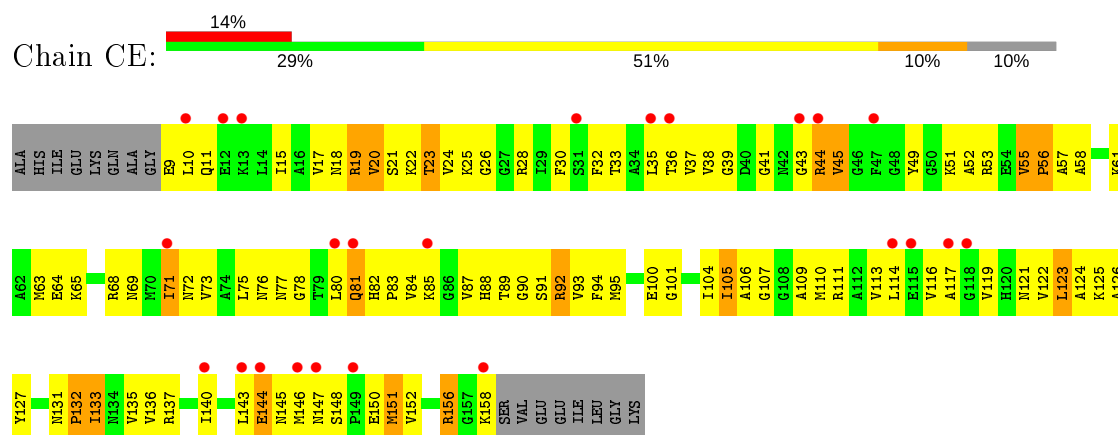
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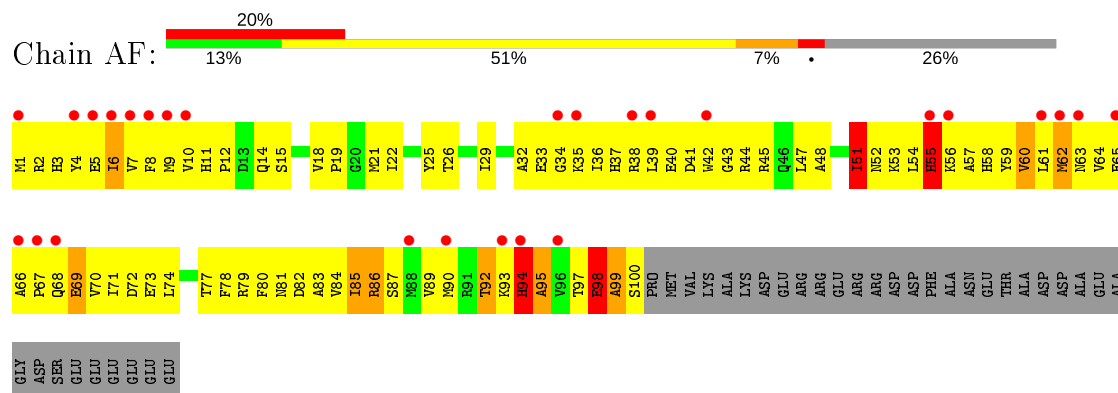
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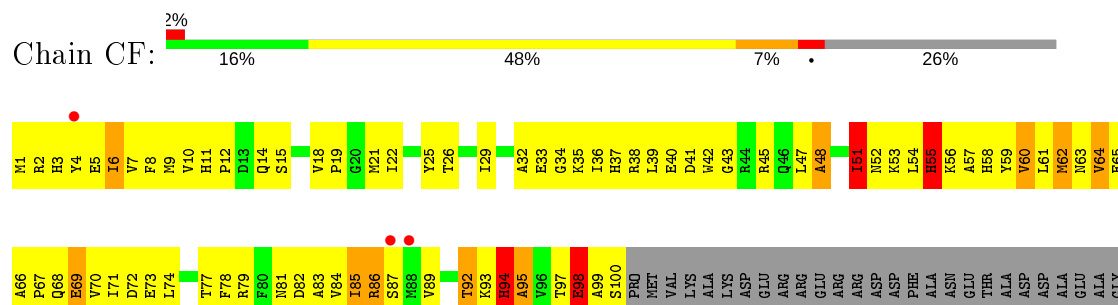
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6

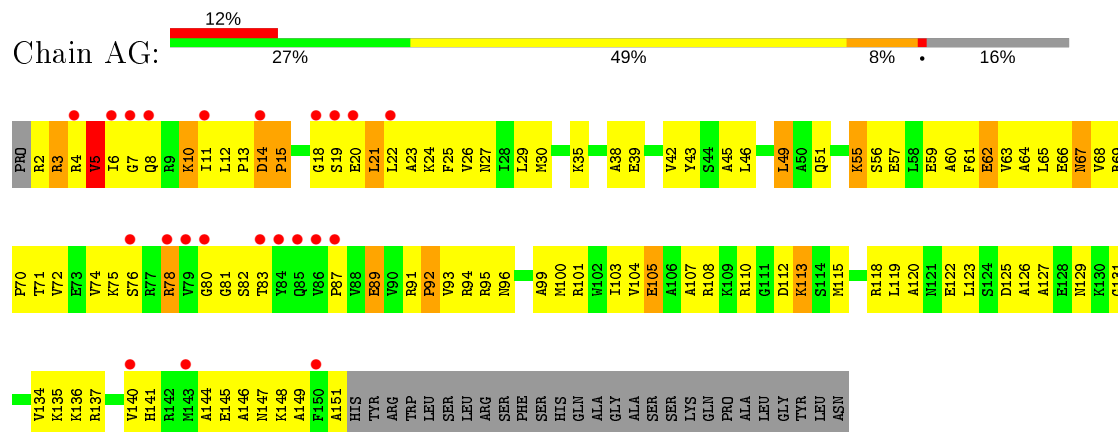


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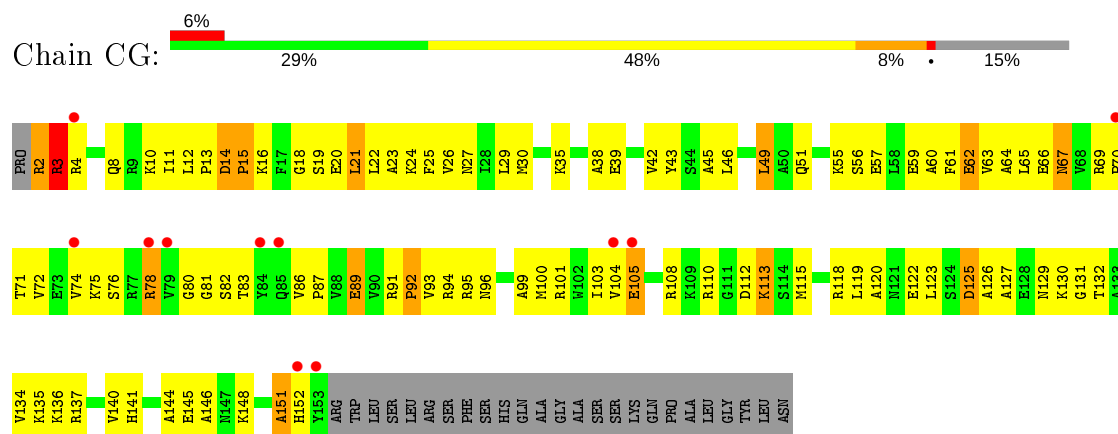


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SER
GLU
GLU
GLU
GLU

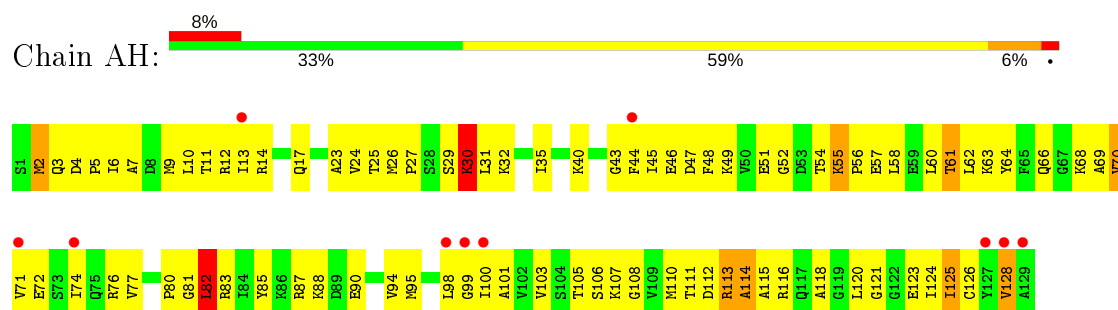
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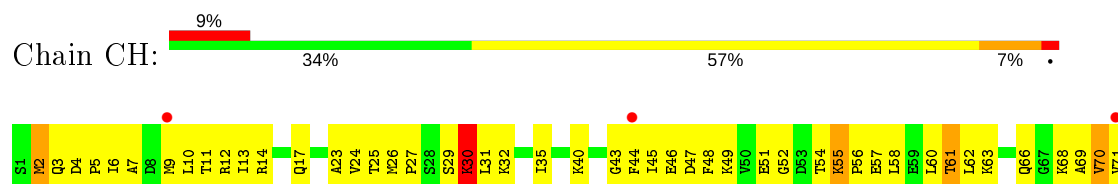
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

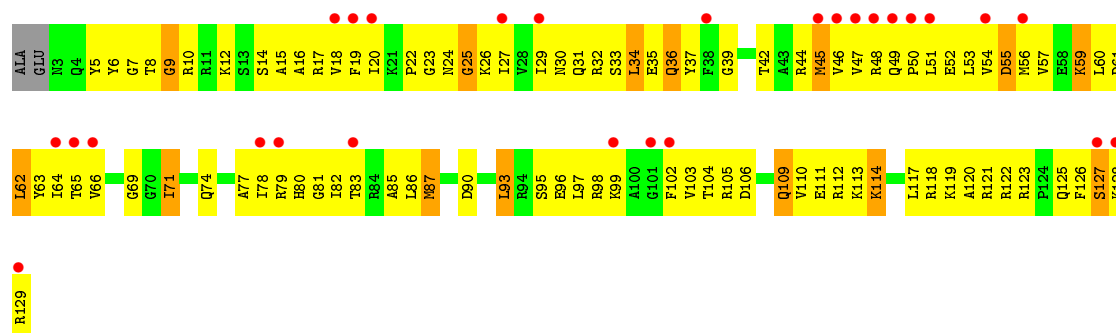


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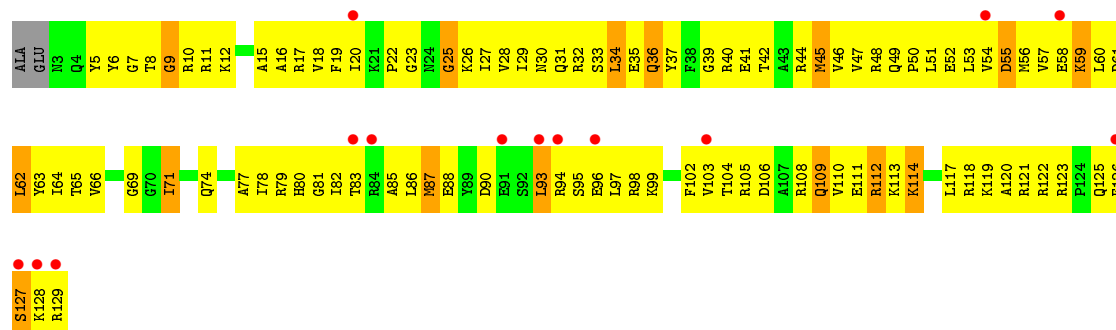




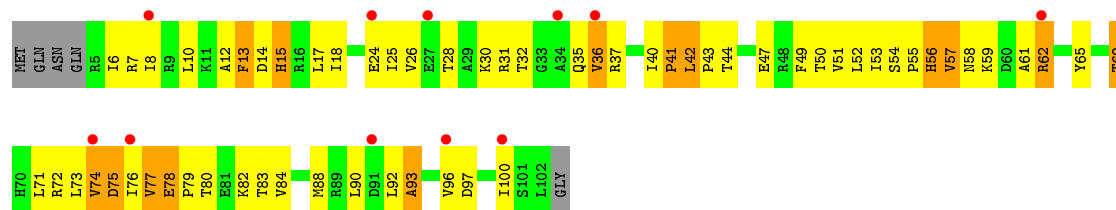
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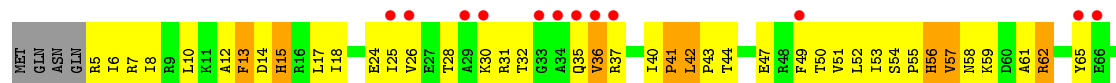
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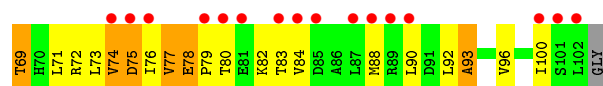


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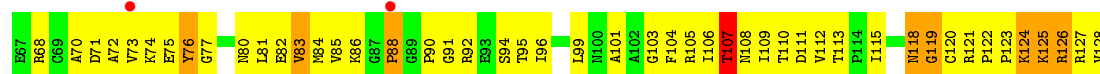


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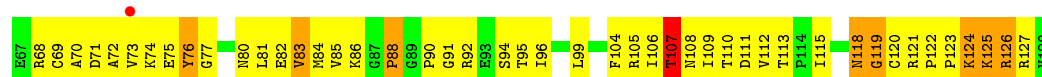




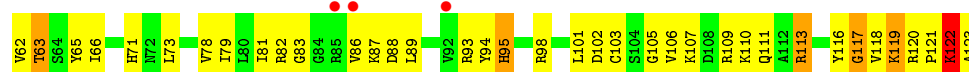
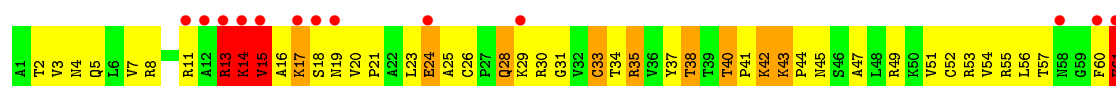
• Molecule 10: 30S ribosomal protein S11



• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12

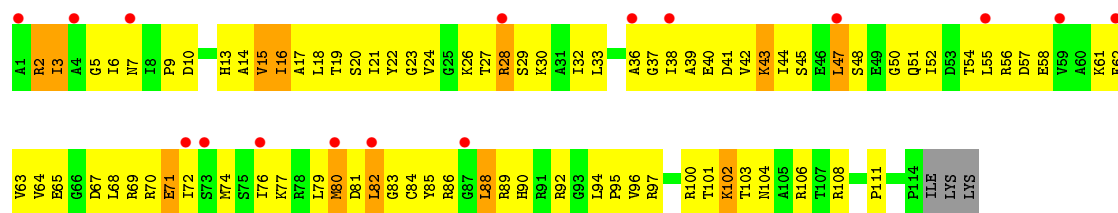


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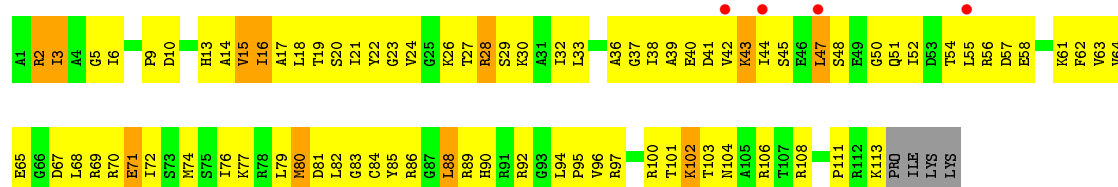


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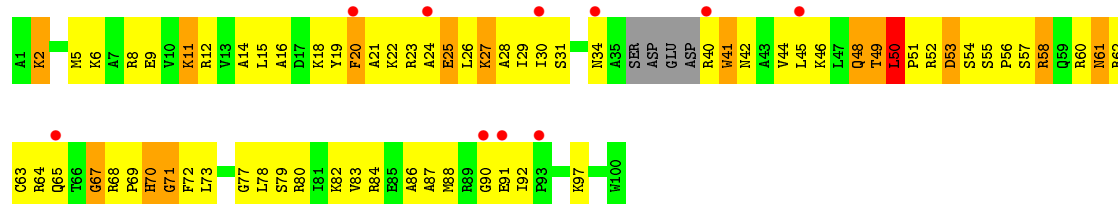




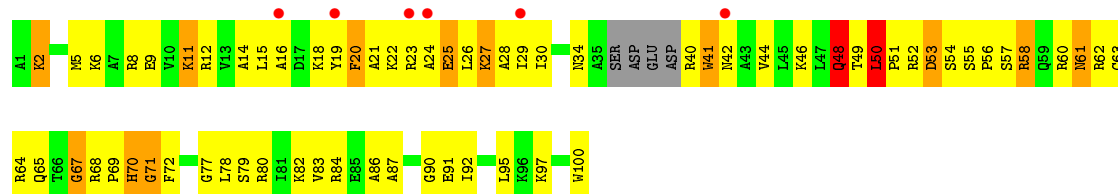
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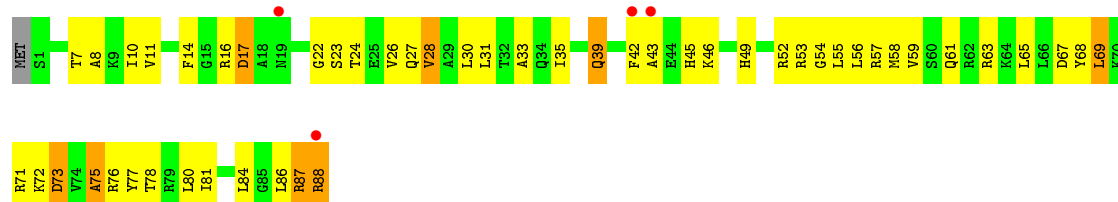
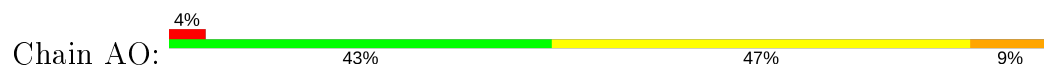
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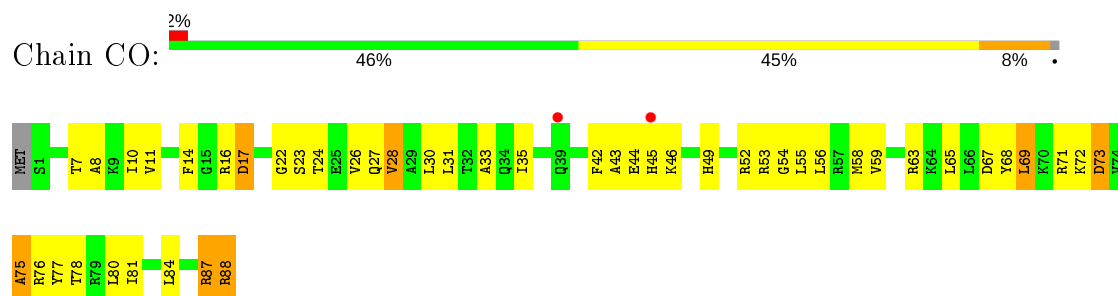
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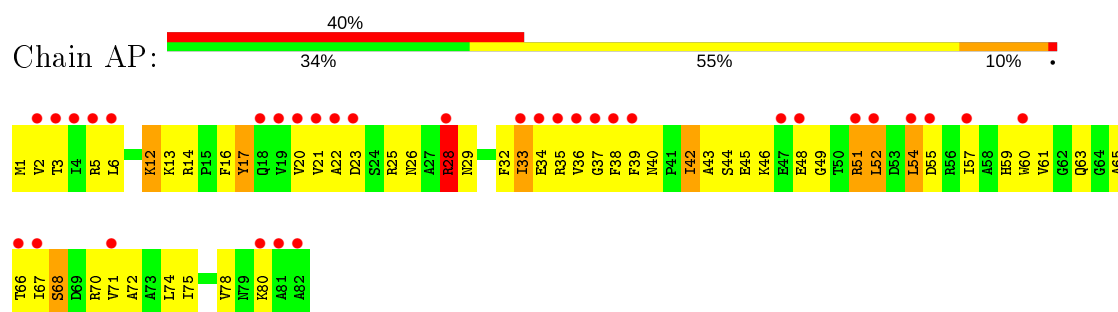
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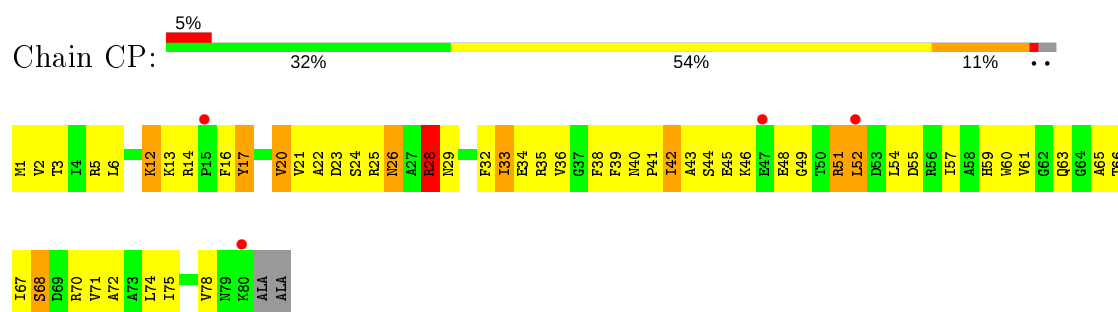
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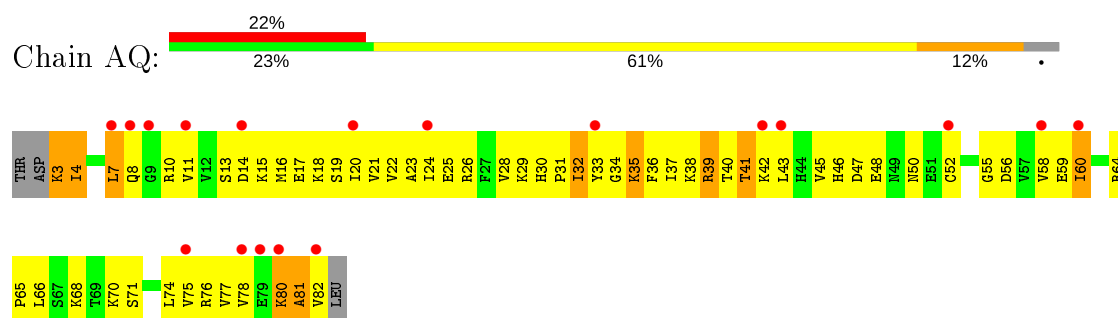
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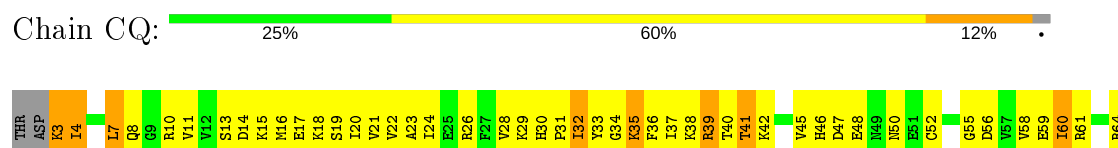
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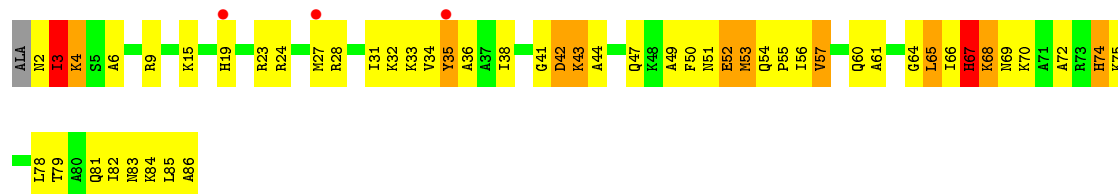


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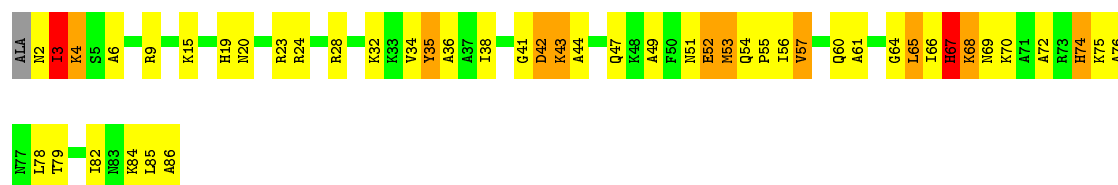
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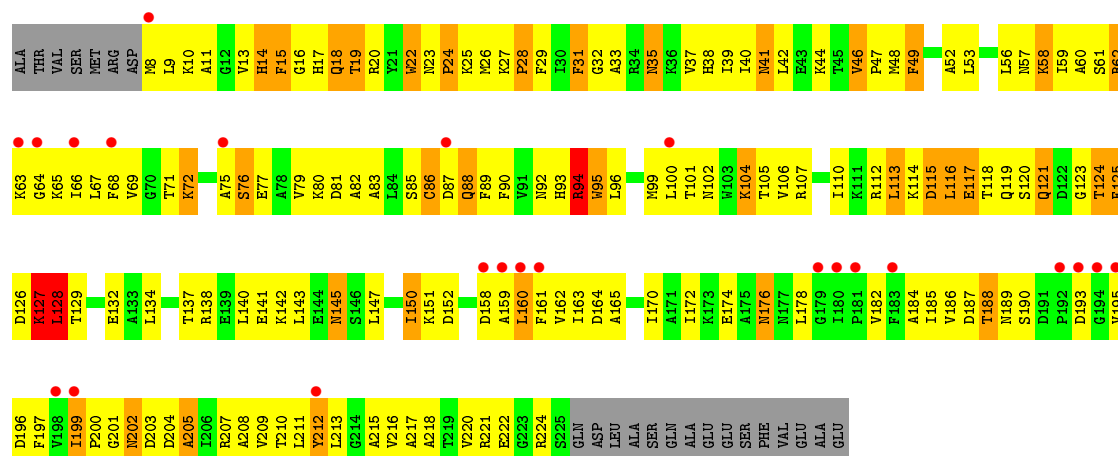
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Chain CT: 43% 42% 12% ..



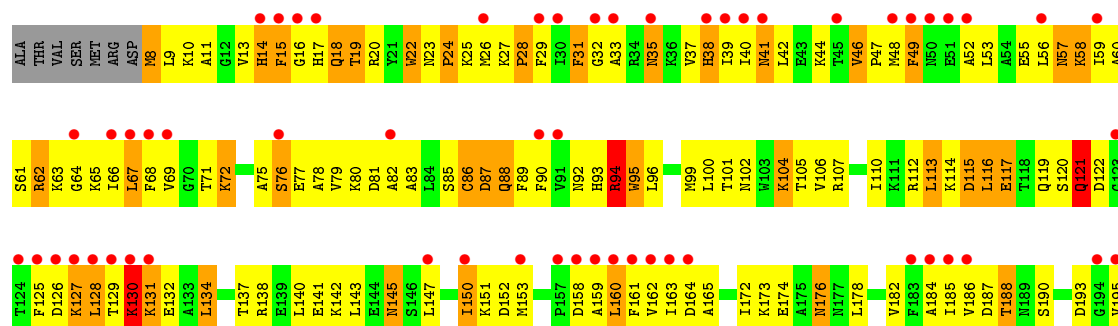
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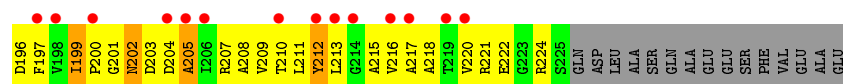
Chain AB: 10% 25% 50% 15% 9%



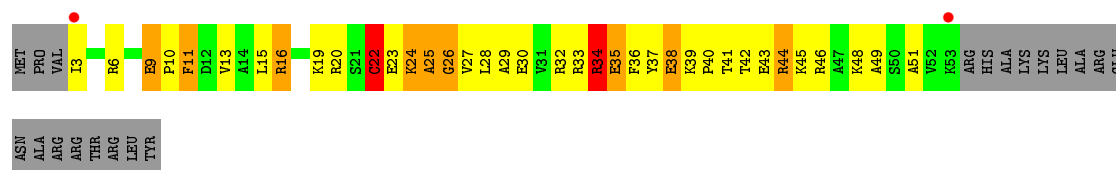
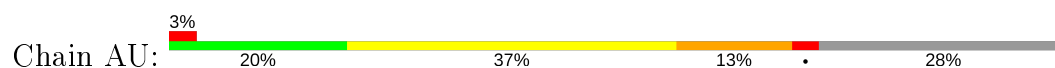
• Molecule 20: 30S ribosomal protein S2

Chain CB: 30% 24% 48% 18% 9%

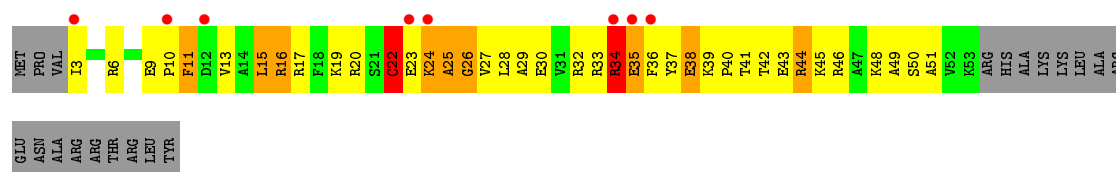
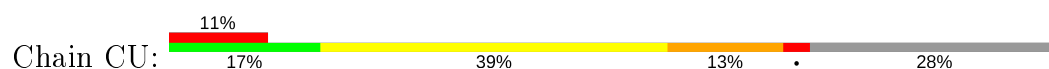




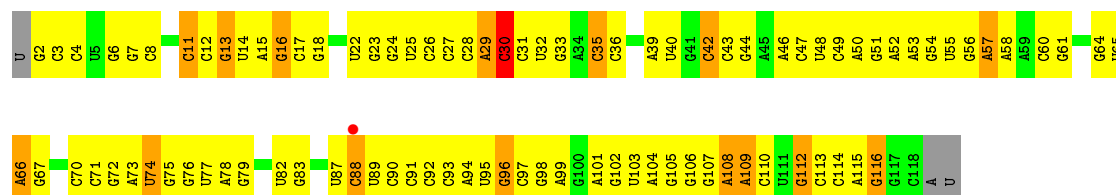
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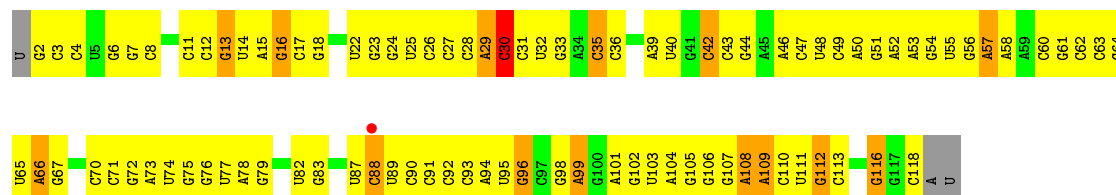
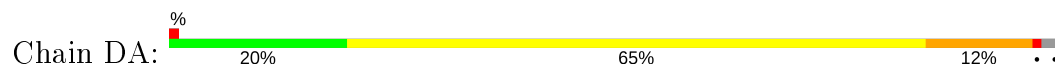
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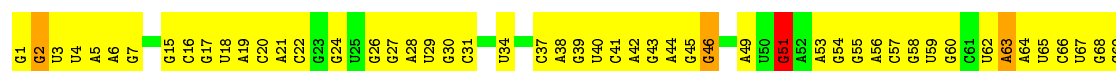
- Molecule 22: 5S ribosomal RNA



- Molecule 22: 5S ribosomal RNA



- Molecule 23: 23S ribosomal RNA



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| C1999 | A1927 | U1859 | C1790 | G1721 | U1649 | U1578 | G1516 | A1453 | A1392 | U1318 | A1247 | U1182 | G1112 |
| C2000 | A1928 | G1860 | A1791 | A1722 | A1654 | A1579 | G1517 | C1454 | A1393 | C1319 | G1248 | U1183 | |
| | G1929 | | G1792 | G1723 | A1655 | A1580 | C1518 | | U1394 | U1249 | U1249 | U1184 | G1116 |
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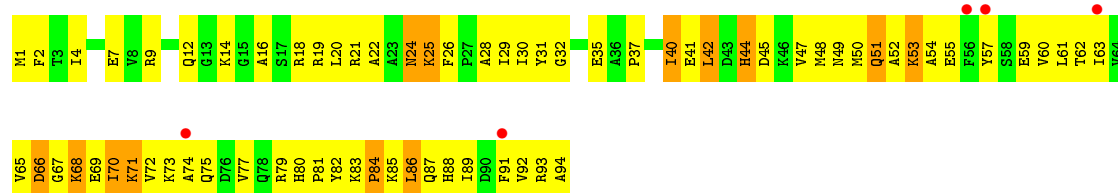
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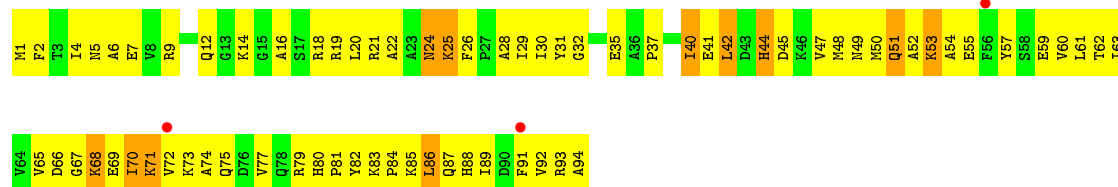
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| U970 | C902 | U841 | U773 | G704 | G636 | A572 | A507 | A442 | C366 | C305 | A241 | C106 | C107 | C41 |
| G971 | G903 | U842 | G774 | U573 | A637 | U574 | A508 | A443 | C367 | U306 | G242 | A172 | G108 | A42 |
| A972 | G904 | | G775 | A705 | G638 | A574 | C509 | C444 | | G307 | U243 | A173 | G109 | G43 |
| U973 | A905 | | G776 | A706 | U639 | A575 | C510 | C445 | G370 | G308 | A244 | U174 | | A44 |
| G974 | | U846 | G777 | G707 | C640 | U576 | U511 | G446 | A371 | A309 | G245 | G175 | | G45 |
| A975 | A909 | U847 | | G708 | U641 | U580 | G512 | | G372 | A310 | C246 | U113 | G46 | |
| | | C848 | G780 | U709 | U642 | U581 | A513 | U451 | U373 | A311 | G247 | U114 | C47 | C47 |
| A979 | A911 | A849 | A781 | U710 | A643 | C581 | A514 | G452 | A374 | G312 | G248 | C115 | G48 | G48 |
| U980 | C912 | U850 | A782 | G711 | A644 | A582 | A515 | A453 | | G315 | C249 | C116 | A49 | A49 |
| A981 | U913 | C851 | A783 | G712 | C645 | G583 | | A454 | G379 | G316 | G250 | A118 | U50 | U50 |
| C982 | | U852 | G784 | G713 | U646 | C584 | G518 | C455 | | G317 | A251 | A181 | G51 | G51 |
| A983 | G916 | C853 | G785 | U714 | G647 | G585 | U519 | C456 | G386 | C318 | G252 | A182 | A52 | A52 |
| A984 | A917 | C854 | C786 | U715 | G648 | A586 | G520 | A457 | U387 | G319 | | A183 | A53 | A53 |
| | | G855 | | A716 | G649 | C587 | U521 | U459 | | A320 | A256 | C183 | G54 | G54 |
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| C989 | C921 | G858 | C795 | C719 | A854 | U590 | U525 | G463 | U394 | C323 | | G189 | G58 | G58 |
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| A996 | A928 | C865 | U803 | G726 | A661 | G597 | A532 | G469 | | A330 | C269 | A196 | U65 | U65 |
| G997 | U929 | A866 | A804 | A727 | G662 | U598 | G533 | A470 | | C331 | U404 | G132 | C66 | C66 |
| C998 | G930 | C867 | G805 | G728 | G663 | U599 | U534 | A471 | | A332 | A270 | U133 | U67 | U67 |
| U999 | U931 | U868 | U907 | G729 | G664 | G600 | | | | | G271 | A199 | | |

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| G1945 | U1880 | A1815 | A1746 | G1682 | G1537 | U1474 | U1411 | G1344 | A1274 | C1208 | C1146 | A1080 | A1001 |
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| | | A1847 | G1776 | U1712 | C1565 | | U1438 | C1376 | A1302 | A1237 | A1175 | U1108 | U1033 |
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| A2015 | A1937 | G1673 | G1673 | A1593 | G1630 | U1467 | U1468 | U1404 | C1335 | U1267 | U1201 | G1139 | |
| U2016 | G1938 | C1874 | G1674 | U1594 | C1531 | U1468 | U1469 | U1405 | G1336 | A1268 | U1203 | G1140 | G1068 |
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| G2018 | A1940 | U1811 | A1676 | A1596 | C1533 | A1470 | A1470 | G1407 | G1338 | G1270 | A1204 | U1141 | A1070 |
| A2019 | | G1877 | G1677 | A1597 | U1534 | G1471 | G1471 | G1408 | G1339 | G1271 | A1205 | U1141 | |
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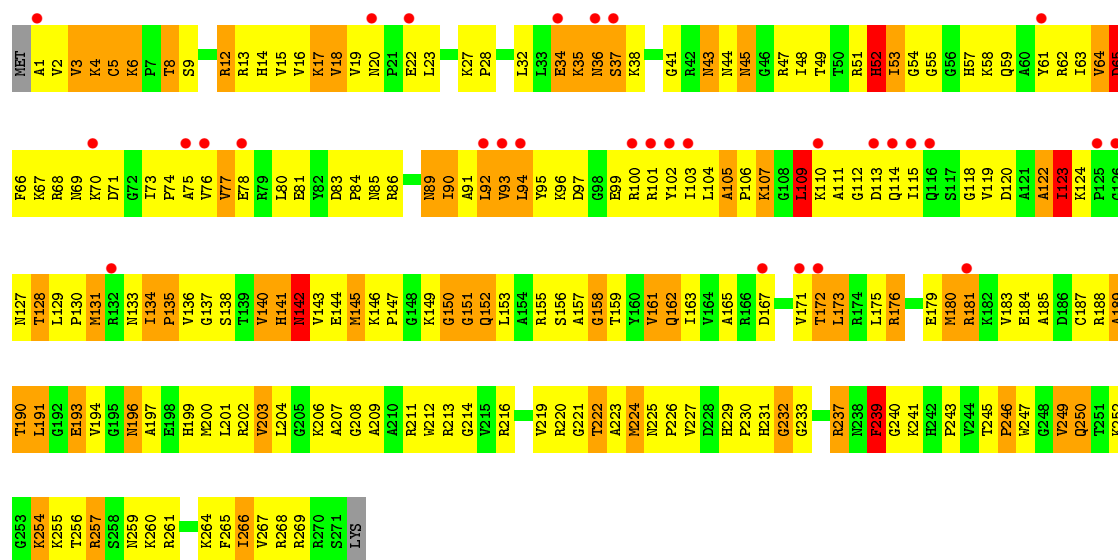




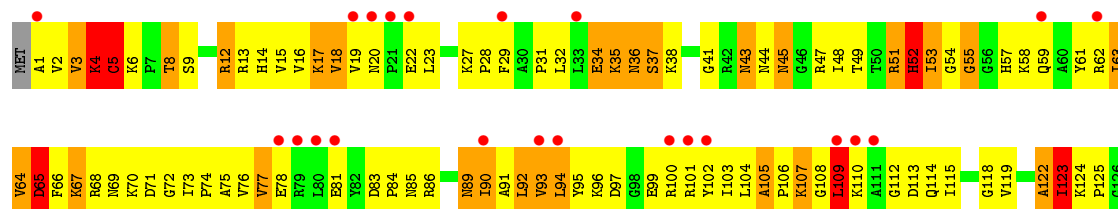
• Molecule 24: 50S ribosomal protein L25



• Molecule 25: 50S ribosomal protein L2

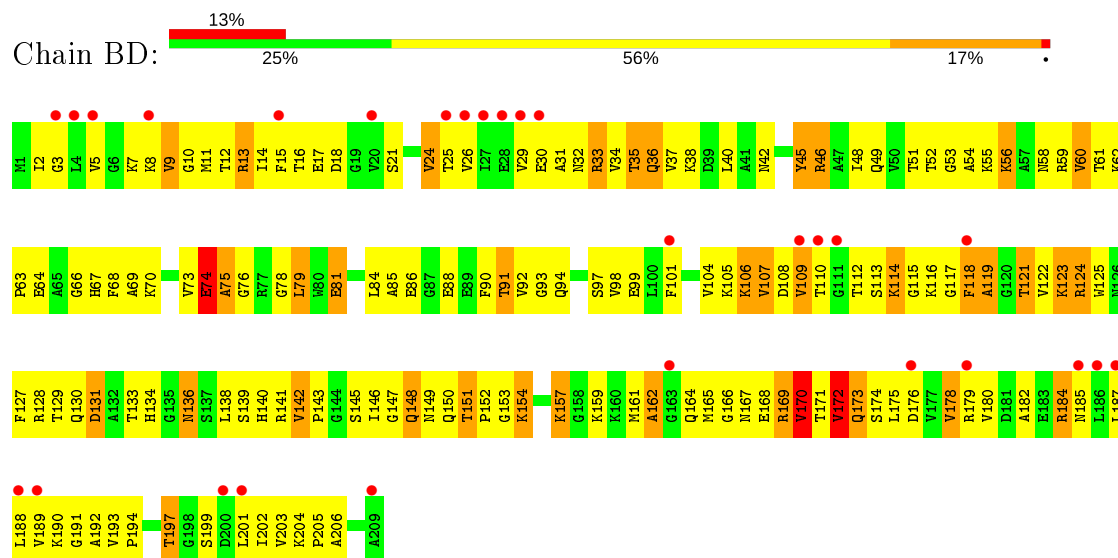


• Molecule 25: 50S ribosomal protein L2

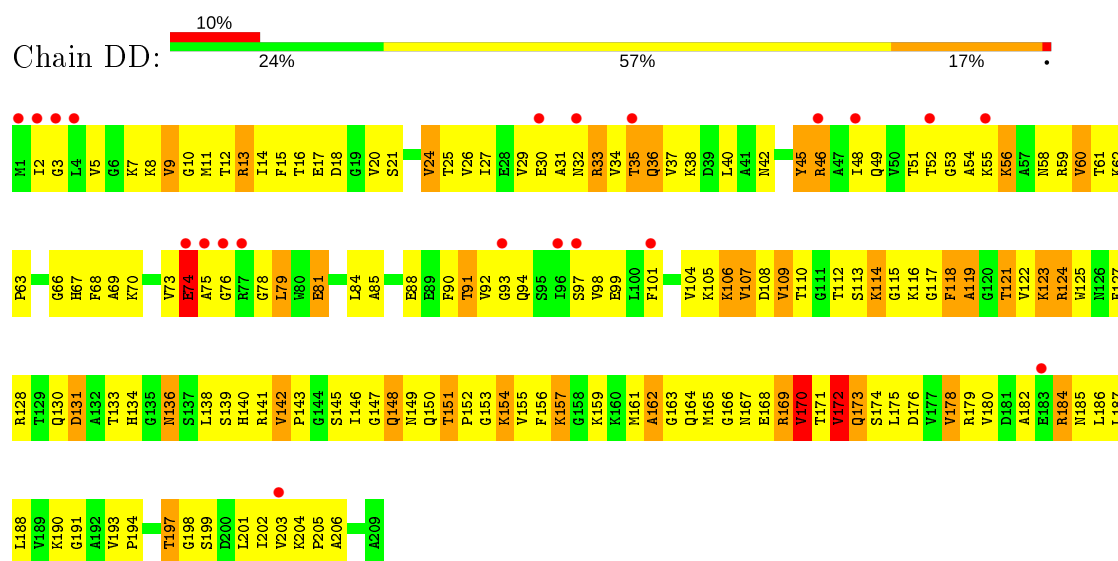




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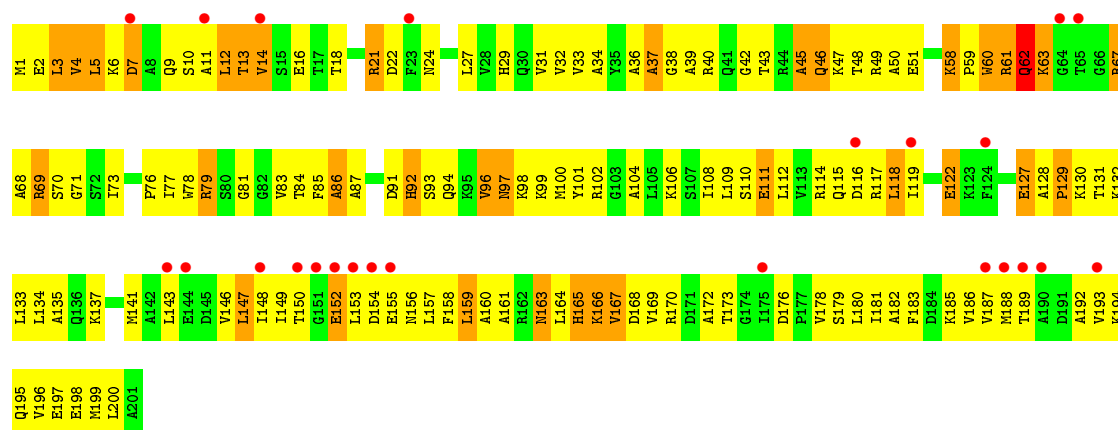


• Molecule 26: 50S ribosomal protein L3

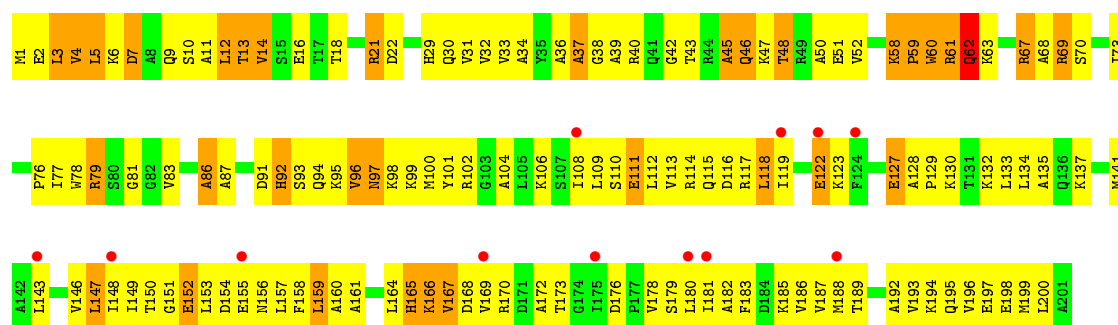


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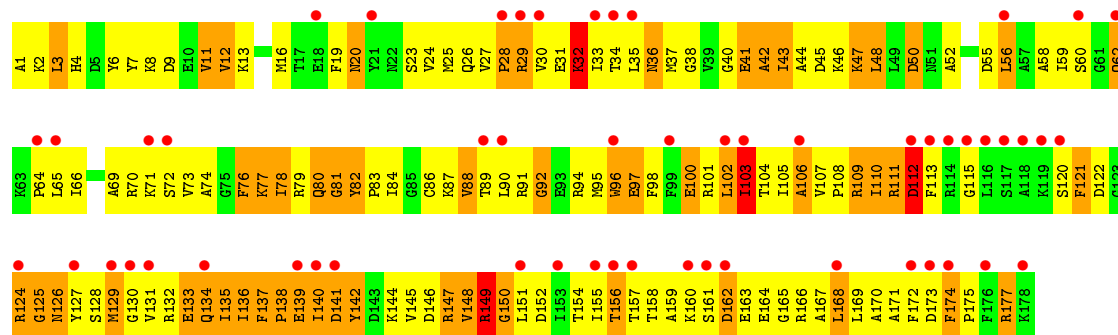
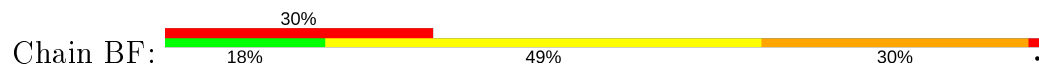




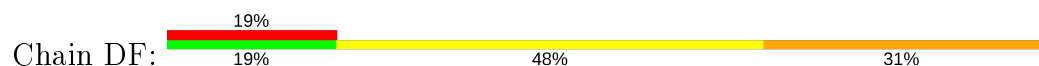
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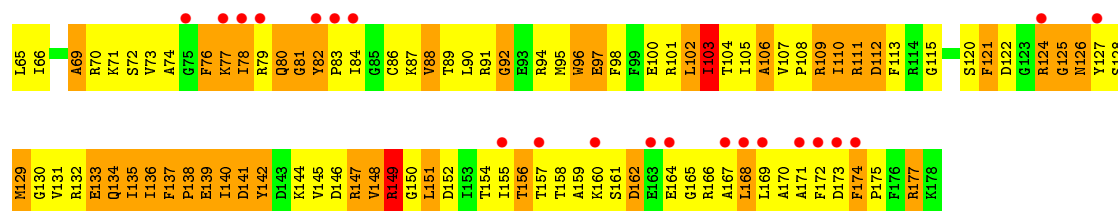


• Molecule 28: 50S ribosomal protein L5

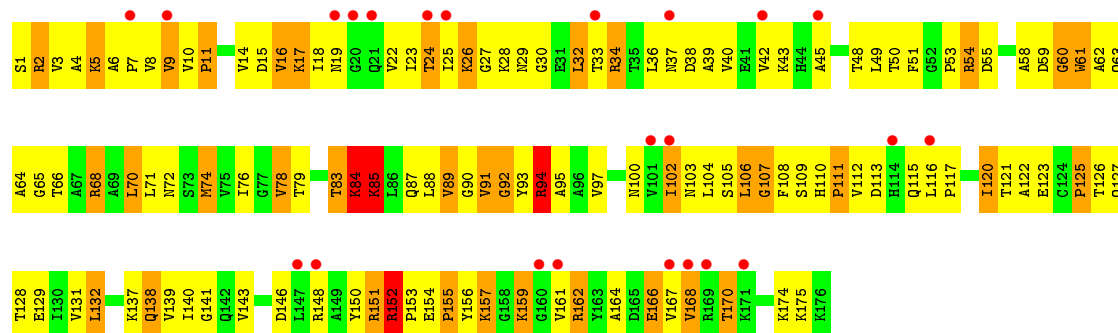


• Molecule 28: 50S ribosomal protein L5

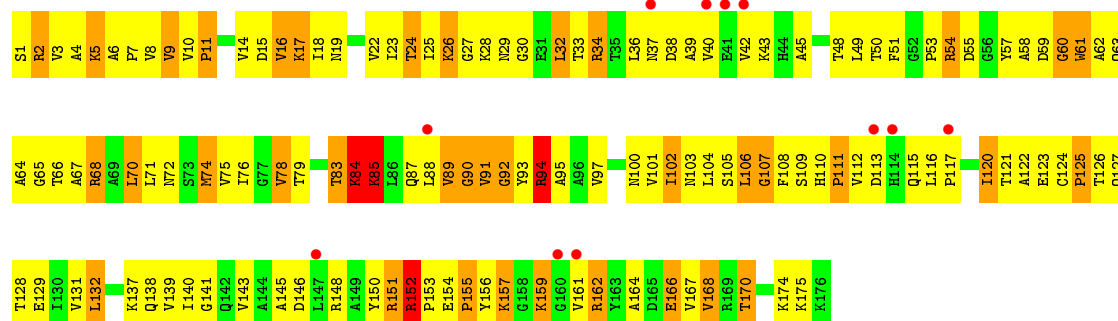




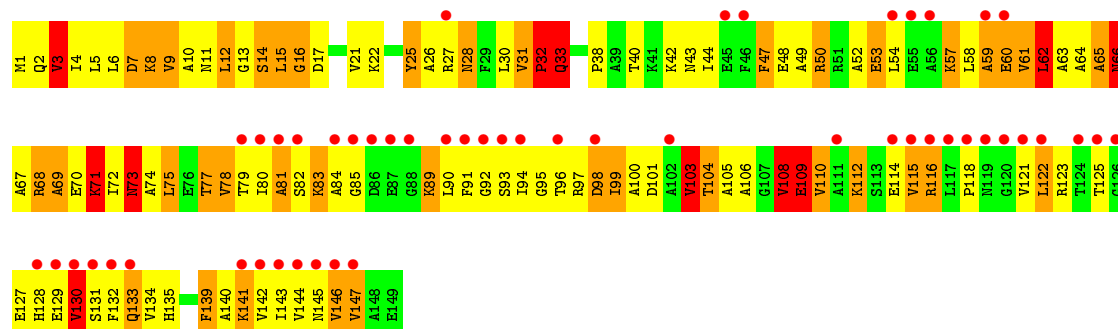
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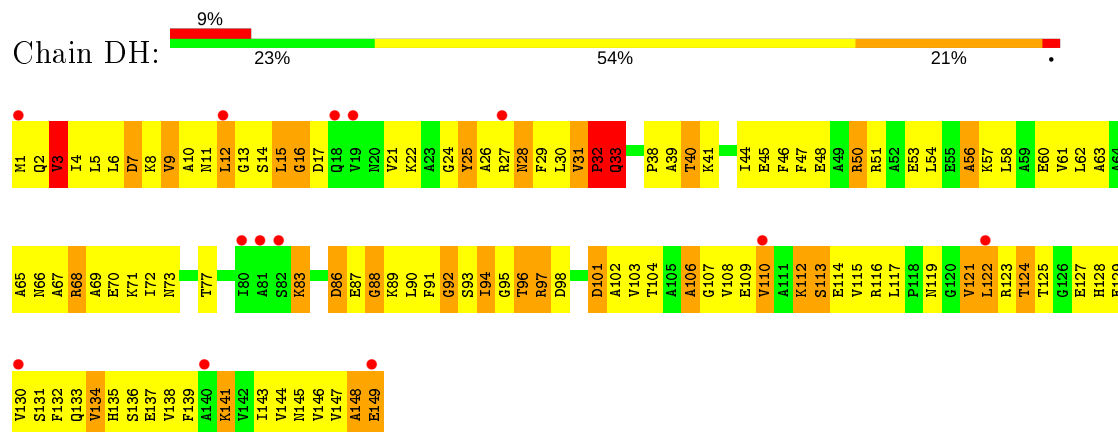
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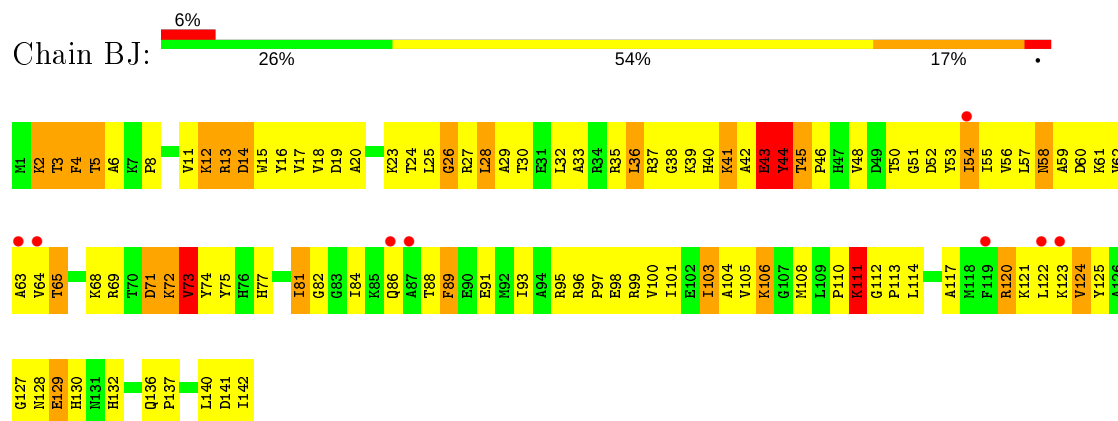
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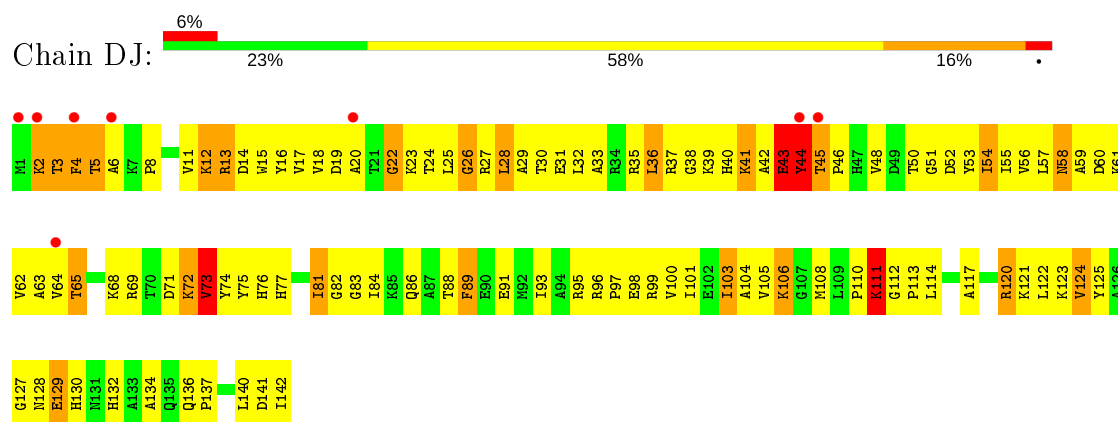
- Molecule 30: 50S ribosomal protein L9



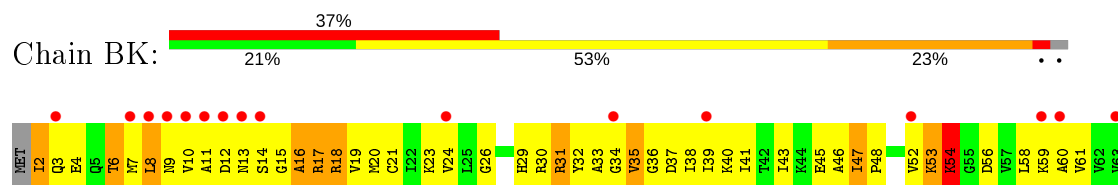
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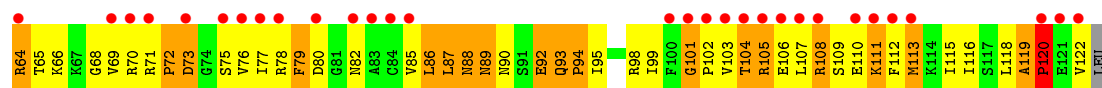


- Molecule 31: 50S ribosomal protein L13

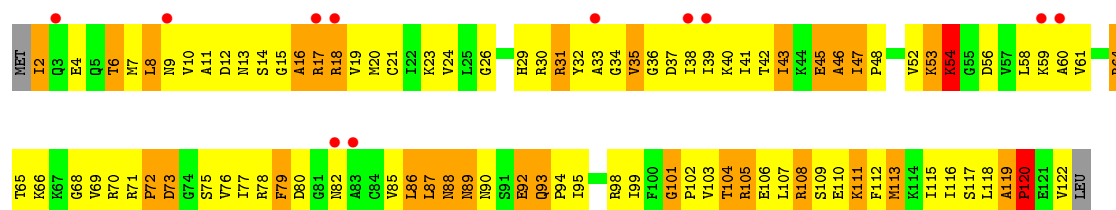


- Molecule 32: 50S ribosomal protein L14

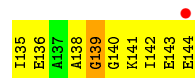
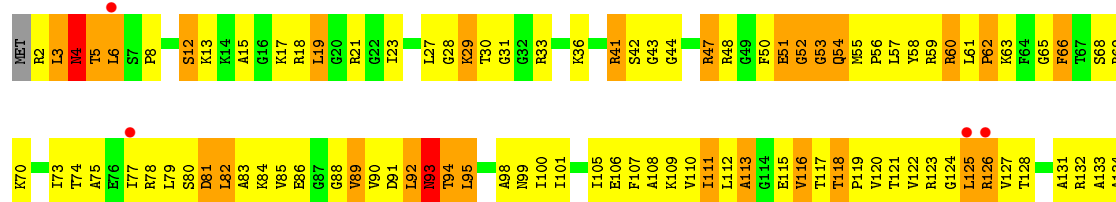




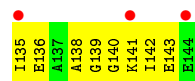
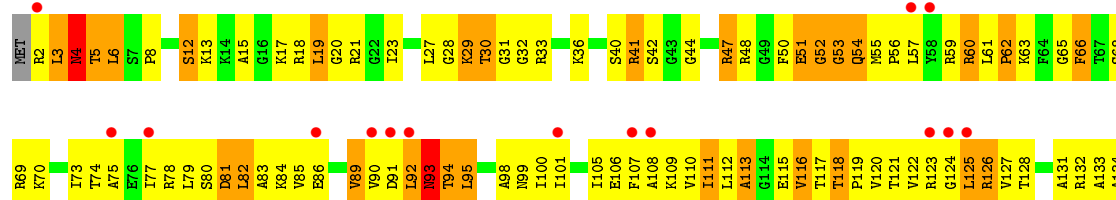
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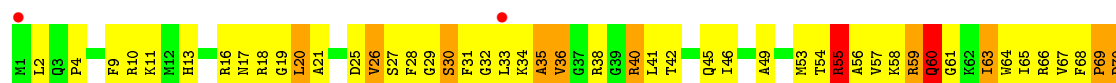
- Molecule 33: 50S ribosomal protein L15

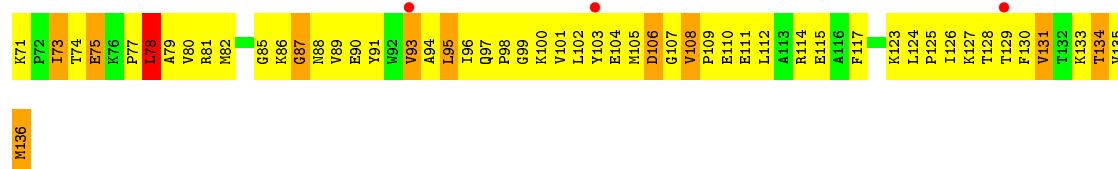


- Molecule 33: 50S ribosomal protein L15

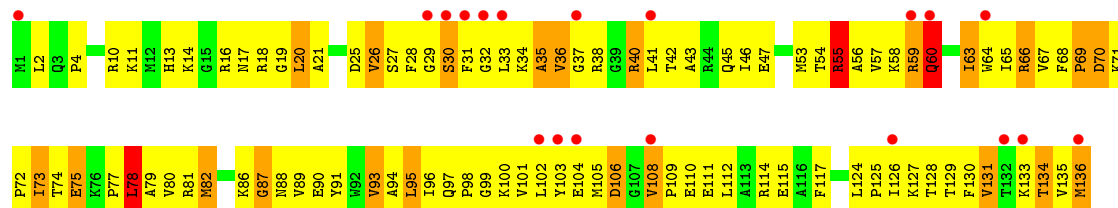


- Molecule 34: 50S ribosomal protein L16

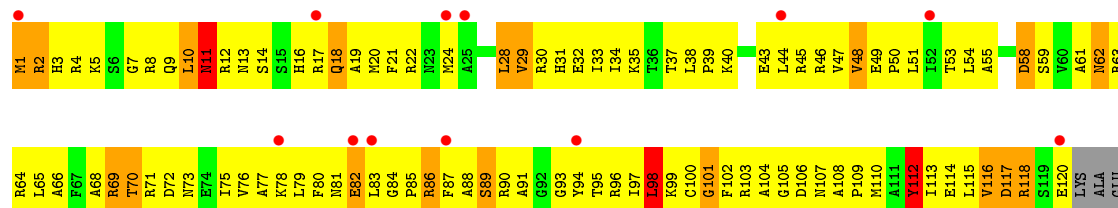




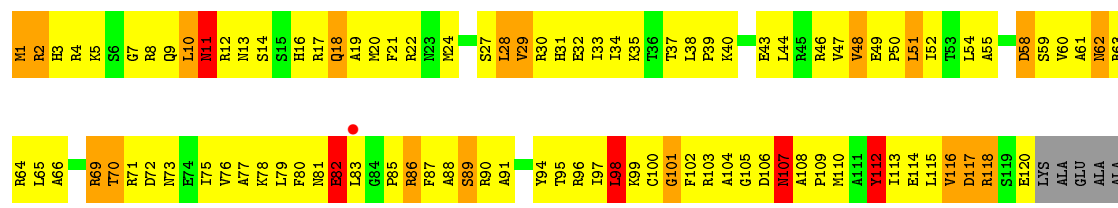
• Molecule 34: 50S ribosomal protein L16



• Molecule 35: 50S ribosomal protein L17

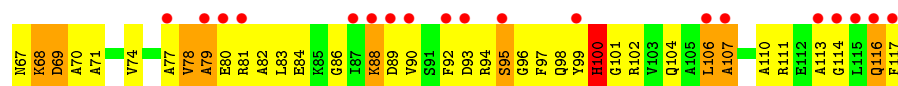


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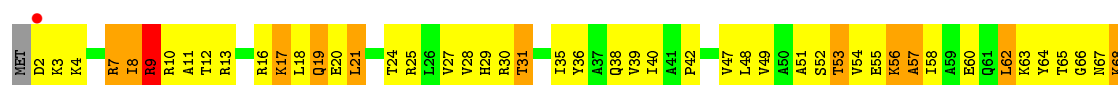


• Molecule 36: 50S ribosomal protein L18

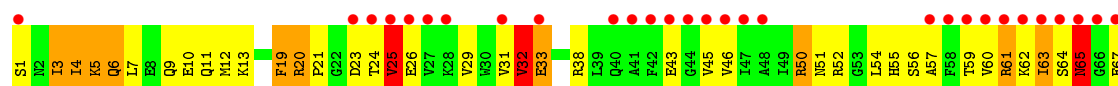




- Molecule 36: 50S ribosomal protein L18



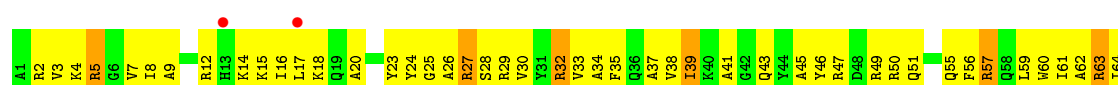
- Molecule 37: 50S ribosomal protein L19



- Molecule 37: 50S ribosomal protein L19

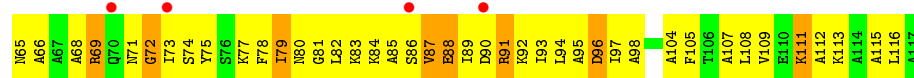


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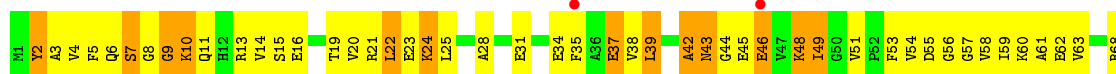


- Molecule 38: 50S ribosomal protein L20

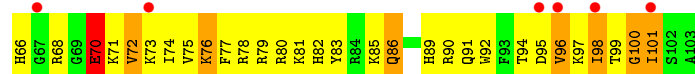
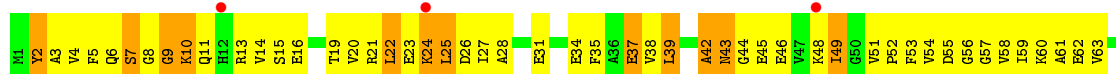




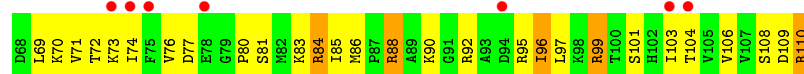
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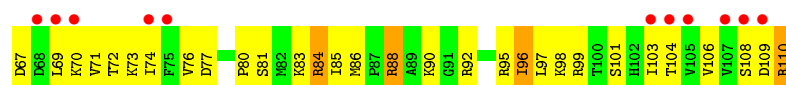
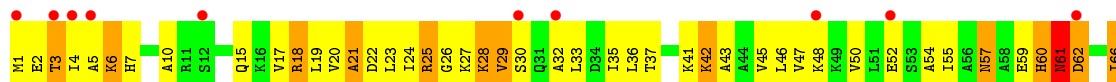
• Molecule 39: 50S ribosomal protein L21



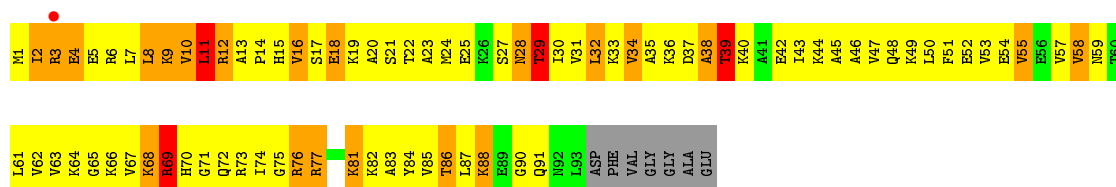
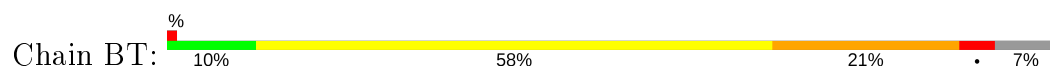
• Molecule 40: 50S ribosomal protein L22



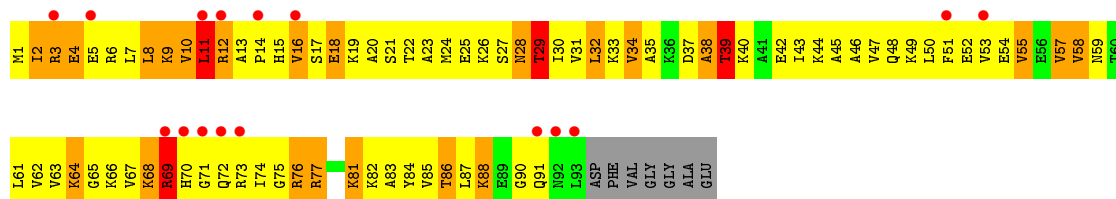
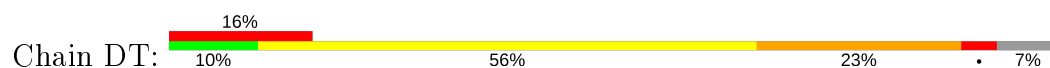
• Molecule 40: 50S ribosomal protein L22



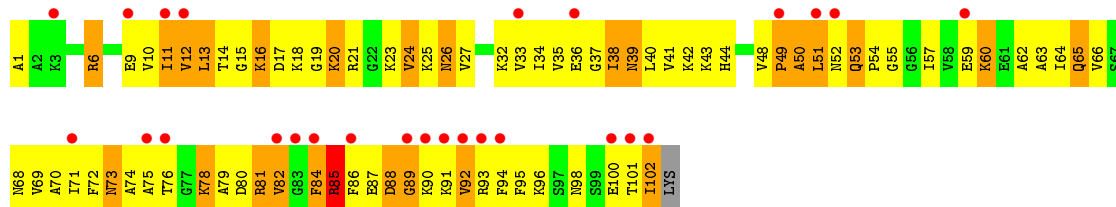
• Molecule 41: 50S ribosomal protein L23



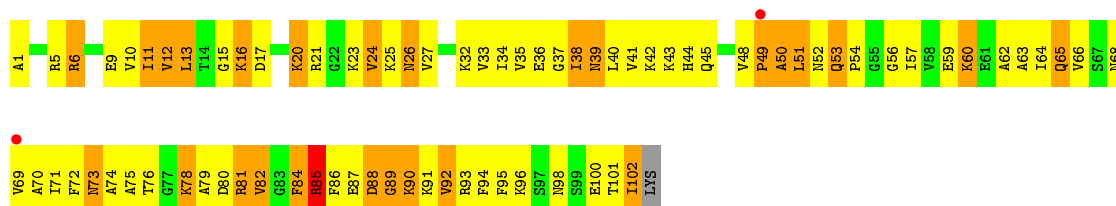
• Molecule 41: 50S ribosomal protein L23



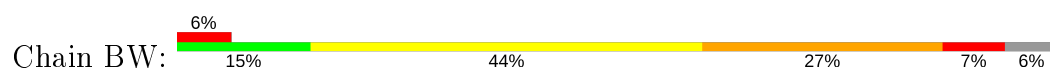
• Molecule 42: 50S ribosomal protein L24

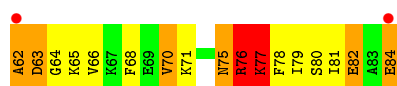


• Molecule 42: 50S ribosomal protein L24

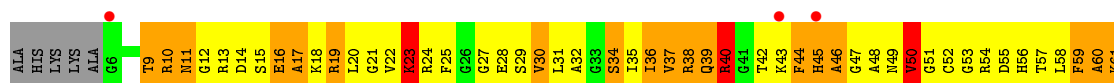
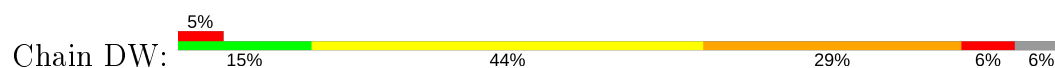


• Molecule 43: 50S ribosomal protein L27





- Molecule 43: 50S ribosomal protein L27



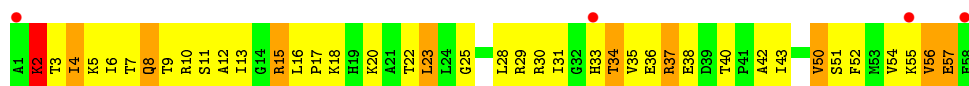
- Molecule 44: 50S ribosomal protein L29



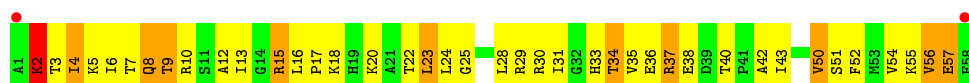
- Molecule 44: 50S ribosomal protein L29



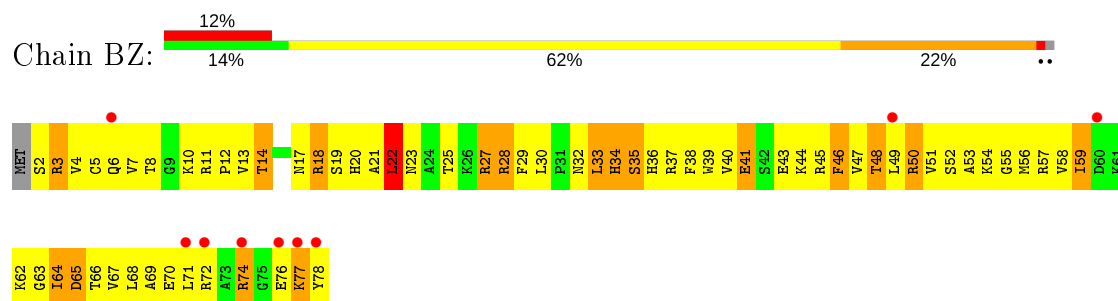
- Molecule 45: 50S ribosomal protein L30



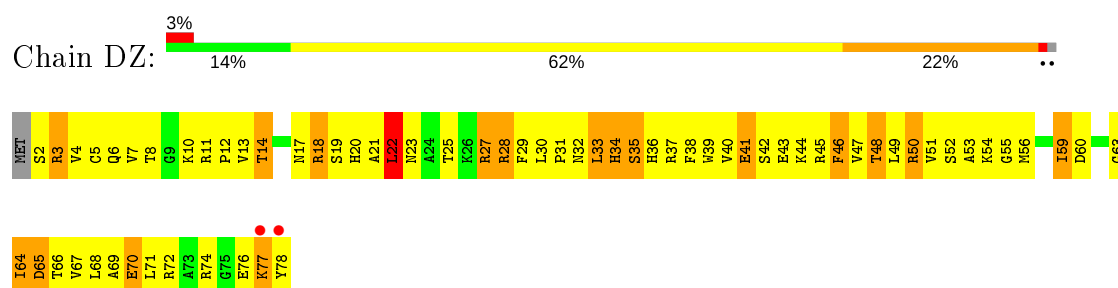
- Molecule 45: 50S ribosomal protein L30



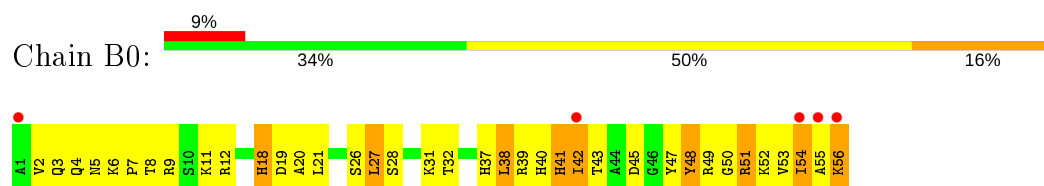
- Molecule 46: 50S ribosomal protein L28



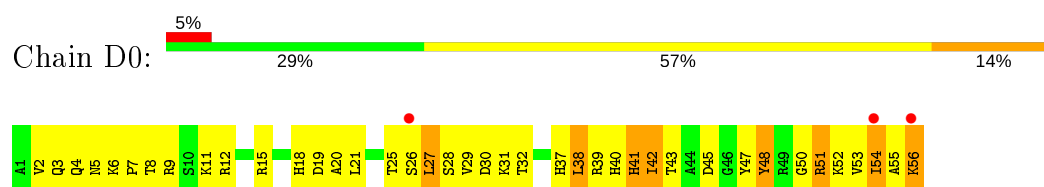
- Molecule 46: 50S ribosomal protein L28



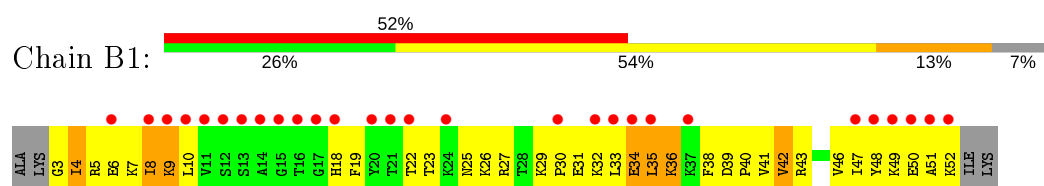
- Molecule 47: 50S ribosomal protein L32



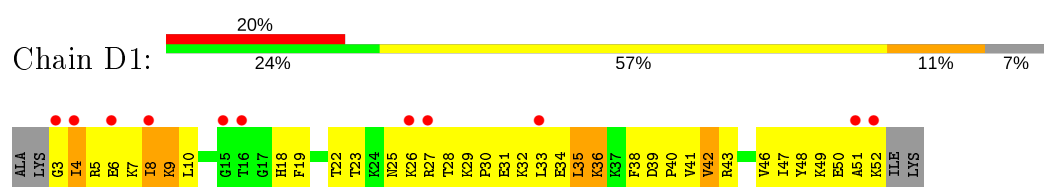
- Molecule 47: 50S ribosomal protein L32



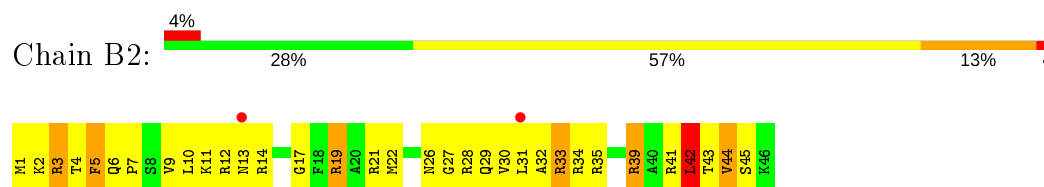
- Molecule 48: 50S ribosomal protein L33



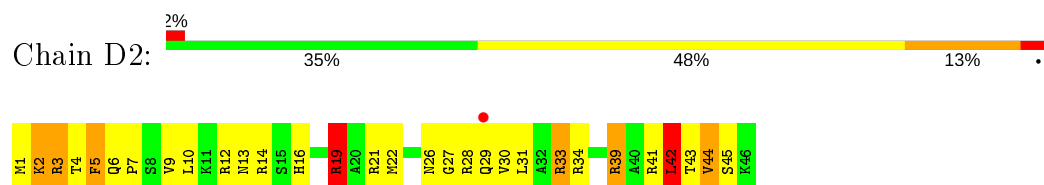
- Molecule 48: 50S ribosomal protein L33



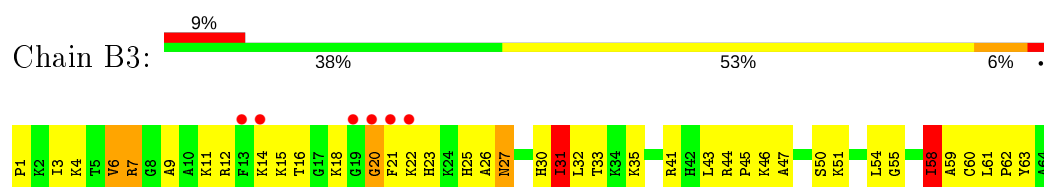
- Molecule 49: 50S ribosomal protein L34



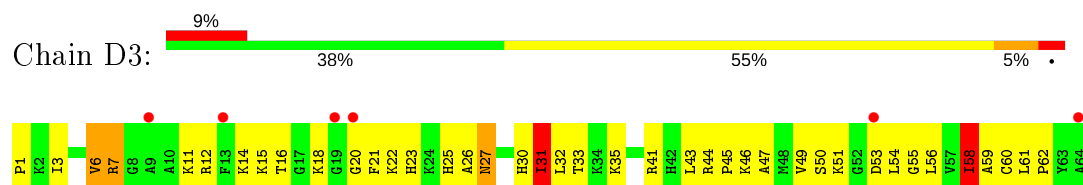
- Molecule 49: 50S ribosomal protein L34



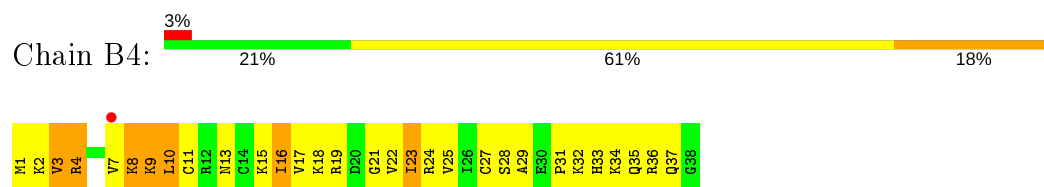
- Molecule 50: 50S ribosomal protein L35



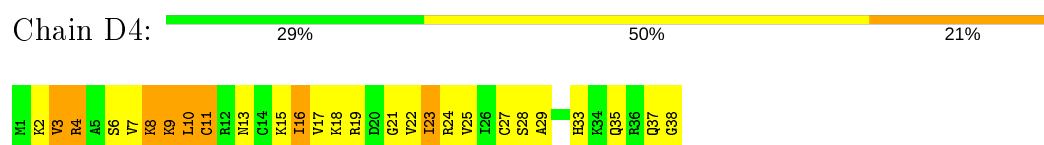
- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36

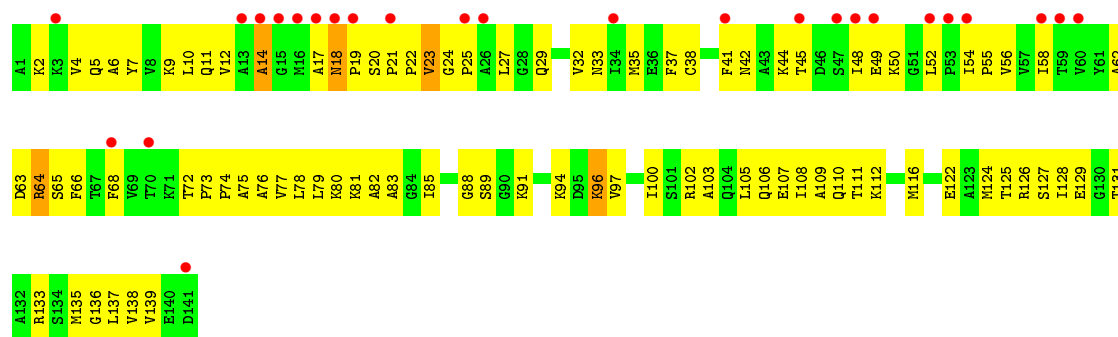


- Molecule 51: 50S ribosomal protein L36

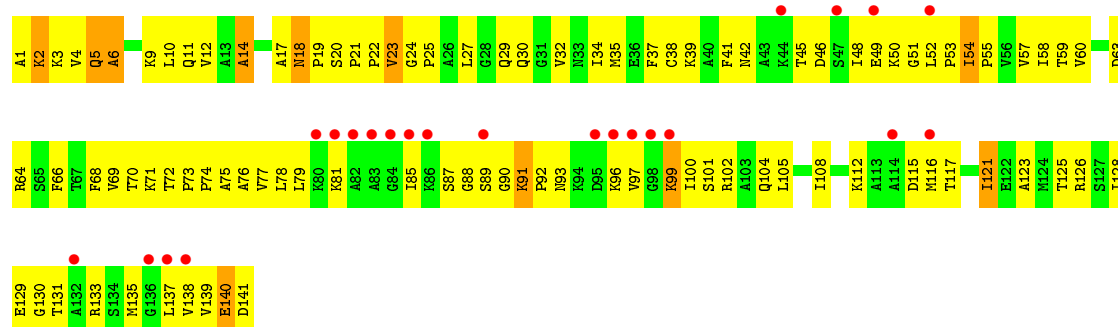


- Molecule 52: 50S ribosomal protein L11





● Molecule 52: 50S ribosomal protein L11



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.70 Å 379.50 Å 739.30 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 70.00 – 3.50 137.77 – 3.50 | Depositor EDS |
| % Data completeness (in resolution range) | 62.1 (70.00-3.50) 62.3 (137.77-3.50) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.07 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.88 (at 3.49 Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.269 , 0.318 0.234 , 0.279 | Depositor DCC |
| R_{free} test set | 22229 reflections (4.89%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 117.9 | Xtriage |
| Anisotropy | 0.294 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.23 , 67.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 284077 | wwPDB-VP |
| Average B, all atoms (Å ²) | 70.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.26 | 1/36762 (0.0%) | 0.77 | 13/57350 (0.0%) |
| 1 | CA | 0.26 | 1/36762 (0.0%) | 0.77 | 17/57350 (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 | 0.43 | 0/2227 |
| 3 | CD | 0.23 | 0/1665 | 0.43 | 0/2227 |
| 4 | AE | 0.23 | 0/1118 | 0.45 | 0/1504 |
| 4 | CE | 0.23 | 0/1118 | 0.45 | 0/1504 |
| 5 | AF | 0.24 | 0/835 | 0.44 | 0/1128 |
| 5 | CF | 0.24 | 0/835 | 0.44 | 0/1128 |
| 6 | AG | 0.23 | 0/1187 | 0.45 | 0/1591 |
| 6 | CG | 0.23 | 0/1211 | 0.44 | 0/1624 |
| 7 | AH | 0.23 | 0/989 | 0.45 | 0/1326 |
| 7 | CH | 0.23 | 0/989 | 0.45 | 0/1326 |
| 8 | AI | 0.24 | 0/1034 | 0.44 | 0/1375 |
| 8 | CI | 0.24 | 0/1034 | 0.44 | 0/1375 |
| 9 | AJ | 0.22 | 0/796 | 0.47 | 0/1077 |
| 9 | CJ | 0.22 | 0/796 | 0.47 | 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 | 0.47 | 0/1300 |
| 11 | CL | 0.22 | 0/969 | 0.47 | 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 | 0.43 | 0/1043 |
| 13 | CN | 0.24 | 0/785 | 0.43 | 0/1043 |
| 14 | AO | 0.22 | 0/723 | 0.44 | 0/966 |
| 14 | CO | 0.22 | 0/723 | 0.44 | 0/966 |
| 15 | AP | 0.25 | 0/659 | 0.45 | 0/884 |
| 15 | CP | 0.25 | 0/648 | 0.44 | 0/870 |
| 16 | AQ | 0.24 | 0/657 | 0.46 | 0/881 |
| 16 | CQ | 0.24 | 0/665 | 0.48 | 0/892 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AR | 0.23 | 0/462 | 0.44 | 0/621 |
| 17 | CR | 0.23 | 0/462 | 0.44 | 0/621 |
| 18 | AS | 0.25 | 0/652 | 0.45 | 0/877 |
| 18 | CS | 0.25 | 0/660 | 0.46 | 0/888 |
| 19 | AT | 0.23 | 0/671 | 0.41 | 0/888 |
| 19 | CT | 0.24 | 0/671 | 0.41 | 0/888 |
| 20 | AB | 0.25 | 0/1735 | 0.44 | 0/2338 |
| 20 | CB | 0.25 | 0/1735 | 0.44 | 0/2338 |
| 21 | AU | 0.26 | 0/430 | 0.46 | 0/570 |
| 21 | CU | 0.26 | 0/430 | 0.46 | 0/570 |
| 22 | BA | 0.24 | 0/2803 | 0.75 | 2/4371 (0.0%) |
| 22 | DA | 0.25 | 0/2803 | 0.75 | 1/4371 (0.0%) |
| 23 | BB | 0.27 | 7/68314 (0.0%) | 0.78 | 41/106569 (0.0%) |
| 23 | DB | 0.28 | 7/68314 (0.0%) | 0.78 | 49/106569 (0.0%) |
| 24 | BV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 24 | DV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 25 | BC | 0.22 | 0/2121 | 0.47 | 0/2852 |
| 25 | DC | 0.22 | 0/2121 | 0.47 | 0/2852 |
| 26 | BD | 0.24 | 0/1586 | 0.46 | 0/2134 |
| 26 | DD | 0.24 | 0/1586 | 0.47 | 0/2134 |
| 27 | BE | 0.23 | 0/1571 | 0.49 | 0/2113 |
| 27 | DE | 0.24 | 0/1571 | 0.49 | 0/2113 |
| 28 | BF | 0.26 | 0/1444 | 0.51 | 0/1937 |
| 28 | DF | 0.26 | 0/1444 | 0.51 | 0/1937 |
| 29 | BG | 0.23 | 0/1343 | 0.46 | 0/1816 |
| 29 | DG | 0.23 | 0/1343 | 0.46 | 0/1816 |
| 30 | BH | 0.25 | 0/1122 | 0.46 | 0/1515 |
| 30 | DH | 0.25 | 0/1122 | 0.46 | 0/1515 |
| 31 | BJ | 0.23 | 0/1152 | 0.47 | 0/1551 |
| 31 | DJ | 0.23 | 0/1152 | 0.47 | 0/1551 |
| 32 | BK | 0.24 | 0/939 | 0.52 | 0/1258 |
| 32 | DK | 0.23 | 0/939 | 0.52 | 0/1258 |
| 33 | BL | 0.23 | 0/1054 | 0.47 | 0/1403 |
| 33 | DL | 0.23 | 0/1054 | 0.47 | 0/1403 |
| 34 | BM | 0.25 | 0/1093 | 0.47 | 0/1460 |
| 34 | DM | 0.25 | 0/1093 | 0.47 | 0/1460 |
| 35 | BN | 0.24 | 0/973 | 0.51 | 0/1301 |
| 35 | DN | 0.24 | 0/973 | 0.51 | 0/1301 |
| 36 | BO | 0.23 | 0/902 | 0.47 | 0/1209 |
| 36 | DO | 0.23 | 0/902 | 0.48 | 0/1209 |
| 37 | BP | 0.24 | 0/929 | 0.48 | 0/1242 |
| 37 | DP | 0.24 | 0/929 | 0.48 | 0/1242 |
| 38 | BQ | 0.25 | 0/960 | 0.46 | 0/1278 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DQ | 0.25 | 0/960 | 0.46 | 0/1278 |
| 39 | BR | 0.25 | 0/829 | 0.48 | 0/1107 |
| 39 | DR | 0.25 | 0/829 | 0.48 | 0/1107 |
| 40 | BS | 0.22 | 0/864 | 0.49 | 0/1156 |
| 40 | DS | 0.22 | 0/864 | 0.49 | 0/1156 |
| 41 | BT | 0.23 | 0/744 | 0.52 | 0/994 |
| 41 | DT | 0.23 | 0/744 | 0.52 | 0/994 |
| 42 | BU | 0.25 | 0/787 | 0.45 | 0/1051 |
| 42 | DU | 0.25 | 0/787 | 0.45 | 0/1051 |
| 43 | BW | 0.28 | 0/603 | 0.48 | 0/797 |
| 43 | DW | 0.27 | 0/603 | 0.48 | 0/797 |
| 44 | BX | 0.23 | 0/510 | 0.51 | 0/677 |
| 44 | DX | 0.23 | 0/510 | 0.51 | 0/677 |
| 45 | BY | 0.23 | 0/453 | 0.49 | 0/605 |
| 45 | DY | 0.23 | 0/453 | 0.49 | 0/605 |
| 46 | BZ | 0.25 | 0/635 | 0.51 | 0/848 |
| 46 | DZ | 0.25 | 0/635 | 0.51 | 0/848 |
| 47 | B0 | 0.22 | 0/450 | 0.52 | 0/599 |
| 47 | D0 | 0.22 | 0/450 | 0.52 | 0/599 |
| 48 | B1 | 0.27 | 0/416 | 0.47 | 0/554 |
| 48 | D1 | 0.27 | 0/416 | 0.47 | 0/554 |
| 49 | B2 | 0.25 | 0/380 | 0.49 | 0/498 |
| 49 | D2 | 0.26 | 0/380 | 0.49 | 0/498 |
| 50 | B3 | 0.24 | 0/513 | 0.46 | 0/676 |
| 50 | D3 | 0.24 | 0/513 | 0.46 | 0/676 |
| 51 | B4 | 0.22 | 0/303 | 0.46 | 0/397 |
| 51 | D4 | 0.22 | 0/303 | 0.46 | 0/397 |
| 52 | BI | 0.24 | 0/1046 | 0.46 | 0/1410 |
| 52 | DI | 0.25 | 0/1046 | 0.47 | 0/1410 |
| All | All | 0.26 | 16/306361 (0.0%) | 0.70 | 123/457973 (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 | 13 |
| 1 | CA | 0 | 13 |
| 23 | BB | 0 | 36 |
| 23 | DB | 0 | 38 |
| All | All | 0 | 100 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23 | DB | 1086 | A | C5-C6 | -16.14 | 1.26 | 1.41 |
| 23 | BB | 1086 | A | C5-C6 | -16.11 | 1.26 | 1.41 |
| 23 | BB | 1088 | A | C6-N1 | -10.49 | 1.28 | 1.35 |
| 23 | DB | 1088 | A | C6-N1 | -10.45 | 1.28 | 1.35 |
| 23 | DB | 1060 | U | C2-N3 | 7.89 | 1.43 | 1.37 |
| 23 | BB | 1060 | U | C2-N3 | 7.86 | 1.43 | 1.37 |
| 23 | BB | 1086 | A | N3-C4 | -7.29 | 1.30 | 1.34 |
| 23 | DB | 1086 | A | N3-C4 | -7.04 | 1.30 | 1.34 |
| 23 | DB | 1086 | A | N7-C5 | -6.41 | 1.35 | 1.39 |
| 23 | BB | 1086 | A | N7-C5 | -6.28 | 1.35 | 1.39 |
| 1 | AA | 495 | A | N3-C4 | -5.62 | 1.31 | 1.34 |
| 1 | CA | 495 | A | N3-C4 | -5.48 | 1.31 | 1.34 |
| 23 | DB | 2272 | U | C2-N3 | 5.41 | 1.41 | 1.37 |
| 23 | BB | 2272 | U | C2-N3 | 5.34 | 1.41 | 1.37 |
| 23 | BB | 2267 | A | C6-N6 | -5.14 | 1.29 | 1.33 |
| 23 | DB | 2267 | A | C6-N6 | -5.13 | 1.29 | 1.33 |

All (123) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 23 | BB | 2791 | G | O5'-P-OP1 | -31.87 | 72.45 | 110.70 |
| 23 | DB | 2791 | G | O5'-P-OP2 | -31.41 | 73.01 | 110.70 |
| 23 | DB | 2204 | G | O5'-P-OP1 | -29.65 | 75.12 | 110.70 |
| 1 | AA | 1213 | A | O5'-P-OP2 | -29.58 | 75.21 | 110.70 |
| 23 | BB | 2204 | G | O5'-P-OP2 | -28.34 | 76.69 | 110.70 |
| 1 | CA | 1213 | A | O5'-P-OP1 | -26.18 | 79.28 | 110.70 |
| 23 | DB | 2204 | G | O5'-P-OP2 | 17.93 | 132.22 | 110.70 |
| 23 | BB | 2204 | G | O5'-P-OP1 | 17.70 | 131.94 | 110.70 |
| 1 | CA | 1213 | A | O5'-P-OP2 | 17.64 | 131.86 | 110.70 |
| 1 | AA | 1213 | A | O5'-P-OP1 | 16.79 | 130.85 | 110.70 |
| 23 | BB | 2791 | G | O5'-P-OP2 | 16.25 | 130.19 | 110.70 |
| 1 | CA | 1212 | U | OP1-P-O3' | 15.45 | 139.18 | 105.20 |
| 23 | DB | 2791 | G | O5'-P-OP1 | 15.06 | 128.77 | 110.70 |
| 23 | DB | 2203 | U | OP1-P-O3' | 14.29 | 136.63 | 105.20 |
| 1 | AA | 1212 | U | OP2-P-O3' | 14.25 | 136.56 | 105.20 |
| 23 | DB | 2790 | U | OP2-P-O3' | 14.20 | 136.44 | 105.20 |
| 23 | BB | 2203 | U | OP2-P-O3' | 14.09 | 136.19 | 105.20 |
| 23 | BB | 2790 | U | OP1-P-O3' | 13.23 | 134.30 | 105.20 |
| 23 | DB | 1552 | A | N9-C1'-C2' | -9.81 | 101.21 | 112.00 |
| 23 | BB | 1552 | A | N9-C1'-C2' | -9.76 | 101.26 | 112.00 |
| 23 | DB | 1088 | A | N1-C6-N6 | -8.31 | 113.61 | 118.60 |
| 23 | BB | 1088 | A | N1-C6-N6 | -8.20 | 113.68 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | CA | 1049 | U | O5'-P-OP1 | -7.79 | 98.69 | 105.70 |
| 23 | BB | 1439 | A | N9-C1'-C2' | -7.78 | 103.44 | 112.00 |
| 23 | DB | 1439 | A | N9-C1'-C2' | -7.75 | 103.47 | 112.00 |
| 23 | BB | 773 | U | C5'-C4'-C3' | -7.59 | 103.86 | 116.00 |
| 23 | DB | 1060 | U | C5-C4-O4 | -7.35 | 121.49 | 125.90 |
| 23 | BB | 1060 | U | C5-C4-O4 | -7.29 | 121.53 | 125.90 |
| 1 | CA | 975 | A | C5'-C4'-C3' | -7.25 | 104.41 | 116.00 |
| 23 | DB | 773 | U | C5'-C4'-C3' | -7.14 | 104.57 | 116.00 |
| 23 | BB | 1086 | A | C4-C5-C6 | 7.13 | 120.56 | 117.00 |
| 23 | DB | 1086 | A | C4-C5-C6 | 7.12 | 120.56 | 117.00 |
| 23 | BB | 2733 | A | N9-C1'-C2' | -7.06 | 104.23 | 112.00 |
| 23 | DB | 2272 | U | N3-C4-O4 | -7.05 | 114.47 | 119.40 |
| 23 | BB | 2272 | U | N3-C4-O4 | -6.98 | 114.51 | 119.40 |
| 23 | DB | 2733 | A | N9-C1'-C2' | -6.94 | 104.37 | 112.00 |
| 1 | AA | 975 | A | C5'-C4'-C3' | -6.77 | 105.17 | 116.00 |
| 1 | AA | 1212 | U | O3'-P-O5' | -6.76 | 91.16 | 104.00 |
| 1 | AA | 86 | G | N9-C1'-C2' | 6.63 | 122.62 | 114.00 |
| 23 | DB | 2135 | A | N9-C1'-C2' | -6.63 | 104.71 | 112.00 |
| 23 | DB | 745 | G | C5'-C4'-C3' | -6.61 | 105.42 | 116.00 |
| 23 | DB | 1350 | C | C5'-C4'-C3' | -6.55 | 105.52 | 116.00 |
| 23 | BB | 745 | G | C5'-C4'-C3' | -6.46 | 105.66 | 116.00 |
| 1 | CA | 1212 | U | O3'-P-O5' | -6.43 | 91.78 | 104.00 |
| 23 | BB | 690 | G | C5'-C4'-C3' | -6.42 | 105.72 | 116.00 |
| 23 | DB | 1088 | A | C5-C6-N6 | 6.40 | 128.82 | 123.70 |
| 23 | BB | 1088 | A | C5-C6-N6 | 6.39 | 128.81 | 123.70 |
| 23 | BB | 2283 | C | O5'-P-OP2 | -6.38 | 99.95 | 105.70 |
| 23 | BB | 1251 | C | C5'-C4'-C3' | -6.20 | 106.08 | 116.00 |
| 1 | CA | 1424 | U | C5'-C4'-C3' | -6.11 | 106.23 | 116.00 |
| 23 | DB | 2480 | C | C5'-C4'-C3' | 6.11 | 125.77 | 116.00 |
| 23 | DB | 1086 | A | C6-C5-N7 | -6.08 | 128.04 | 132.30 |
| 23 | BB | 1086 | A | C6-C5-N7 | -6.07 | 128.05 | 132.30 |
| 23 | DB | 2199 | A | C5'-C4'-C3' | -6.07 | 106.29 | 116.00 |
| 23 | BB | 241 | A | C5'-C4'-C3' | -6.01 | 106.38 | 116.00 |
| 23 | BB | 1552 | A | C4'-C3'-O3' | 5.99 | 124.98 | 113.00 |
| 1 | CA | 1534 | A | C2'-C3'-O3' | -5.99 | 96.33 | 109.50 |
| 22 | BA | 108 | A | C5'-C4'-O4' | -5.96 | 101.94 | 109.10 |
| 23 | DB | 1251 | C | C5'-C4'-C3' | -5.89 | 106.57 | 116.00 |
| 23 | DB | 2096 | C | C5'-C4'-C3' | -5.88 | 106.60 | 116.00 |
| 23 | DB | 690 | G | C5'-C4'-C3' | -5.87 | 106.61 | 116.00 |
| 1 | AA | 576 | C | C5'-C4'-C3' | 5.87 | 125.39 | 116.00 |
| 1 | CA | 1213 | A | C5'-C4'-O4' | 5.84 | 116.11 | 109.10 |
| 23 | DB | 241 | A | C5'-C4'-O4' | 5.82 | 116.08 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | DB | 126 | A | C5'-C4'-C3' | 5.82 | 125.30 | 116.00 |
| 1 | CA | 576 | C | O5'-P-OP1 | -5.80 | 100.48 | 105.70 |
| 23 | BB | 1318 | U | C5'-C4'-C3' | -5.77 | 106.77 | 116.00 |
| 23 | DB | 2203 | U | O3'-P-O5' | -5.76 | 93.06 | 104.00 |
| 1 | AA | 1213 | A | C1'-O4'-C4' | -5.75 | 105.30 | 109.90 |
| 23 | BB | 1060 | U | N1-C2-O2 | -5.71 | 118.81 | 122.80 |
| 23 | DB | 1397 | U | C5'-C4'-C3' | -5.68 | 106.91 | 116.00 |
| 23 | DB | 242 | G | C4'-C3'-O3' | -5.68 | 97.48 | 109.40 |
| 23 | BB | 2480 | C | C5'-C4'-C3' | 5.67 | 125.08 | 116.00 |
| 23 | DB | 2790 | U | C4'-C3'-O3' | 5.61 | 124.23 | 113.00 |
| 23 | DB | 1086 | A | C2-N3-C4 | -5.61 | 107.79 | 110.60 |
| 23 | BB | 1086 | A | C2-N3-C4 | -5.61 | 107.79 | 110.60 |
| 23 | DB | 1552 | A | C4'-C3'-O3' | 5.58 | 124.16 | 113.00 |
| 23 | DB | 1060 | U | N1-C2-O2 | -5.57 | 118.90 | 122.80 |
| 23 | DB | 2894 | G | C5'-C4'-C3' | -5.57 | 107.09 | 116.00 |
| 23 | DB | 1318 | U | C5'-C4'-C3' | -5.56 | 107.10 | 116.00 |
| 23 | BB | 2199 | A | C5'-C4'-C3' | -5.55 | 107.12 | 116.00 |
| 23 | BB | 479 | A | C4'-C3'-O3' | -5.54 | 97.77 | 109.40 |
| 1 | CA | 1213 | A | C1'-O4'-C4' | -5.54 | 105.47 | 109.90 |
| 1 | CA | 765 | G | N9-C1'-C2' | -5.51 | 105.94 | 112.00 |
| 1 | AA | 765 | G | N9-C1'-C2' | -5.51 | 105.94 | 112.00 |
| 23 | DB | 2109 | U | N1-C1'-C2' | -5.51 | 105.94 | 112.00 |
| 23 | BB | 2471 | A | C5'-C4'-C3' | -5.44 | 107.30 | 116.00 |
| 1 | CA | 67 | C | C5'-C4'-C3' | -5.42 | 107.33 | 116.00 |
| 23 | BB | 2894 | G | C5'-C4'-C3' | -5.41 | 107.34 | 116.00 |
| 23 | DB | 2619 | C | C5'-C4'-C3' | -5.41 | 107.35 | 116.00 |
| 23 | BB | 1382 | G | C5'-C4'-C3' | 5.39 | 124.63 | 116.00 |
| 23 | DB | 140 | C | C5'-C4'-C3' | 5.39 | 124.62 | 116.00 |
| 23 | DB | 1654 | A | C5'-C4'-C3' | -5.38 | 107.40 | 116.00 |
| 23 | BB | 2716 | C | C5'-C4'-C3' | 5.37 | 124.59 | 116.00 |
| 23 | BB | 1350 | C | C5'-C4'-C3' | -5.37 | 107.41 | 116.00 |
| 23 | BB | 242 | G | C4'-C3'-O3' | -5.36 | 98.15 | 109.40 |
| 23 | BB | 1060 | U | N3-C2-O2 | 5.34 | 125.94 | 122.20 |
| 23 | DB | 1280 | G | C5'-C4'-C3' | -5.34 | 107.46 | 116.00 |
| 23 | DB | 2471 | A | C5'-C4'-C3' | -5.33 | 107.47 | 116.00 |
| 23 | BB | 2203 | U | O3'-P-O5' | -5.30 | 93.93 | 104.00 |
| 23 | BB | 2272 | U | N1-C2-O2 | -5.30 | 119.09 | 122.80 |
| 23 | DB | 1060 | U | N3-C2-O2 | 5.29 | 125.91 | 122.20 |
| 23 | BB | 2790 | U | O3'-P-O5' | -5.29 | 93.95 | 104.00 |
| 23 | DB | 1382 | G | C5'-C4'-C3' | 5.28 | 124.45 | 116.00 |
| 23 | DB | 2138 | G | C5'-C4'-C3' | -5.28 | 107.55 | 116.00 |
| 1 | CA | 437 | U | N1-C1'-C2' | 5.28 | 120.86 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | BB | 1397 | U | C5'-C4'-C3' | -5.27 | 107.56 | 116.00 |
| 1 | AA | 437 | U | N1-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 23 | DB | 1634 | A | C5'-C4'-C3' | -5.26 | 107.58 | 116.00 |
| 1 | AA | 1362 | A | C5'-C4'-O4' | 5.23 | 115.38 | 109.10 |
| 1 | CA | 1362 | A | C5'-C4'-O4' | 5.23 | 115.38 | 109.10 |
| 23 | BB | 2134 | A | C5'-C4'-C3' | 5.21 | 124.34 | 116.00 |
| 23 | DB | 2272 | U | N1-C2-O2 | -5.19 | 119.17 | 122.80 |
| 1 | CA | 1362 | A | C5'-C4'-C3' | 5.18 | 124.30 | 116.00 |
| 22 | BA | 30 | C | C5'-C4'-C3' | -5.18 | 107.71 | 116.00 |
| 23 | DB | 2716 | C | C5'-C4'-C3' | 5.17 | 124.27 | 116.00 |
| 1 | AA | 1049 | U | O5'-P-OP1 | 5.12 | 116.84 | 110.70 |
| 1 | AA | 1049 | U | O5'-P-OP2 | -5.11 | 101.11 | 105.70 |
| 23 | BB | 268 | C | C5'-C4'-C3' | -5.07 | 107.89 | 116.00 |
| 23 | DB | 747 | U | C5'-C4'-C3' | 5.05 | 124.08 | 116.00 |
| 1 | CA | 1301 | U | N1-C1'-C2' | 5.02 | 120.52 | 114.00 |
| 22 | DA | 30 | C | C5'-C4'-C3' | -5.01 | 107.98 | 116.00 |
| 23 | DB | 134 | G | C5'-C4'-C3' | -5.00 | 108.00 | 116.00 |

There are no chirality outliers.

All (100) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | AA | 1006 | G | Sidechain |
| 1 | AA | 1047 | 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 | 703 | G | Sidechain |
| 1 | AA | 83 | C | Sidechain |
| 1 | AA | 832 | G | Sidechain |
| 1 | AA | 992 | U | 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 | 1439 | A | Sidechain |
| 23 | BB | 1533 | C | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 23 | BB | 1538 | G | Sidechain |
| 23 | BB | 1546 | G | Sidechain |
| 23 | BB | 1572 | A | Sidechain |
| 23 | BB | 1645 | G | Sidechain |
| 23 | BB | 1734 | G | Sidechain |
| 23 | BB | 1792 | 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 | 2319 | G | Sidechain |
| 23 | BB | 2471 | A | Sidechain |
| 23 | BB | 2503 | A | Sidechain |
| 23 | BB | 2638 | G | Sidechain |
| 23 | BB | 2733 | A | Sidechain |
| 23 | BB | 2848 | G | Sidechain |
| 23 | BB | 2857 | G | Sidechain |
| 23 | BB | 2868 | A | Sidechain |
| 23 | BB | 299 | A | Sidechain |
| 23 | BB | 361 | G | Sidechain |
| 23 | BB | 427 | U | Sidechain |
| 23 | BB | 51 | G | Sidechain |
| 23 | BB | 630 | G | Sidechain |
| 23 | BB | 727 | A | Sidechain |
| 23 | BB | 729 | G | Sidechain |
| 23 | BB | 757 | G | Sidechain |
| 1 | CA | 1006 | G | Sidechain |
| 1 | CA | 1047 | 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 | 703 | G | Sidechain |
| 1 | CA | 82 | G | Sidechain |
| 1 | CA | 832 | G | Sidechain |
| 1 | CA | 992 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 23 | DB | 1047 | G | Sidechain |
| 23 | DB | 1060 | U | Sidechain |
| 23 | DB | 1086 | A | Sidechain |
| 23 | DB | 1088 | A | Sidechain |
| 23 | DB | 1439 | A | Sidechain |
| 23 | DB | 1533 | C | Sidechain |
| 23 | DB | 1538 | G | Sidechain |
| 23 | DB | 1546 | G | Sidechain |
| 23 | DB | 1572 | A | Sidechain |
| 23 | DB | 1645 | G | Sidechain |
| 23 | DB | 1734 | G | Sidechain |
| 23 | DB | 1792 | G | Sidechain |
| 23 | DB | 1814 | G | Sidechain |
| 23 | DB | 1828 | G | Sidechain |
| 23 | DB | 2062 | A | Sidechain |
| 23 | DB | 2109 | U | Sidechain |
| 23 | DB | 2135 | A | Sidechain |
| 23 | DB | 2136 | G | Sidechain |
| 23 | DB | 2155 | U | Sidechain |
| 23 | DB | 221 | A | Sidechain |
| 23 | DB | 222 | A | Sidechain |
| 23 | DB | 2272 | U | Sidechain |
| 23 | DB | 2319 | G | Sidechain |
| 23 | DB | 2471 | A | Sidechain |
| 23 | DB | 2503 | A | Sidechain |
| 23 | DB | 2638 | G | Sidechain |
| 23 | DB | 2733 | A | Sidechain |
| 23 | DB | 2848 | G | Sidechain |
| 23 | DB | 2857 | G | Sidechain |
| 23 | DB | 2868 | A | Sidechain |
| 23 | DB | 299 | A | Sidechain |
| 23 | DB | 356 | G | Sidechain |
| 23 | DB | 427 | U | Sidechain |
| 23 | DB | 51 | G | Sidechain |
| 23 | DB | 630 | G | Sidechain |
| 23 | DB | 727 | A | Sidechain |
| 23 | DB | 729 | G | Sidechain |
| 23 | DB | 757 | G | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32831 | 0 | 16521 | 1355 | 0 |
| 1 | CA | 32831 | 0 | 16521 | 1385 | 0 |
| 2 | AC | 1624 | 0 | 1699 | 137 | 0 |
| 2 | CC | 1624 | 0 | 1699 | 145 | 0 |
| 3 | AD | 1643 | 0 | 1710 | 166 | 0 |
| 3 | CD | 1643 | 0 | 1710 | 156 | 0 |
| 4 | AE | 1105 | 0 | 1148 | 105 | 0 |
| 4 | CE | 1105 | 0 | 1148 | 115 | 0 |
| 5 | AF | 817 | 0 | 808 | 98 | 0 |
| 5 | CF | 817 | 0 | 808 | 88 | 0 |
| 6 | AG | 1174 | 0 | 1230 | 118 | 0 |
| 6 | CG | 1196 | 0 | 1246 | 110 | 0 |
| 7 | AH | 979 | 0 | 1034 | 93 | 0 |
| 7 | CH | 979 | 0 | 1034 | 93 | 0 |
| 8 | AI | 1022 | 0 | 1070 | 153 | 0 |
| 8 | CI | 1022 | 0 | 1070 | 151 | 0 |
| 9 | AJ | 786 | 0 | 828 | 78 | 0 |
| 9 | CJ | 786 | 0 | 828 | 84 | 0 |
| 10 | AK | 877 | 0 | 887 | 100 | 0 |
| 10 | CK | 877 | 0 | 887 | 101 | 0 |
| 11 | AL | 955 | 0 | 1019 | 90 | 0 |
| 11 | CL | 955 | 0 | 1019 | 94 | 0 |
| 12 | AM | 883 | 0 | 944 | 110 | 0 |
| 12 | CM | 876 | 0 | 937 | 109 | 0 |
| 13 | AN | 774 | 0 | 827 | 96 | 0 |
| 13 | CN | 774 | 0 | 827 | 90 | 0 |
| 14 | AO | 715 | 0 | 742 | 48 | 0 |
| 14 | CO | 715 | 0 | 742 | 41 | 0 |
| 15 | AP | 649 | 0 | 666 | 53 | 0 |
| 15 | CP | 638 | 0 | 656 | 55 | 0 |
| 16 | AQ | 648 | 0 | 691 | 73 | 0 |
| 16 | CQ | 656 | 0 | 702 | 73 | 0 |
| 17 | AR | 455 | 0 | 478 | 34 | 0 |
| 17 | CR | 455 | 0 | 478 | 34 | 0 |
| 18 | AS | 637 | 0 | 665 | 101 | 0 |
| 18 | CS | 644 | 0 | 675 | 98 | 0 |
| 19 | AT | 665 | 0 | 714 | 49 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | CT | 665 | 0 | 714 | 49 | 0 |
| 20 | AB | 1704 | 0 | 1732 | 205 | 0 |
| 20 | CB | 1704 | 0 | 1732 | 208 | 0 |
| 21 | AU | 425 | 0 | 449 | 75 | 0 |
| 21 | CU | 425 | 0 | 449 | 68 | 0 |
| 22 | BA | 2507 | 0 | 1270 | 109 | 0 |
| 22 | DA | 2507 | 0 | 1270 | 111 | 0 |
| 23 | BB | 60995 | 0 | 30678 | 2412 | 0 |
| 23 | DB | 60995 | 0 | 30677 | 2498 | 0 |
| 24 | BV | 753 | 0 | 780 | 89 | 0 |
| 24 | DV | 753 | 0 | 780 | 90 | 0 |
| 25 | BC | 2082 | 0 | 2157 | 261 | 0 |
| 25 | DC | 2082 | 0 | 2157 | 274 | 0 |
| 26 | BD | 1565 | 0 | 1616 | 216 | 0 |
| 26 | DD | 1565 | 0 | 1616 | 220 | 0 |
| 27 | BE | 1552 | 0 | 1619 | 180 | 0 |
| 27 | DE | 1552 | 0 | 1619 | 170 | 0 |
| 28 | BF | 1420 | 0 | 1460 | 236 | 0 |
| 28 | DF | 1420 | 0 | 1460 | 238 | 0 |
| 29 | BG | 1323 | 0 | 1374 | 163 | 0 |
| 29 | DG | 1323 | 0 | 1374 | 161 | 0 |
| 30 | BH | 1111 | 0 | 1148 | 176 | 0 |
| 30 | DH | 1111 | 0 | 1148 | 146 | 0 |
| 31 | BJ | 1129 | 0 | 1162 | 150 | 0 |
| 31 | DJ | 1129 | 0 | 1162 | 154 | 0 |
| 32 | BK | 930 | 0 | 1000 | 122 | 0 |
| 32 | DK | 930 | 0 | 1000 | 134 | 0 |
| 33 | BL | 1045 | 0 | 1117 | 150 | 0 |
| 33 | DL | 1045 | 0 | 1117 | 155 | 0 |
| 34 | BM | 1074 | 0 | 1157 | 114 | 0 |
| 34 | DM | 1074 | 0 | 1157 | 112 | 0 |
| 35 | BN | 960 | 0 | 1000 | 135 | 0 |
| 35 | DN | 960 | 0 | 1000 | 129 | 0 |
| 36 | BO | 892 | 0 | 923 | 97 | 0 |
| 36 | DO | 892 | 0 | 923 | 104 | 0 |
| 37 | BP | 917 | 0 | 965 | 112 | 0 |
| 37 | DP | 917 | 0 | 965 | 113 | 0 |
| 38 | BQ | 947 | 0 | 1022 | 156 | 0 |
| 38 | DQ | 947 | 0 | 1022 | 167 | 0 |
| 39 | BR | 816 | 0 | 839 | 123 | 0 |
| 39 | DR | 816 | 0 | 839 | 138 | 0 |
| 40 | BS | 857 | 0 | 922 | 93 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | DS | 857 | 0 | 922 | 93 | 0 |
| 41 | BT | 738 | 0 | 807 | 127 | 0 |
| 41 | DT | 738 | 0 | 807 | 122 | 0 |
| 42 | BU | 779 | 0 | 834 | 132 | 0 |
| 42 | DU | 779 | 0 | 834 | 121 | 0 |
| 43 | BW | 596 | 0 | 610 | 128 | 0 |
| 43 | DW | 596 | 0 | 610 | 137 | 0 |
| 44 | BX | 509 | 0 | 543 | 54 | 0 |
| 44 | DX | 509 | 0 | 543 | 50 | 0 |
| 45 | BY | 449 | 0 | 491 | 48 | 0 |
| 45 | DY | 449 | 0 | 491 | 50 | 0 |
| 46 | BZ | 625 | 0 | 652 | 89 | 0 |
| 46 | DZ | 625 | 0 | 652 | 92 | 0 |
| 47 | B0 | 444 | 0 | 461 | 40 | 0 |
| 47 | D0 | 444 | 0 | 461 | 42 | 0 |
| 48 | B1 | 409 | 0 | 440 | 57 | 0 |
| 48 | D1 | 409 | 0 | 440 | 44 | 0 |
| 49 | B2 | 377 | 0 | 418 | 43 | 0 |
| 49 | D2 | 377 | 0 | 418 | 43 | 0 |
| 50 | B3 | 504 | 0 | 574 | 40 | 0 |
| 50 | D3 | 504 | 0 | 574 | 40 | 0 |
| 51 | B4 | 302 | 0 | 340 | 40 | 0 |
| 51 | D4 | 302 | 0 | 340 | 35 | 0 |
| 52 | BI | 1032 | 0 | 1088 | 111 | 0 |
| 52 | DI | 1032 | 0 | 1088 | 182 | 0 |
| 53 | AA | 58 | 0 | 0 | 0 | 0 |
| 53 | AE | 1 | 0 | 0 | 0 | 0 |
| 53 | AN | 1 | 0 | 0 | 0 | 0 |
| 53 | BB | 110 | 0 | 0 | 0 | 0 |
| 53 | CA | 61 | 0 | 0 | 0 | 0 |
| 53 | CE | 1 | 0 | 0 | 0 | 0 |
| 53 | DB | 111 | 0 | 0 | 0 | 0 |
| 54 | AA | 36 | 0 | 37 | 2 | 0 |
| 54 | CA | 36 | 0 | 37 | 1 | 0 |
| 55 | B4 | 1 | 0 | 0 | 0 | 0 |
| 55 | D4 | 1 | 0 | 0 | 0 | 0 |
| 56 | AA | 282 | 0 | 0 | 4 | 0 |
| 56 | AE | 4 | 0 | 0 | 0 | 0 |
| 56 | AK | 2 | 0 | 0 | 0 | 0 |
| 56 | AL | 5 | 0 | 0 | 0 | 0 |
| 56 | AN | 4 | 0 | 0 | 0 | 0 |
| 56 | AT | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56 | B2 | 1 | 0 | 0 | 0 | 0 |
| 56 | BB | 492 | 0 | 0 | 5 | 0 |
| 56 | BC | 8 | 0 | 0 | 0 | 0 |
| 56 | BD | 1 | 0 | 0 | 0 | 0 |
| 56 | BE | 2 | 0 | 0 | 0 | 0 |
| 56 | BH | 1 | 0 | 0 | 0 | 0 |
| 56 | BL | 2 | 0 | 0 | 0 | 0 |
| 56 | CA | 294 | 0 | 0 | 0 | 0 |
| 56 | CE | 4 | 0 | 0 | 0 | 0 |
| 56 | CI | 1 | 0 | 0 | 0 | 0 |
| 56 | CK | 1 | 0 | 0 | 0 | 0 |
| 56 | CL | 3 | 0 | 0 | 0 | 0 |
| 56 | CN | 3 | 0 | 0 | 0 | 0 |
| 56 | CT | 1 | 0 | 0 | 0 | 0 |
| 56 | D2 | 1 | 0 | 0 | 0 | 0 |
| 56 | DB | 499 | 0 | 0 | 8 | 0 |
| 56 | DC | 5 | 0 | 0 | 0 | 0 |
| 56 | DD | 1 | 0 | 0 | 0 | 0 |
| 56 | DE | 1 | 0 | 0 | 0 | 0 |
| 56 | DL | 5 | 0 | 0 | 1 | 0 |
| 56 | DP | 1 | 0 | 0 | 0 | 0 |
| All | All | 284077 | 0 | 190751 | 17232 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (17232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:DB:1099:G:H8 | 52:DI:3:LYS:N | 1.38 | 1.20 |
| 23:BB:855:G:H21 | 43:BW:23:LYS:HG2 | 1.08 | 1.15 |
| 42:DU:85:ARG:HD3 | 42:DU:86:PHE:H | 1.13 | 1.14 |
| 41:DT:5:GLU:HA | 41:DT:8:LEU:HB2 | 1.25 | 1.13 |
| 42:BU:85:ARG:HD3 | 42:BU:86:PHE:H | 1.11 | 1.12 |
| 41:BT:5:GLU:HA | 41:BT:8:LEU:HB2 | 1.25 | 1.12 |
| 1:CA:1533:C:H2' | 1:CA:1534:A:H3' | 1.34 | 1.08 |
| 23:DB:545:U:H5'' | 23:DB:546:U:H4' | 1.25 | 1.08 |
| 23:DB:1098:A:H3' | 52:DI:3:LYS:HA | 1.38 | 1.05 |
| 21:AU:16:ARG:HE | 21:AU:16:ARG:HA | 1.20 | 1.04 |
| 23:BB:1338:G:H4' | 41:BT:18:GLU:HG3 | 1.40 | 1.04 |
| 23:DB:1099:G:C8 | 52:DI:3:LYS:N | 2.26 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BD:106:LYS:HB3 | 26:BD:206:ALA:H | 1.23 | 1.03 |
| 31:DJ:58:ASN:HA | 31:DJ:127:GLY:HA2 | 1.40 | 1.03 |
| 1:AA:1221:G:H4' | 18:AS:76:THR:HG21 | 1.40 | 1.03 |
| 31:BJ:58:ASN:HA | 31:BJ:127:GLY:HA2 | 1.38 | 1.03 |
| 45:DY:8:GLN:HG2 | 45:DY:31:ILE:HA | 1.40 | 1.02 |
| 8:AI:20:ILE:HA | 8:AI:62:LEU:HD12 | 1.37 | 1.02 |
| 28:DF:36:ASN:HD22 | 28:DF:152:ASP:HB2 | 1.24 | 1.02 |
| 23:DB:1099:G:O5' | 52:DI:4:VAL:N | 1.92 | 1.02 |
| 32:DK:35:VAL:HG23 | 32:DK:36:GLY:H | 1.23 | 1.02 |
| 1:CA:1221:G:H4' | 18:CS:76:THR:HG21 | 1.41 | 1.02 |
| 23:DB:1098:A:H3' | 52:DI:3:LYS:CA | 1.87 | 1.02 |
| 21:CU:16:ARG:HE | 21:CU:16:ARG:HA | 1.23 | 1.02 |
| 32:BK:35:VAL:HG23 | 32:BK:36:GLY:H | 1.24 | 1.01 |
| 8:CI:20:ILE:HA | 8:CI:62:LEU:HD12 | 1.37 | 1.01 |
| 28:DF:126:ASN:HD22 | 28:DF:156:THR:HG23 | 1.20 | 1.01 |
| 42:BU:80:ASP:HB3 | 42:BU:96:LYS:H | 1.25 | 1.01 |
| 28:BF:126:ASN:HD22 | 28:BF:156:THR:HG23 | 1.20 | 1.01 |
| 35:BN:2:ARG:HA | 35:BN:5:LYS:HD3 | 1.43 | 1.01 |
| 23:DB:1812:U:H1' | 25:DC:43:ASN:HD21 | 1.23 | 1.01 |
| 31:DJ:17:VAL:HG23 | 31:DJ:137:PRO:HB2 | 1.42 | 1.01 |
| 23:BB:1812:U:H1' | 25:BC:43:ASN:HD21 | 1.25 | 1.01 |
| 23:DB:1338:G:H4' | 41:DT:18:GLU:HG3 | 1.40 | 1.01 |
| 28:BF:65:LEU:H | 28:BF:88:VAL:HG22 | 1.24 | 1.00 |
| 35:DN:29:VAL:HG12 | 35:DN:83:LEU:HD21 | 1.40 | 1.00 |
| 25:BC:77:VAL:HG23 | 25:BC:112:GLY:H | 1.23 | 1.00 |
| 31:BJ:17:VAL:HG23 | 31:BJ:137:PRO:HB2 | 1.39 | 1.00 |
| 23:DB:1244:A:H5'' | 33:DL:8:PRO:HD3 | 1.41 | 1.00 |
| 38:DQ:63:ARG:HH22 | 38:DQ:96:ASP:HA | 1.26 | 1.00 |
| 1:AA:1086:U:H3 | 1:AA:1099:G:H22 | 1.10 | 1.00 |
| 45:BY:8:GLN:HG2 | 45:BY:31:ILE:HA | 1.42 | 1.00 |
| 23:DB:137:U:H2' | 23:DB:138:U:O4' | 1.59 | 1.00 |
| 35:BN:96:ARG:HH11 | 35:BN:116:VAL:HG23 | 1.24 | 1.00 |
| 20:CB:202:ASN:HD22 | 20:CB:204:ASP:H | 1.06 | 1.00 |
| 13:AN:51:PRO:HB2 | 13:AN:54:SER:HB3 | 1.44 | 1.00 |
| 28:BF:36:ASN:HD22 | 28:BF:152:ASP:HB2 | 1.26 | 1.00 |
| 42:BU:38:ILE:HG23 | 42:BU:39:ASN:H | 1.25 | 1.00 |
| 42:DU:80:ASP:HB3 | 42:DU:96:LYS:H | 1.22 | 1.00 |
| 5:CF:92:THR:HG22 | 5:CF:94:HIS:H | 1.26 | 1.00 |
| 25:DC:77:VAL:HG23 | 25:DC:112:GLY:H | 1.23 | 1.00 |
| 30:BH:7:ASP:HA | 30:BH:15:LEU:HD22 | 1.44 | 0.99 |
| 23:DB:1174:U:H1' | 23:DB:1176:U:H1' | 1.43 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BN:2:ARG:HG2 | 35:BN:5:LYS:HB2 | 1.43 | 0.99 |
| 30:DH:127:GLU:HA | 30:DH:145:ASN:HA | 1.44 | 0.99 |
| 10:CK:33:ILE:HB | 10:CK:73:VAL:HG11 | 1.42 | 0.99 |
| 23:BB:1203:U:H1' | 33:BL:4:ASN:HD21 | 1.21 | 0.99 |
| 35:DN:2:ARG:HA | 35:DN:5:LYS:HD3 | 1.44 | 0.99 |
| 26:DD:106:LYS:HB3 | 26:DD:206:ALA:H | 1.24 | 0.98 |
| 42:DU:38:ILE:HG23 | 42:DU:39:ASN:H | 1.26 | 0.98 |
| 20:CB:46:VAL:HG13 | 20:CB:47:PRO:HD3 | 1.45 | 0.98 |
| 40:BS:24:ILE:HD11 | 40:BS:36:LEU:HD11 | 1.43 | 0.98 |
| 1:CA:1086:U:H3 | 1:CA:1099:G:H22 | 1.11 | 0.98 |
| 13:CN:51:PRO:HB2 | 13:CN:54:SER:HB3 | 1.45 | 0.98 |
| 2:AC:128:MET:HB2 | 2:AC:131:ARG:HB2 | 1.46 | 0.98 |
| 30:DH:7:ASP:HA | 30:DH:15:LEU:HD22 | 1.45 | 0.98 |
| 38:BQ:63:ARG:HH22 | 38:BQ:96:ASP:HA | 1.28 | 0.98 |
| 31:BJ:112:GLY:H | 31:BJ:113:PRO:HD2 | 1.29 | 0.97 |
| 33:DL:79:LEU:HB2 | 33:DL:113:ALA:HB3 | 1.45 | 0.97 |
| 2:CC:48:LYS:HE2 | 2:CC:48:LYS:H | 1.29 | 0.97 |
| 5:AF:92:THR:HG22 | 5:AF:94:HIS:H | 1.26 | 0.97 |
| 35:BN:29:VAL:HG12 | 35:BN:83:LEU:HD21 | 1.43 | 0.97 |
| 25:DC:144:GLU:HG3 | 25:DC:151:GLY:H | 1.23 | 0.97 |
| 31:DJ:112:GLY:H | 31:DJ:113:PRO:HD2 | 1.28 | 0.97 |
| 20:AB:202:ASN:HD22 | 20:AB:204:ASP:H | 1.07 | 0.96 |
| 23:DB:1654:A:O2' | 26:DD:118:PHE:HB2 | 1.65 | 0.96 |
| 10:AK:33:ILE:HB | 10:AK:73:VAL:HG11 | 1.44 | 0.96 |
| 33:BL:79:LEU:HB2 | 33:BL:113:ALA:HB3 | 1.47 | 0.96 |
| 1:CA:465:A:H2' | 1:CA:466:A:H3' | 1.46 | 0.96 |
| 20:AB:46:VAL:HG13 | 20:AB:47:PRO:HD3 | 1.47 | 0.96 |
| 23:BB:1420:A:H2' | 23:BB:2211:A:H62 | 1.28 | 0.96 |
| 25:BC:144:GLU:HG3 | 25:BC:151:GLY:H | 1.28 | 0.96 |
| 23:BB:460:A:H4' | 41:BT:72:GLN:HB2 | 1.45 | 0.96 |
| 2:CC:69:THR:HG21 | 2:CC:75:VAL:HG21 | 1.48 | 0.96 |
| 28:DF:65:LEU:H | 28:DF:88:VAL:HG22 | 1.25 | 0.96 |
| 23:DB:1420:A:H2' | 23:DB:2211:A:H62 | 1.28 | 0.95 |
| 23:BB:2502:G:H5' | 23:BB:2503:A:H5'' | 1.49 | 0.95 |
| 23:BB:962:G:H21 | 23:BB:2250:G:H22 | 1.13 | 0.95 |
| 33:DL:29:LYS:HG3 | 33:DL:30:THR:HG23 | 1.48 | 0.95 |
| 1:AA:1399:C:H4' | 1:AA:1400:C:H5'' | 1.48 | 0.95 |
| 34:BM:40:ARG:HD3 | 34:BM:93:VAL:HG21 | 1.48 | 0.95 |
| 34:DM:40:ARG:HD3 | 34:DM:93:VAL:HG21 | 1.45 | 0.95 |
| 2:AC:69:THR:HG21 | 2:AC:75:VAL:HG21 | 1.48 | 0.95 |
| 25:BC:183:VAL:HG13 | 25:BC:185:ALA:H | 1.29 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:CF:29:ILE:HG21 | 5:CF:64:VAL:HG11 | 1.48 | 0.95 |
| 35:DN:2:ARG:HG2 | 35:DN:5:LYS:HB2 | 1.47 | 0.95 |
| 23:BB:1244:A:H5'' | 33:BL:8:PRO:HD3 | 1.48 | 0.95 |
| 18:AS:18:VAL:HG21 | 18:AS:43:MET:HG2 | 1.48 | 0.95 |
| 23:DB:2502:G:H5' | 23:DB:2503:A:H5'' | 1.47 | 0.95 |
| 25:DC:27:LYS:HG3 | 25:DC:28:PRO:HD2 | 1.46 | 0.94 |
| 15:AP:28:ARG:HD2 | 15:AP:29:ASN:H | 1.32 | 0.94 |
| 25:DC:183:VAL:HG13 | 25:DC:185:ALA:H | 1.28 | 0.94 |
| 5:AF:29:ILE:HG21 | 5:AF:64:VAL:HG11 | 1.49 | 0.94 |
| 23:BB:1283:G:H22 | 23:BB:1286:A:H5' | 1.31 | 0.94 |
| 1:CA:1399:C:H4' | 1:CA:1400:C:H5'' | 1.48 | 0.94 |
| 44:DX:39:GLN:HB3 | 44:DX:42:LEU:HD13 | 1.48 | 0.94 |
| 1:AA:465:A:H2' | 1:AA:466:A:H3' | 1.49 | 0.94 |
| 25:BC:146:LYS:HB3 | 25:BC:147:PRO:HD2 | 1.47 | 0.94 |
| 23:DB:1099:G:H8 | 52:DI:3:LYS:H | 1.01 | 0.94 |
| 2:CC:128:MET:HB2 | 2:CC:131:ARG:HB2 | 1.46 | 0.94 |
| 23:DB:855:G:H21 | 43:DW:23:LYS:HG2 | 1.33 | 0.93 |
| 25:BC:27:LYS:HG3 | 25:BC:28:PRO:HD2 | 1.49 | 0.93 |
| 23:DB:1283:G:H22 | 23:DB:1286:A:H5' | 1.29 | 0.93 |
| 10:AK:88:PRO:HD3 | 21:AU:28:LEU:HD11 | 1.49 | 0.93 |
| 40:DS:24:ILE:HD11 | 40:DS:36:LEU:HD11 | 1.48 | 0.93 |
| 46:DZ:40:VAL:HG21 | 46:DZ:43:GLU:HB3 | 1.50 | 0.93 |
| 23:BB:855:G:N2 | 43:BW:23:LYS:HG2 | 1.82 | 0.93 |
| 21:CU:24:LYS:HZ3 | 21:CU:25:ALA:H | 1.17 | 0.93 |
| 33:BL:29:LYS:HG3 | 33:BL:30:THR:HG23 | 1.50 | 0.93 |
| 20:CB:65:LYS:HB2 | 20:CB:158:ASP:H | 1.34 | 0.93 |
| 3:CD:116:LEU:HB3 | 3:CD:122:ILE:HD11 | 1.50 | 0.93 |
| 26:DD:106:LYS:HB3 | 26:DD:206:ALA:N | 1.84 | 0.93 |
| 44:BX:39:GLN:HB3 | 44:BX:42:LEU:HD13 | 1.49 | 0.92 |
| 1:CA:1003:G:H21 | 1:CA:1005:A:H5' | 1.33 | 0.92 |
| 26:BD:114:LYS:HZ2 | 26:BD:116:LYS:HZ2 | 0.96 | 0.92 |
| 1:AA:1432:G:H5'' | 37:BP:105:LYS:HG2 | 1.47 | 0.92 |
| 12:CM:21:ILE:HB | 12:CM:24:VAL:HG22 | 1.48 | 0.92 |
| 2:AC:48:LYS:HE2 | 2:AC:48:LYS:H | 1.33 | 0.92 |
| 10:CK:88:PRO:HD3 | 21:CU:28:LEU:HD11 | 1.50 | 0.92 |
| 35:DN:37:THR:HG22 | 35:DN:39:PRO:HD2 | 1.50 | 0.92 |
| 28:BF:62:GLN:HE22 | 28:BF:90:LEU:HD13 | 1.35 | 0.92 |
| 15:CP:28:ARG:HD2 | 15:CP:29:ASN:H | 1.33 | 0.92 |
| 25:DC:146:LYS:HB3 | 25:DC:147:PRO:HD2 | 1.48 | 0.92 |
| 3:CD:90:LEU:HA | 3:CD:93:LEU:HD12 | 1.50 | 0.92 |
| 12:AM:21:ILE:HB | 12:AM:24:VAL:HG22 | 1.49 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BD:106:LYS:HB3 | 26:BD:206:ALA:N | 1.83 | 0.92 |
| 1:AA:1003:G:N2 | 1:AA:1005:A:H5' | 1.85 | 0.91 |
| 30:BH:31:VAL:HB | 30:BH:32:PRO:HD3 | 1.50 | 0.91 |
| 28:DF:43:ILE:HG23 | 28:DF:44:ALA:H | 1.34 | 0.91 |
| 43:DW:51:GLY:HA3 | 43:DW:59:PHE:HB2 | 1.53 | 0.91 |
| 23:BB:856:G:H1' | 43:BW:23:LYS:HB3 | 1.53 | 0.91 |
| 23:DB:2365:G:H4' | 43:DW:59:PHE:HE1 | 1.34 | 0.91 |
| 52:DI:11:GLN:HG2 | 52:DI:55:PRO:HB3 | 1.52 | 0.91 |
| 25:BC:128:THR:HA | 25:BC:190:THR:HG22 | 1.52 | 0.91 |
| 30:BH:128:HIS:HB2 | 30:BH:144:VAL:HB | 1.51 | 0.91 |
| 3:AD:116:LEU:HB3 | 3:AD:122:ILE:HD11 | 1.51 | 0.91 |
| 28:DF:62:GLN:HE22 | 28:DF:90:LEU:HD13 | 1.33 | 0.91 |
| 5:AF:3:HIS:ND1 | 5:AF:92:THR:HG23 | 1.85 | 0.91 |
| 21:AU:24:LYS:HZ3 | 21:AU:25:ALA:H | 1.17 | 0.91 |
| 26:BD:5:VAL:H | 26:BD:32:ASN:HD21 | 1.13 | 0.91 |
| 30:DH:131:SER:HB2 | 30:DH:141:LYS:HA | 1.52 | 0.91 |
| 20:AB:65:LYS:HB2 | 20:AB:158:ASP:H | 1.34 | 0.91 |
| 26:BD:113:SER:HB3 | 26:BD:168:GLU:H | 1.36 | 0.91 |
| 23:BB:2787:C:H1' | 26:BD:63:PRO:HG3 | 1.50 | 0.91 |
| 31:BJ:72:LYS:HB2 | 31:BJ:89:PHE:HB2 | 1.53 | 0.91 |
| 5:CF:38:ARG:HH21 | 5:CF:63:ASN:ND2 | 1.69 | 0.91 |
| 1:AA:1003:G:H21 | 1:AA:1005:A:H5' | 1.33 | 0.90 |
| 23:BB:470:A:H61 | 41:BT:72:GLN:HE22 | 1.12 | 0.90 |
| 8:AI:5:TYR:HB2 | 8:AI:20:ILE:HB | 1.51 | 0.90 |
| 32:BK:47:ILE:HG12 | 32:BK:48:PRO:HD2 | 1.53 | 0.90 |
| 8:CI:5:TYR:HB2 | 8:CI:20:ILE:HB | 1.51 | 0.90 |
| 30:DH:31:VAL:HB | 30:DH:32:PRO:HD3 | 1.51 | 0.90 |
| 30:DH:48:GLU:HB2 | 30:DH:51:ARG:HH21 | 1.34 | 0.90 |
| 28:BF:11:VAL:HG12 | 28:BF:12:VAL:H | 1.36 | 0.90 |
| 28:BF:43:ILE:HG23 | 28:BF:44:ALA:H | 1.34 | 0.90 |
| 23:BB:547:A:H3' | 23:BB:548:G:H8 | 1.35 | 0.90 |
| 27:BE:58:LYS:H | 27:BE:58:LYS:HD3 | 1.34 | 0.90 |
| 23:DB:962:G:H21 | 23:DB:2250:G:H22 | 1.13 | 0.90 |
| 30:BH:116:ARG:HB2 | 30:BH:116:ARG:HH11 | 1.36 | 0.90 |
| 43:BW:18:LYS:HA | 43:BW:36:ILE:HG12 | 1.54 | 0.90 |
| 28:DF:3:LEU:HD21 | 28:DF:172:PHE:HB3 | 1.53 | 0.90 |
| 16:AQ:74:LEU:HD22 | 16:AQ:75:VAL:H | 1.35 | 0.90 |
| 40:BS:26:GLY:H | 40:BS:71:VAL:HG13 | 1.37 | 0.90 |
| 1:AA:699:C:H2' | 1:AA:700:G:H5'' | 1.49 | 0.90 |
| 1:CA:1003:G:N2 | 1:CA:1005:A:H5' | 1.87 | 0.90 |
| 20:CB:85:SER:HB3 | 20:CB:221:ARG:HD3 | 1.54 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CF:3:HIS:ND1 | 5:CF:92:THR:HG23 | 1.86 | 0.90 |
| 26:DD:5:VAL:H | 26:DD:32:ASN:HD21 | 1.11 | 0.90 |
| 23:DB:1060:U:N3 | 23:DB:1088:A:N7 | 2.20 | 0.90 |
| 3:AD:160:LEU:H | 3:AD:160:LEU:HD13 | 1.37 | 0.90 |
| 6:AG:3:ARG:H | 6:AG:3:ARG:HD3 | 1.36 | 0.90 |
| 23:BB:858:G:N3 | 23:BB:2268:A:H2' | 1.87 | 0.90 |
| 43:DW:9:THR:HG23 | 43:DW:10:ARG:HD3 | 1.52 | 0.90 |
| 46:DZ:6:GLN:HE22 | 46:DZ:50:ARG:H | 1.17 | 0.90 |
| 27:DE:58:LYS:HD3 | 27:DE:58:LYS:H | 1.36 | 0.89 |
| 3:AD:90:LEU:HA | 3:AD:93:LEU:HD12 | 1.51 | 0.89 |
| 23:BB:136:G:H2' | 23:BB:137:U:C6 | 2.07 | 0.89 |
| 18:CS:18:VAL:HG21 | 18:CS:43:MET:HG2 | 1.51 | 0.89 |
| 38:BQ:79:ILE:HA | 38:BQ:82:LEU:HD12 | 1.53 | 0.89 |
| 23:BB:2356:U:H5'' | 43:BW:16:GLU:HG3 | 1.54 | 0.89 |
| 35:DN:32:GLU:HG3 | 35:DN:115:LEU:HD12 | 1.51 | 0.89 |
| 30:BH:116:ARG:HE | 30:BH:139:PHE:HB2 | 1.37 | 0.89 |
| 20:AB:112:ARG:HD2 | 20:AB:116:LEU:HD12 | 1.54 | 0.89 |
| 23:BB:1173:U:H2' | 23:BB:1174:U:H4' | 1.52 | 0.89 |
| 3:CD:160:LEU:H | 3:CD:160:LEU:HD13 | 1.36 | 0.89 |
| 1:AA:812:G:HO2' | 1:AA:813:U:H6 | 0.92 | 0.89 |
| 1:AA:600:A:H5'' | 7:AH:88:LYS:HD2 | 1.54 | 0.89 |
| 8:AI:34:LEU:HD21 | 8:AI:48:ARG:HH21 | 1.37 | 0.89 |
| 35:BN:37:THR:HG22 | 35:BN:39:PRO:HD2 | 1.53 | 0.89 |
| 23:DB:1024:G:H3' | 23:DB:1025:G:H5'' | 1.53 | 0.89 |
| 31:DJ:36:LEU:HD21 | 31:DJ:122:LEU:HB2 | 1.53 | 0.89 |
| 35:DN:96:ARG:HH11 | 35:DN:116:VAL:HG23 | 1.35 | 0.89 |
| 1:CA:812:G:HO2' | 1:CA:813:U:H6 | 0.94 | 0.89 |
| 4:CE:21:SER:HB2 | 4:CE:28:ARG:HE | 1.37 | 0.89 |
| 23:DB:117:G:H5' | 23:DB:126:A:H8 | 1.36 | 0.89 |
| 23:DB:79:C:HO2' | 23:DB:346:A:H8 | 1.20 | 0.89 |
| 26:DD:113:SER:HB3 | 26:DD:168:GLU:H | 1.37 | 0.89 |
| 23:BB:1060:U:N3 | 23:BB:1088:A:N7 | 2.20 | 0.89 |
| 23:BB:1654:A:O2' | 26:BD:118:PHE:HB2 | 1.72 | 0.89 |
| 23:BB:2305:U:H5'' | 28:BF:130:GLY:HA3 | 1.55 | 0.89 |
| 28:BF:3:LEU:HD21 | 28:BF:172:PHE:HB3 | 1.54 | 0.89 |
| 25:DC:128:THR:HA | 25:DC:190:THR:HG22 | 1.53 | 0.89 |
| 33:BL:57:LEU:HD12 | 33:BL:60:ARG:HH22 | 1.36 | 0.89 |
| 40:DS:26:GLY:H | 40:DS:71:VAL:HG13 | 1.34 | 0.89 |
| 24:DV:44:HIS:HE1 | 24:DV:86:LEU:H | 1.20 | 0.89 |
| 16:CQ:74:LEU:HD22 | 16:CQ:75:VAL:H | 1.38 | 0.89 |
| 12:AM:52:ILE:HD12 | 12:AM:55:LEU:HD12 | 1.54 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BZ:40:VAL:HG21 | 46:BZ:43:GLU:HB3 | 1.53 | 0.88 |
| 28:DF:11:VAL:HG12 | 28:DF:12:VAL:H | 1.36 | 0.88 |
| 31:DJ:72:LYS:HB2 | 31:DJ:89:PHE:HB2 | 1.53 | 0.88 |
| 1:AA:429:U:H5' | 3:AD:8:LEU:HG | 1.56 | 0.88 |
| 23:BB:27:G:H22 | 23:BB:512:G:H2' | 1.38 | 0.88 |
| 52:BI:129:GLU:HB3 | 52:BI:133:ARG:HH12 | 1.35 | 0.88 |
| 23:DB:27:G:H22 | 23:DB:512:G:H2' | 1.38 | 0.88 |
| 23:DB:858:G:N3 | 23:DB:2268:A:H2' | 1.88 | 0.88 |
| 5:CF:3:HIS:HB2 | 5:CF:92:THR:HA | 1.55 | 0.88 |
| 20:CB:112:ARG:HD2 | 20:CB:116:LEU:HD12 | 1.55 | 0.88 |
| 25:DC:180:MET:HB2 | 25:DC:268:ARG:HB2 | 1.56 | 0.88 |
| 20:AB:85:SER:HB3 | 20:AB:221:ARG:HD3 | 1.52 | 0.88 |
| 5:AF:3:HIS:HB2 | 5:AF:92:THR:HA | 1.56 | 0.88 |
| 30:BH:73:ASN:HD22 | 30:BH:74:ALA:H | 1.21 | 0.88 |
| 31:BJ:36:LEU:HD21 | 31:BJ:122:LEU:HB2 | 1.54 | 0.88 |
| 1:CA:699:C:H2' | 1:CA:700:G:H5'' | 1.53 | 0.88 |
| 30:DH:31:VAL:HB | 30:DH:32:PRO:CD | 2.04 | 0.88 |
| 23:DB:2882:A:H4' | 35:DN:97:ILE:HD11 | 1.56 | 0.88 |
| 6:CG:14:ASP:H | 6:CG:23:ALA:HB2 | 1.38 | 0.88 |
| 6:CG:46:LEU:HG | 6:CG:57:GLU:HB3 | 1.56 | 0.88 |
| 37:DP:4:ILE:HG22 | 37:DP:5:LYS:H | 1.39 | 0.88 |
| 8:CI:34:LEU:HD21 | 8:CI:48:ARG:HH21 | 1.37 | 0.87 |
| 19:CT:24:ARG:HG3 | 19:CT:65:LEU:HD11 | 1.55 | 0.87 |
| 39:DR:14:VAL:HG22 | 39:DR:15:SER:H | 1.36 | 0.87 |
| 43:BW:9:THR:HG23 | 43:BW:10:ARG:HD3 | 1.53 | 0.87 |
| 48:D1:7:LYS:HA | 48:D1:23:THR:HG22 | 1.57 | 0.87 |
| 6:AG:14:ASP:H | 6:AG:23:ALA:HB2 | 1.37 | 0.87 |
| 26:BD:29:VAL:HB | 26:BD:98:VAL:HG22 | 1.56 | 0.87 |
| 12:AM:70:ARG:HH12 | 28:BF:112:ASP:HB2 | 1.37 | 0.87 |
| 3:AD:105:GLY:HA3 | 3:AD:158:LEU:HD23 | 1.55 | 0.87 |
| 43:BW:51:GLY:HA3 | 43:BW:59:PHE:HB2 | 1.55 | 0.87 |
| 23:DB:2179:C:H2' | 23:DB:2179:C:O2 | 1.75 | 0.87 |
| 30:BH:31:VAL:HB | 30:BH:32:PRO:CD | 2.04 | 0.87 |
| 1:AA:981:U:H4' | 13:AN:60:ARG:HD2 | 1.55 | 0.87 |
| 37:BP:4:ILE:HG22 | 37:BP:5:LYS:H | 1.39 | 0.87 |
| 42:DU:81:ARG:HH21 | 42:DU:81:ARG:H | 1.22 | 0.87 |
| 29:DG:8:VAL:HG11 | 29:DG:49:LEU:HB3 | 1.57 | 0.87 |
| 23:BB:470:A:H61 | 41:BT:72:GLN:NE2 | 1.72 | 0.86 |
| 24:BV:44:HIS:HE1 | 24:BV:86:LEU:H | 1.21 | 0.86 |
| 40:DS:29:VAL:HG11 | 40:DS:55:ILE:HD13 | 1.54 | 0.86 |
| 1:CA:817:C:H1' | 1:CA:819:A:H5' | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1084:A:H1' | 23:DB:1106:G:H5' | 1.55 | 0.86 |
| 4:AE:81:GLN:HG2 | 4:AE:148:SER:HA | 1.57 | 0.86 |
| 48:B1:7:LYS:HA | 48:B1:23:THR:HG22 | 1.54 | 0.86 |
| 1:CA:600:A:H5'' | 7:CH:88:LYS:HD2 | 1.57 | 0.86 |
| 32:DK:47:ILE:HG12 | 32:DK:48:PRO:HD2 | 1.54 | 0.86 |
| 33:DL:57:LEU:HD12 | 33:DL:60:ARG:HH22 | 1.40 | 0.86 |
| 52:BI:27:LEU:HD23 | 52:BI:27:LEU:H | 1.40 | 0.86 |
| 1:AA:72:A:H61 | 1:AA:99:C:H1' | 1.41 | 0.86 |
| 6:CG:129:ASN:HA | 6:CG:134:VAL:HG11 | 1.57 | 0.86 |
| 23:DB:2787:C:H1' | 26:DD:63:PRO:HG3 | 1.58 | 0.86 |
| 24:BV:72:VAL:HG12 | 24:BV:93:ARG:HA | 1.58 | 0.86 |
| 1:CA:981:U:H4' | 13:CN:60:ARG:HD2 | 1.58 | 0.86 |
| 23:DB:1437:C:H2' | 23:DB:1438:U:C6 | 2.10 | 0.86 |
| 20:AB:125:PHE:HD2 | 20:AB:125:PHE:H | 1.24 | 0.86 |
| 26:DD:29:VAL:HB | 26:DD:98:VAL:HG22 | 1.57 | 0.86 |
| 23:DB:996:A:H4' | 38:DQ:91:ARG:HD2 | 1.56 | 0.86 |
| 39:DR:19:THR:HG22 | 39:DR:97:LYS:HA | 1.58 | 0.86 |
| 46:BZ:6:GLN:HE22 | 46:BZ:50:ARG:H | 1.21 | 0.86 |
| 1:CA:1328:C:H5'' | 12:CM:27:THR:HG21 | 1.56 | 0.86 |
| 26:DD:114:LYS:NZ | 26:DD:116:LYS:HZ2 | 1.73 | 0.86 |
| 6:AG:149:ALA:H | 10:AK:55:ARG:NH2 | 1.73 | 0.86 |
| 10:AK:86:LYS:HB3 | 10:AK:112:VAL:HG23 | 1.58 | 0.86 |
| 15:AP:61:VAL:HA | 15:AP:65:ALA:HB3 | 1.57 | 0.86 |
| 35:BN:102:PHE:H | 35:BN:109:PRO:HA | 1.40 | 0.86 |
| 23:BB:1024:G:H3' | 23:BB:1025:G:H5'' | 1.57 | 0.85 |
| 23:BB:2769:U:H2' | 23:BB:2770:G:H8 | 1.39 | 0.85 |
| 42:BU:81:ARG:HH21 | 42:BU:81:ARG:H | 1.23 | 0.85 |
| 38:DQ:105:PHE:HA | 38:DQ:108:LEU:HD13 | 1.57 | 0.85 |
| 48:B1:26:LYS:HD3 | 48:B1:52:LYS:HB3 | 1.56 | 0.85 |
| 23:DB:2269:G:H4' | 43:DW:19:ARG:HH12 | 1.41 | 0.85 |
| 26:DD:148:GLN:HB2 | 26:DD:152:PRO:HG2 | 1.58 | 0.85 |
| 39:BR:19:THR:HG22 | 39:BR:97:LYS:HA | 1.58 | 0.85 |
| 1:CA:426:U:H4' | 3:CD:39:GLN:HA | 1.59 | 0.85 |
| 49:B2:30:VAL:HG22 | 49:B2:33:ARG:HH22 | 1.41 | 0.85 |
| 23:BB:546:U:H4' | 23:BB:547:A:OP1 | 1.77 | 0.85 |
| 29:BG:8:VAL:HG11 | 29:BG:49:LEU:HB3 | 1.56 | 0.85 |
| 37:BP:20:ARG:HD2 | 37:BP:21:PRO:HD2 | 1.56 | 0.85 |
| 3:AD:138:PRO:HA | 3:AD:181:PHE:HD2 | 1.42 | 0.85 |
| 25:BC:180:MET:HB2 | 25:BC:268:ARG:HB2 | 1.58 | 0.85 |
| 30:BH:100:ALA:HA | 30:BH:110:VAL:HG22 | 1.56 | 0.85 |
| 31:BJ:25:LEU:HD22 | 31:BJ:26:GLY:H | 1.39 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:CA:429:U:H5' | 3:CD:8:LEU:HG | 1.56 | 0.85 |
| 15:CP:40:ASN:HD21 | 15:CP:43:ALA:N | 1.74 | 0.85 |
| 26:DD:14:ILE:HA | 37:DP:11:GLN:HE22 | 1.41 | 0.85 |
| 35:DN:102:PHE:H | 35:DN:109:PRO:HA | 1.39 | 0.85 |
| 41:DT:11:LEU:HD22 | 41:DT:11:LEU:H | 1.42 | 0.85 |
| 6:AG:46:LEU:HG | 6:AG:57:GLU:HB3 | 1.56 | 0.85 |
| 9:AJ:42:LEU:HD11 | 9:AJ:73:LEU:HB2 | 1.58 | 0.85 |
| 37:DP:20:ARG:HD2 | 37:DP:21:PRO:HD2 | 1.58 | 0.85 |
| 32:BK:71:ARG:HD2 | 32:BK:105:ARG:HE | 1.40 | 0.85 |
| 39:BR:14:VAL:HG22 | 39:BR:15:SER:H | 1.40 | 0.85 |
| 8:CI:26:LYS:H | 8:CI:61:ASP:HB3 | 1.42 | 0.85 |
| 34:DM:19:GLY:HA2 | 34:DM:97:GLN:HB2 | 1.58 | 0.85 |
| 43:DW:18:LYS:HA | 43:DW:36:ILE:HG12 | 1.56 | 0.85 |
| 20:AB:221:ARG:HG3 | 20:AB:222:GLU:HG2 | 1.57 | 0.85 |
| 24:DV:72:VAL:HG12 | 24:DV:93:ARG:HA | 1.55 | 0.85 |
| 29:BG:15:ASP:HB3 | 29:BG:26:LYS:H | 1.41 | 0.85 |
| 41:BT:53:VAL:HG11 | 41:BT:87:LEU:HD13 | 1.58 | 0.85 |
| 1:CA:120:A:H2' | 1:CA:121:U:H5'' | 1.57 | 0.85 |
| 27:DE:31:VAL:HG21 | 27:DE:104:ALA:HB2 | 1.59 | 0.85 |
| 33:DL:6:LEU:H | 33:DL:6:LEU:HD23 | 1.42 | 0.85 |
| 19:AT:24:ARG:HG3 | 19:AT:65:LEU:HD11 | 1.57 | 0.85 |
| 1:CA:1323:G:H2' | 1:CA:1324:A:C8 | 2.12 | 0.85 |
| 34:DM:55:ARG:HH21 | 34:DM:55:ARG:HA | 1.42 | 0.85 |
| 36:DO:11:ALA:HB3 | 36:DO:96:GLY:H | 1.42 | 0.85 |
| 3:CD:105:GLY:HA3 | 3:CD:158:LEU:HD23 | 1.58 | 0.84 |
| 29:DG:26:LYS:HA | 29:DG:32:LEU:H | 1.40 | 0.84 |
| 6:AG:129:ASN:HA | 6:AG:134:VAL:HG11 | 1.57 | 0.84 |
| 15:AP:40:ASN:HD21 | 15:AP:43:ALA:N | 1.75 | 0.84 |
| 9:CJ:42:LEU:HD11 | 9:CJ:73:LEU:HB2 | 1.59 | 0.84 |
| 32:DK:71:ARG:HD2 | 32:DK:105:ARG:HE | 1.40 | 0.84 |
| 41:DT:57:VAL:HG22 | 41:DT:58:VAL:H | 1.42 | 0.84 |
| 1:AA:1493:A:H1' | 54:AA:2059:HYG:H362 | 1.41 | 0.84 |
| 23:BB:2039:U:H2' | 23:BB:2040:G:H8 | 1.43 | 0.84 |
| 23:BB:532:A:H2' | 38:BQ:27:ARG:HH22 | 1.41 | 0.84 |
| 20:CB:221:ARG:HG3 | 20:CB:222:GLU:HG2 | 1.58 | 0.84 |
| 1:AA:1060:U:H4' | 9:AJ:54:SER:HB2 | 1.57 | 0.84 |
| 8:AI:26:LYS:H | 8:AI:61:ASP:HB3 | 1.41 | 0.84 |
| 15:CP:61:VAL:HA | 15:CP:65:ALA:HB3 | 1.58 | 0.84 |
| 23:DB:2769:U:H2' | 23:DB:2770:G:H8 | 1.43 | 0.84 |
| 1:AA:1323:G:H2' | 1:AA:1324:A:C8 | 2.13 | 0.84 |
| 23:BB:140:C:H4' | 23:BB:141:G:H21 | 1.40 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1437:C:H2' | 23:BB:1438:U:C6 | 2.13 | 0.84 |
| 32:BK:86:LEU:H | 32:BK:86:LEU:HD23 | 1.42 | 0.84 |
| 1:AA:781:A:H2' | 1:AA:782:A:H5' | 1.59 | 0.84 |
| 49:B2:10:LEU:HD21 | 49:B2:14:ARG:HH11 | 1.41 | 0.84 |
| 29:BG:26:LYS:HA | 29:BG:32:LEU:H | 1.41 | 0.84 |
| 34:DM:19:GLY:H | 34:DM:38:ARG:HH12 | 1.26 | 0.84 |
| 41:DT:29:THR:HA | 41:DT:86:THR:HA | 1.59 | 0.84 |
| 4:AE:21:SER:HB2 | 4:AE:28:ARG:HE | 1.40 | 0.84 |
| 14:AO:88:ARG:HA | 14:AO:88:ARG:HH11 | 1.43 | 0.84 |
| 1:AA:120:A:H2' | 1:AA:121:U:H5'' | 1.59 | 0.83 |
| 21:CU:36:PHE:HB3 | 21:CU:40:PRO:HD3 | 1.59 | 0.83 |
| 26:DD:114:LYS:HZ2 | 26:DD:116:LYS:NZ | 1.75 | 0.83 |
| 34:BM:19:GLY:H | 34:BM:38:ARG:HH12 | 1.26 | 0.83 |
| 41:BT:57:VAL:HG22 | 41:BT:58:VAL:H | 1.43 | 0.83 |
| 1:CA:1060:U:H4' | 9:CJ:54:SER:HB2 | 1.59 | 0.83 |
| 23:DB:2743:U:H2' | 23:DB:2744:G:H5'' | 1.58 | 0.83 |
| 26:DD:114:LYS:HZ2 | 26:DD:116:LYS:HZ2 | 0.86 | 0.83 |
| 2:AC:70:ALA:HA | 2:AC:105:VAL:HG21 | 1.59 | 0.83 |
| 23:BB:1674:G:H21 | 23:BB:1677:A:H61 | 1.26 | 0.83 |
| 10:CK:105:ARG:HH21 | 21:CU:10:PRO:HD3 | 1.43 | 0.83 |
| 23:DB:1099:G:H5'' | 52:DI:3:LYS:N | 1.93 | 0.83 |
| 41:DT:39:THR:HG22 | 41:DT:42:GLU:H | 1.43 | 0.83 |
| 28:BF:42:ALA:HA | 28:BF:48:LEU:HD21 | 1.58 | 0.83 |
| 28:BF:42:ALA:H | 28:BF:48:LEU:HD11 | 1.42 | 0.83 |
| 41:BT:29:THR:HA | 41:BT:86:THR:HA | 1.57 | 0.83 |
| 49:D2:10:LEU:HD21 | 49:D2:14:ARG:HH11 | 1.41 | 0.83 |
| 23:DB:704:G:H2' | 23:DB:726:G:H22 | 1.41 | 0.83 |
| 41:BT:39:THR:HG22 | 41:BT:42:GLU:H | 1.41 | 0.83 |
| 23:DB:2039:U:H2' | 23:DB:2040:G:H8 | 1.44 | 0.83 |
| 23:BB:979:A:H2' | 23:BB:982:C:H41 | 1.42 | 0.83 |
| 34:BM:55:ARG:HH21 | 34:BM:55:ARG:HA | 1.42 | 0.83 |
| 39:BR:16:GLU:HA | 39:BR:98:ILE:HG22 | 1.60 | 0.83 |
| 44:BX:17:GLU:HB3 | 44:BX:53:VAL:HG11 | 1.61 | 0.83 |
| 11:AL:13:ARG:H | 11:AL:13:ARG:HD2 | 1.44 | 0.83 |
| 20:CB:116:LEU:HD22 | 20:CB:140:LEU:HD11 | 1.61 | 0.83 |
| 48:D1:26:LYS:HD3 | 48:D1:52:LYS:HB3 | 1.60 | 0.83 |
| 52:DI:27:LEU:HD23 | 52:DI:27:LEU:H | 1.44 | 0.83 |
| 17:AR:40:PRO:HD2 | 17:AR:43:ILE:HD12 | 1.59 | 0.83 |
| 23:BB:75:G:H4' | 44:BX:48:ARG:HH22 | 1.44 | 0.83 |
| 34:BM:19:GLY:HA2 | 34:BM:97:GLN:HB2 | 1.61 | 0.83 |
| 3:CD:138:PRO:HA | 3:CD:181:PHE:HD2 | 1.42 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CE:81:GLN:HG2 | 4:CE:148:SER:HA | 1.60 | 0.83 |
| 16:CQ:16:MET:HB2 | 16:CQ:19:SER:HB2 | 1.59 | 0.83 |
| 31:DJ:25:LEU:HD22 | 31:DJ:26:GLY:H | 1.42 | 0.83 |
| 6:AG:4:ARG:HG3 | 6:AG:5:VAL:H | 1.44 | 0.83 |
| 10:AK:105:ARG:HH21 | 21:AU:10:PRO:HD3 | 1.42 | 0.83 |
| 23:BB:1082:U:C4 | 23:BB:1086:A:C2 | 2.66 | 0.83 |
| 27:DE:161:ALA:HA | 27:DE:164:LEU:HB2 | 1.61 | 0.83 |
| 1:AA:426:U:H4' | 3:AD:39:GLN:HA | 1.60 | 0.82 |
| 24:DV:72:VAL:HG21 | 24:DV:91:PHE:HB3 | 1.61 | 0.82 |
| 23:BB:1060:U:C2 | 23:BB:1088:A:N7 | 2.48 | 0.82 |
| 28:DF:42:ALA:H | 28:DF:48:LEU:HD11 | 1.43 | 0.82 |
| 1:CA:18:C:H4' | 1:CA:1078:U:O2 | 1.78 | 0.82 |
| 20:CB:19:THR:HG23 | 20:CB:20:ARG:H | 1.44 | 0.82 |
| 35:DN:101:GLY:HA2 | 35:DN:110:MET:N | 1.95 | 0.82 |
| 46:BZ:7:VAL:HG13 | 46:BZ:8:THR:HG23 | 1.61 | 0.82 |
| 28:DF:42:ALA:HA | 28:DF:48:LEU:HD21 | 1.60 | 0.82 |
| 38:BQ:105:PHE:HA | 38:BQ:108:LEU:HD13 | 1.60 | 0.82 |
| 12:CM:52:ILE:HD12 | 12:CM:55:LEU:HD12 | 1.58 | 0.82 |
| 23:DB:979:A:H2' | 23:DB:982:C:H41 | 1.44 | 0.82 |
| 10:AK:22:ILE:HD13 | 10:AK:85:VAL:HG22 | 1.61 | 0.82 |
| 21:AU:36:PHE:HB3 | 21:AU:40:PRO:HD3 | 1.59 | 0.82 |
| 30:DH:68:ARG:HG3 | 30:DH:134:VAL:HG21 | 1.58 | 0.82 |
| 38:DQ:63:ARG:NH2 | 38:DQ:96:ASP:HA | 1.95 | 0.82 |
| 33:BL:6:LEU:HD23 | 33:BL:6:LEU:H | 1.42 | 0.82 |
| 40:BS:29:VAL:HG11 | 40:BS:55:ILE:HD13 | 1.59 | 0.82 |
| 41:BT:67:VAL:HB | 41:BT:76:ARG:HG2 | 1.61 | 0.82 |
| 2:CC:70:ALA:HA | 2:CC:105:VAL:HG21 | 1.59 | 0.82 |
| 14:CO:88:ARG:HA | 14:CO:88:ARG:HH11 | 1.42 | 0.82 |
| 17:CR:40:PRO:HD2 | 17:CR:43:ILE:HD12 | 1.61 | 0.82 |
| 23:DB:62:U:H2' | 23:DB:63:A:O4' | 1.80 | 0.82 |
| 6:AG:62:GLU:HG2 | 6:AG:69:ARG:HH21 | 1.44 | 0.82 |
| 36:BO:11:ALA:HB3 | 36:BO:96:GLY:H | 1.43 | 0.82 |
| 10:AK:31:VAL:HG21 | 10:AK:66:ALA:HA | 1.62 | 0.82 |
| 41:BT:11:LEU:HD22 | 41:BT:11:LEU:H | 1.45 | 0.82 |
| 1:CA:841:C:H3' | 1:CA:843:U:OP2 | 1.79 | 0.82 |
| 23:DB:1475:G:H1' | 23:DB:1514:G:O6 | 1.79 | 0.82 |
| 26:BD:148:GLN:HB2 | 26:BD:152:PRO:HG2 | 1.58 | 0.82 |
| 23:BB:321:U:OP2 | 27:BE:130:LYS:HA | 1.80 | 0.82 |
| 45:BY:35:VAL:HG22 | 45:BY:36:GLU:H | 1.45 | 0.82 |
| 10:CK:124:LYS:HA | 21:CU:34:ARG:HB3 | 1.61 | 0.82 |
| 23:DB:1082:U:C4 | 23:DB:1086:A:C2 | 2.67 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1099:G:P | 52:DI:3:LYS:HA | 2.20 | 0.82 |
| 46:DZ:33:LEU:HA | 46:DZ:52:SER:HA | 1.62 | 0.82 |
| 1:AA:817:C:H1' | 1:AA:819:A:H5' | 1.61 | 0.81 |
| 5:AF:86:ARG:NH1 | 17:AR:63:TYR:HB3 | 1.94 | 0.81 |
| 19:AT:34:VAL:HG11 | 19:AT:78:LEU:HD22 | 1.61 | 0.81 |
| 23:BB:958:U:H3 | 34:BM:16:ARG:HB3 | 1.45 | 0.81 |
| 37:BP:57:ALA:HA | 37:BP:73:PHE:O | 1.80 | 0.81 |
| 10:CK:86:LYS:HB3 | 10:CK:112:VAL:HG23 | 1.60 | 0.81 |
| 27:DE:147:LEU:HB3 | 27:DE:186:VAL:HG23 | 1.62 | 0.81 |
| 52:DI:121:ILE:HD13 | 52:DI:121:ILE:H | 1.45 | 0.81 |
| 32:DK:24:VAL:HA | 32:DK:39:ILE:HD12 | 1.62 | 0.81 |
| 41:DT:53:VAL:HG11 | 41:DT:87:LEU:HD13 | 1.59 | 0.81 |
| 23:BB:704:G:H2' | 23:BB:726:G:H22 | 1.43 | 0.81 |
| 10:CK:31:VAL:HG21 | 10:CK:66:ALA:HA | 1.60 | 0.81 |
| 11:CL:13:ARG:H | 11:CL:13:ARG:HD2 | 1.43 | 0.81 |
| 23:DB:1509:A:H5' | 23:DB:1510:G:H5' | 1.60 | 0.81 |
| 29:DG:15:ASP:HB3 | 29:DG:26:LYS:H | 1.43 | 0.81 |
| 35:BN:101:GLY:HA2 | 35:BN:110:MET:N | 1.95 | 0.81 |
| 3:CD:29:THR:H | 3:CD:33:ILE:HG21 | 1.45 | 0.81 |
| 23:DB:1060:U:C2 | 23:DB:1088:A:N7 | 2.48 | 0.81 |
| 16:AQ:16:MET:HB2 | 16:AQ:19:SER:HB2 | 1.61 | 0.81 |
| 23:BB:1594:U:H2' | 23:BB:1595:C:C6 | 2.16 | 0.81 |
| 23:BB:322:A:H5' | 23:BB:340:A:H1' | 1.62 | 0.81 |
| 25:BC:161:VAL:HG12 | 25:BC:162:GLN:H | 1.46 | 0.81 |
| 30:BH:127:GLU:HG3 | 30:BH:143:ILE:HB | 1.62 | 0.81 |
| 32:BK:87:LEU:HB2 | 32:BK:93:GLN:O | 1.80 | 0.81 |
| 30:DH:86:ASP:HB2 | 30:DH:89:LYS:HD3 | 1.62 | 0.81 |
| 41:DT:67:VAL:HB | 41:DT:76:ARG:HG2 | 1.62 | 0.81 |
| 23:BB:2579:C:O2' | 26:BD:136:ASN:HA | 1.79 | 0.81 |
| 1:CA:1361:G:H2' | 1:CA:1362:A:H5'' | 1.61 | 0.81 |
| 30:DH:135:HIS:HB3 | 30:DH:138:VAL:HB | 1.60 | 0.81 |
| 5:CF:86:ARG:NH1 | 17:CR:63:TYR:HB3 | 1.95 | 0.81 |
| 29:DG:84:LYS:HG2 | 29:DG:85:LYS:H | 1.44 | 0.81 |
| 23:BB:1475:G:H1' | 23:BB:1514:G:O6 | 1.81 | 0.81 |
| 23:BB:1509:A:H5' | 23:BB:1510:G:H5' | 1.61 | 0.81 |
| 23:BB:1729:U:H2' | 23:BB:1730:C:H4' | 1.62 | 0.81 |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:H | 1.46 | 0.81 |
| 12:CM:47:LEU:HD13 | 12:CM:51:GLN:HB3 | 1.63 | 0.81 |
| 23:DB:1203:U:H1' | 33:DL:4:ASN:HD21 | 1.46 | 0.81 |
| 38:DQ:79:ILE:HA | 38:DQ:82:LEU:HD12 | 1.60 | 0.81 |
| 1:AA:1328:C:H5'' | 12:AM:27:THR:HG21 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1178:C:H2' | 23:BB:1179:G:C8 | 2.14 | 0.81 |
| 23:BB:2306:C:H3' | 23:BB:2307:G:H5' | 1.63 | 0.81 |
| 27:BE:31:VAL:HG21 | 27:BE:104:ALA:HB2 | 1.61 | 0.81 |
| 35:BN:97:ILE:HD12 | 35:BN:98:LEU:H | 1.46 | 0.81 |
| 12:CM:2:ARG:HB2 | 12:CM:56:ARG:HH22 | 1.46 | 0.81 |
| 18:CS:51:HIS:HA | 18:CS:56:HIS:HA | 1.63 | 0.81 |
| 32:DK:87:LEU:HB2 | 32:DK:93:GLN:O | 1.81 | 0.81 |
| 20:AB:19:THR:HG23 | 20:AB:20:ARG:H | 1.45 | 0.81 |
| 5:AF:38:ARG:HH21 | 5:AF:63:ASN:ND2 | 1.78 | 0.81 |
| 8:AI:39:GLY:HA2 | 8:AI:44:ARG:HD3 | 1.62 | 0.81 |
| 25:BC:140:VAL:HG12 | 25:BC:141:HIS:H | 1.45 | 0.81 |
| 27:BE:147:LEU:HB3 | 27:BE:186:VAL:HG23 | 1.61 | 0.81 |
| 45:DY:35:VAL:HG22 | 45:DY:36:GLU:H | 1.45 | 0.81 |
| 12:AM:47:LEU:HD13 | 12:AM:51:GLN:HB3 | 1.62 | 0.80 |
| 30:BH:84:ALA:HA | 30:BH:90:LEU:HA | 1.63 | 0.80 |
| 1:AA:935:A:N6 | 6:AG:2:ARG:HD2 | 1.96 | 0.80 |
| 29:BG:84:LYS:HG2 | 29:BG:85:LYS:H | 1.43 | 0.80 |
| 30:BH:83:LYS:HB3 | 30:BH:91:PHE:HB2 | 1.61 | 0.80 |
| 1:CA:1343:G:H1' | 8:CI:122:ARG:HH12 | 1.46 | 0.80 |
| 37:DP:23:ASP:HA | 37:DP:88:ARG:HA | 1.62 | 0.80 |
| 37:DP:57:ALA:HA | 37:DP:73:PHE:O | 1.80 | 0.80 |
| 46:DZ:7:VAL:HG13 | 46:DZ:8:THR:HG23 | 1.62 | 0.80 |
| 18:AS:51:HIS:HA | 18:AS:56:HIS:HA | 1.63 | 0.80 |
| 23:DB:2306:C:H3' | 23:DB:2307:G:H5' | 1.63 | 0.80 |
| 25:DC:144:GLU:HA | 25:DC:151:GLY:HA2 | 1.63 | 0.80 |
| 52:DI:21:PRO:HB2 | 52:DI:22:PRO:HD3 | 1.64 | 0.80 |
| 2:AC:137:VAL:HA | 2:AC:148:ILE:HD13 | 1.63 | 0.80 |
| 22:BA:104:A:H2' | 22:BA:105:G:O4' | 1.81 | 0.80 |
| 31:DJ:81:ILE:HG23 | 31:DJ:82:GLY:H | 1.44 | 0.80 |
| 1:AA:841:C:H3' | 1:AA:843:U:OP2 | 1.81 | 0.80 |
| 6:CG:2:ARG:HB3 | 6:CG:2:ARG:NH1 | 1.97 | 0.80 |
| 49:D2:30:VAL:HG22 | 49:D2:33:ARG:HH22 | 1.47 | 0.80 |
| 23:DB:2153:C:H2' | 23:DB:2154:A:H8 | 1.47 | 0.80 |
| 23:DB:322:A:H5' | 23:DB:340:A:H1' | 1.63 | 0.80 |
| 1:AA:1343:G:H1' | 8:AI:122:ARG:HH12 | 1.47 | 0.80 |
| 2:CC:137:VAL:HA | 2:CC:148:ILE:HD13 | 1.61 | 0.80 |
| 23:DB:479:A:O2' | 23:DB:481:G:H5' | 1.82 | 0.80 |
| 39:DR:16:GLU:HA | 39:DR:98:ILE:HG22 | 1.63 | 0.80 |
| 23:BB:1141:U:H4' | 23:BB:1142:A:O4' | 1.82 | 0.80 |
| 42:BU:85:ARG:HD3 | 42:BU:86:PHE:N | 1.94 | 0.80 |
| 46:BZ:33:LEU:HA | 46:BZ:52:SER:HA | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1451:C:H4' | 23:DB:1452:G:H5' | 1.64 | 0.80 |
| 32:DK:86:LEU:HD23 | 32:DK:86:LEU:H | 1.45 | 0.80 |
| 35:DN:38:LEU:HB3 | 35:DN:39:PRO:HD3 | 1.63 | 0.80 |
| 32:BK:13:ASN:HD21 | 32:BK:98:ARG:H | 1.30 | 0.80 |
| 23:DB:1141:U:H4' | 23:DB:1142:A:O4' | 1.81 | 0.80 |
| 29:BG:122:ALA:HB2 | 29:BG:132:LEU:HB3 | 1.64 | 0.80 |
| 20:CB:32:GLY:H | 20:CB:39:ILE:HB | 1.46 | 0.80 |
| 1:AA:1361:G:H2' | 1:AA:1362:A:H5'' | 1.64 | 0.80 |
| 35:BN:38:LEU:HB3 | 35:BN:39:PRO:HD3 | 1.62 | 0.80 |
| 35:DN:97:ILE:HD12 | 35:DN:98:LEU:H | 1.46 | 0.80 |
| 29:DG:40:VAL:HG22 | 29:DG:64:ALA:HA | 1.62 | 0.79 |
| 6:AG:21:LEU:H | 6:AG:21:LEU:HD23 | 1.46 | 0.79 |
| 23:BB:100:U:O2 | 23:BB:100:U:H2' | 1.81 | 0.79 |
| 27:BE:161:ALA:HA | 27:BE:164:LEU:HB2 | 1.62 | 0.79 |
| 13:CN:15:LEU:HB3 | 13:CN:54:SER:HB2 | 1.64 | 0.79 |
| 22:DA:98:G:H1 | 24:DV:14:LYS:HB2 | 1.47 | 0.79 |
| 29:DG:122:ALA:HB2 | 29:DG:132:LEU:HB3 | 1.64 | 0.79 |
| 10:AK:124:LYS:HA | 21:AU:34:ARG:HB3 | 1.63 | 0.79 |
| 12:AM:44:ILE:HD12 | 12:AM:44:ILE:H | 1.48 | 0.79 |
| 23:BB:1925:C:H2' | 23:BB:1926:U:H5'' | 1.64 | 0.79 |
| 28:DF:141:ASP:HB3 | 28:DF:144:LYS:HB3 | 1.62 | 0.79 |
| 23:DB:1099:G:OP2 | 52:DI:3:LYS:HA | 1.81 | 0.79 |
| 34:DM:60:GLN:H | 34:DM:60:GLN:NE2 | 1.80 | 0.79 |
| 38:DQ:57:ARG:HB3 | 38:DQ:57:ARG:HH11 | 1.46 | 0.79 |
| 24:DV:66:ASP:HB2 | 24:DV:68:LYS:HE3 | 1.64 | 0.79 |
| 23:BB:2151:U:H2' | 23:BB:2152:G:C8 | 2.16 | 0.79 |
| 23:BB:2680:U:OP2 | 26:BD:114:LYS:HB3 | 1.82 | 0.79 |
| 24:BV:66:ASP:HB2 | 24:BV:68:LYS:HE3 | 1.64 | 0.79 |
| 14:AO:35:ILE:HD11 | 14:AO:58:MET:HG3 | 1.65 | 0.79 |
| 8:CI:29:ILE:HG12 | 8:CI:64:ILE:HB | 1.63 | 0.79 |
| 23:DB:532:A:H2' | 38:DQ:27:ARG:HH22 | 1.46 | 0.79 |
| 25:DC:140:VAL:HG12 | 25:DC:141:HIS:H | 1.46 | 0.79 |
| 11:AL:20:VAL:HG12 | 11:AL:93:ARG:HB3 | 1.63 | 0.79 |
| 23:BB:855:G:H21 | 43:BW:23:LYS:CG | 1.94 | 0.79 |
| 28:BF:65:LEU:HD23 | 28:BF:87:LYS:HD2 | 1.63 | 0.79 |
| 1:CA:1032:G:H2' | 1:CA:1033:G:O4' | 1.83 | 0.79 |
| 8:CI:39:GLY:HA2 | 8:CI:44:ARG:HD3 | 1.64 | 0.79 |
| 13:CN:87:ALA:HB2 | 13:CN:92:ILE:HD12 | 1.65 | 0.79 |
| 23:DB:2356:U:H5'' | 43:DW:16:GLU:HG3 | 1.64 | 0.79 |
| 32:DK:13:ASN:HD21 | 32:DK:98:ARG:H | 1.29 | 0.79 |
| 23:BB:2748:A:H1' | 29:BG:66:THR:HB | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:141:ASP:HB3 | 28:BF:144:LYS:HB3 | 1.63 | 0.79 |
| 43:BW:39:GLN:HG2 | 43:BW:40:ARG:N | 1.97 | 0.79 |
| 22:DA:104:A:H2' | 22:DA:105:G:O4' | 1.81 | 0.79 |
| 23:DB:1674:G:H21 | 23:DB:1677:A:H61 | 1.27 | 0.79 |
| 2:AC:122:GLN:HB3 | 2:AC:127:VAL:HG21 | 1.63 | 0.79 |
| 1:AA:264:C:H4' | 16:AQ:64:ARG:HD2 | 1.64 | 0.79 |
| 22:BA:75:G:H1 | 22:BA:102:G:N2 | 1.79 | 0.79 |
| 52:BI:21:PRO:HB2 | 52:BI:22:PRO:HD3 | 1.62 | 0.79 |
| 31:BJ:77:HIS:HD2 | 31:BJ:84:ILE:H | 1.31 | 0.79 |
| 19:CT:34:VAL:HG11 | 19:CT:78:LEU:HD22 | 1.63 | 0.79 |
| 1:AA:1032:G:H2' | 1:AA:1033:G:O4' | 1.83 | 0.79 |
| 20:AB:116:LEU:HD22 | 20:AB:140:LEU:HD11 | 1.64 | 0.79 |
| 42:DU:85:ARG:HD3 | 42:DU:86:PHE:N | 1.96 | 0.79 |
| 20:AB:32:GLY:H | 20:AB:39:ILE:HB | 1.48 | 0.79 |
| 25:BC:226:PRO:HG3 | 25:BC:233:GLY:H | 1.48 | 0.79 |
| 35:BN:32:GLU:HG3 | 35:BN:115:LEU:HD12 | 1.64 | 0.79 |
| 23:DB:90:U:H3' | 23:DB:91:A:H5'' | 1.64 | 0.79 |
| 4:AE:104:ILE:HG23 | 4:AE:111:ARG:HH12 | 1.47 | 0.78 |
| 25:BC:144:GLU:HA | 25:BC:151:GLY:HA2 | 1.65 | 0.78 |
| 52:BI:33:ASN:HD21 | 52:BI:64:ARG:HH11 | 1.31 | 0.78 |
| 37:DP:97:TYR:O | 37:DP:100:ARG:HB2 | 1.83 | 0.78 |
| 13:AN:87:ALA:HB2 | 13:AN:92:ILE:HD12 | 1.65 | 0.78 |
| 23:BB:364:C:H2' | 23:BB:365:U:C6 | 2.18 | 0.78 |
| 38:BQ:65:ASN:HB2 | 38:BQ:75:TYR:HB2 | 1.65 | 0.78 |
| 23:DB:899:A:H2' | 23:DB:900:A:O4' | 1.82 | 0.78 |
| 25:DC:161:VAL:HG12 | 25:DC:162:GLN:H | 1.49 | 0.78 |
| 23:BB:172:A:H2' | 23:BB:173:A:C8 | 2.18 | 0.78 |
| 23:BB:62:U:H2' | 23:BB:63:A:O4' | 1.83 | 0.78 |
| 23:BB:1060:U:OP2 | 52:BI:74:PRO:HA | 1.84 | 0.78 |
| 6:CG:62:GLU:HG2 | 6:CG:69:ARG:HH21 | 1.48 | 0.78 |
| 22:DA:116:G:H4' | 36:DO:54:VAL:HG22 | 1.64 | 0.78 |
| 12:AM:89:ARG:HH22 | 12:AM:94:LEU:HD12 | 1.48 | 0.78 |
| 37:BP:7:LEU:HD12 | 37:BP:7:LEU:H | 1.47 | 0.78 |
| 37:BP:97:TYR:O | 37:BP:100:ARG:HB2 | 1.84 | 0.78 |
| 38:BQ:63:ARG:NH2 | 38:BQ:96:ASP:HA | 1.97 | 0.78 |
| 6:CG:91:ARG:HD2 | 6:CG:91:ARG:H | 1.46 | 0.78 |
| 25:DC:226:PRO:HG3 | 25:DC:233:GLY:H | 1.47 | 0.78 |
| 2:CC:122:GLN:HB3 | 2:CC:127:VAL:HG21 | 1.64 | 0.78 |
| 15:CP:3:THR:HG22 | 15:CP:66:THR:HB | 1.65 | 0.78 |
| 23:DB:958:U:H3 | 34:DM:16:ARG:HB3 | 1.44 | 0.78 |
| 23:BB:2734:A:H2' | 23:BB:2735:G:H5' | 1.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:781:A:H2' | 1:CA:782:A:H5' | 1.63 | 0.78 |
| 43:DW:39:GLN:HG3 | 43:DW:42:THR:HB | 1.66 | 0.78 |
| 44:DX:17:GLU:HB3 | 44:DX:53:VAL:HG11 | 1.65 | 0.78 |
| 3:AD:29:THR:H | 3:AD:33:ILE:HG21 | 1.47 | 0.78 |
| 8:AI:29:ILE:HG12 | 8:AI:64:ILE:HB | 1.64 | 0.78 |
| 13:AN:15:LEU:HB3 | 13:AN:54:SER:HB2 | 1.65 | 0.78 |
| 23:BB:479:A:O2' | 23:BB:481:G:H5' | 1.84 | 0.78 |
| 7:CH:103:VAL:HG22 | 7:CH:124:ILE:HA | 1.65 | 0.78 |
| 6:AG:91:ARG:H | 6:AG:91:ARG:HD2 | 1.49 | 0.78 |
| 29:BG:126:THR:HB | 29:BG:129:GLU:HG3 | 1.64 | 0.78 |
| 52:BI:55:PRO:HD3 | 52:BI:74:PRO:HD3 | 1.65 | 0.78 |
| 1:CA:1144:G:N2 | 1:CA:1146:A:H62 | 1.82 | 0.78 |
| 23:DB:2365:G:H4' | 43:DW:59:PHE:CE1 | 2.17 | 0.78 |
| 28:DF:65:LEU:HD23 | 28:DF:87:LYS:HD2 | 1.66 | 0.78 |
| 22:BA:116:G:H4' | 36:BO:54:VAL:HG22 | 1.64 | 0.78 |
| 11:CL:20:VAL:HG12 | 11:CL:93:ARG:HB3 | 1.65 | 0.78 |
| 23:DB:1099:G:H8 | 52:DI:3:LYS:CA | 1.97 | 0.78 |
| 23:DB:1729:U:H2' | 23:DB:1730:C:H4' | 1.65 | 0.78 |
| 19:AT:85:LEU:HD23 | 19:AT:86:ALA:H | 1.49 | 0.78 |
| 23:BB:2010:G:H5'' | 40:BS:42:LYS:HB2 | 1.66 | 0.78 |
| 34:BM:21:ALA:HB1 | 34:BM:100:LYS:HE2 | 1.65 | 0.78 |
| 37:BP:23:ASP:HA | 37:BP:88:ARG:HA | 1.64 | 0.78 |
| 12:AM:19:THR:HA | 12:AM:24:VAL:HG23 | 1.66 | 0.77 |
| 48:B1:33:LEU:HB3 | 48:B1:51:ALA:HB3 | 1.64 | 0.77 |
| 29:BG:40:VAL:HG22 | 29:BG:64:ALA:HA | 1.66 | 0.77 |
| 23:BB:996:A:H4' | 38:BQ:91:ARG:HD2 | 1.66 | 0.77 |
| 42:BU:26:ASN:HD21 | 42:BU:34:ILE:HD12 | 1.49 | 0.77 |
| 1:AA:108:G:H5' | 1:AA:109:A:H5'' | 1.66 | 0.77 |
| 52:DI:45:THR:HA | 52:DI:48:ILE:HG22 | 1.66 | 0.77 |
| 39:DR:60:LYS:H | 39:DR:100:GLY:HA3 | 1.50 | 0.77 |
| 43:DW:17:ALA:HA | 43:DW:35:ILE:HG23 | 1.64 | 0.77 |
| 39:DR:24:LYS:HA | 39:DR:94:THR:HG23 | 1.66 | 0.77 |
| 24:DV:75:GLN:HG2 | 24:DV:92:VAL:HG23 | 1.66 | 0.77 |
| 43:DW:39:GLN:HG2 | 43:DW:40:ARG:N | 1.98 | 0.77 |
| 1:AA:1057:G:H4' | 2:AC:196:GLY:H | 1.50 | 0.77 |
| 25:BC:32:LEU:O | 25:BC:63:ILE:HG12 | 1.85 | 0.77 |
| 29:BG:148:ARG:HA | 29:BG:161:VAL:HB | 1.67 | 0.77 |
| 37:BP:20:ARG:HE | 37:BP:91:VAL:HG21 | 1.47 | 0.77 |
| 46:BZ:30:LEU:HD23 | 46:BZ:30:LEU:H | 1.47 | 0.77 |
| 23:DB:1099:G:H5'' | 52:DI:2:LYS:C | 2.03 | 0.77 |
| 23:DB:2734:A:H2' | 23:DB:2735:G:H5' | 1.65 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DZ:30:LEU:HD23 | 46:DZ:30:LEU:H | 1.47 | 0.77 |
| 23:BB:2769:U:H2' | 23:BB:2770:G:C8 | 2.20 | 0.77 |
| 1:CA:83:C:O2' | 1:CA:84:U:H3' | 1.85 | 0.77 |
| 23:DB:608:A:H2' | 23:DB:609:A:C8 | 2.20 | 0.77 |
| 23:DB:918:A:H2' | 23:DB:919:U:H5' | 1.66 | 0.77 |
| 12:CM:44:ILE:H | 12:CM:44:ILE:HD12 | 1.48 | 0.77 |
| 23:DB:172:A:H2' | 23:DB:173:A:C8 | 2.20 | 0.77 |
| 23:BB:1993:U:H4' | 26:BD:133:THR:CG2 | 2.14 | 0.77 |
| 23:BB:2185:U:H2' | 23:BB:2186:G:H8 | 1.50 | 0.77 |
| 23:BB:90:U:H3' | 23:BB:91:A:H5" | 1.65 | 0.77 |
| 30:BH:57:LYS:HE2 | 30:BH:58:LEU:HB2 | 1.66 | 0.77 |
| 34:BM:60:GLN:H | 34:BM:60:GLN:NE2 | 1.83 | 0.77 |
| 24:BV:72:VAL:HG21 | 24:BV:91:PHE:HB3 | 1.64 | 0.77 |
| 23:DB:532:A:H3' | 38:DQ:27:ARG:HH12 | 1.50 | 0.77 |
| 8:AI:27:ILE:HD12 | 8:AI:34:LEU:HD22 | 1.67 | 0.77 |
| 10:AK:106:ILE:HG13 | 10:AK:107:THR:H | 1.50 | 0.77 |
| 1:CA:1057:G:H4' | 2:CC:196:GLY:H | 1.50 | 0.77 |
| 18:CS:30:LEU:HB2 | 18:CS:48:ILE:HG23 | 1.66 | 0.77 |
| 51:D4:16:ILE:HG12 | 51:D4:25:VAL:HG22 | 1.66 | 0.77 |
| 23:DB:1594:U:H2' | 23:DB:1595:C:C6 | 2.20 | 0.77 |
| 37:DP:88:ARG:HB2 | 37:DP:112:ARG:NH1 | 2.00 | 0.77 |
| 6:AG:74:VAL:HA | 6:AG:87:PRO:HA | 1.67 | 0.77 |
| 22:BA:98:G:H1 | 24:BV:14:LYS:HB2 | 1.50 | 0.77 |
| 43:BW:17:ALA:HA | 43:BW:35:ILE:HG23 | 1.67 | 0.77 |
| 1:CA:1078:U:H4' | 4:CE:137:ARG:NH1 | 2.00 | 0.77 |
| 20:CB:202:ASN:ND2 | 20:CB:204:ASP:H | 1.81 | 0.77 |
| 2:AC:26:LYS:HG3 | 2:AC:27:GLU:HG3 | 1.65 | 0.77 |
| 34:BM:11:LYS:HD3 | 34:BM:86:LYS:HG2 | 1.67 | 0.77 |
| 7:CH:17:GLN:HG2 | 7:CH:62:LEU:HD23 | 1.65 | 0.77 |
| 35:DN:72:ASP:HB3 | 35:DN:75:ILE:HG12 | 1.67 | 0.77 |
| 39:DR:2:TYR:HB2 | 39:DR:42:ALA:HB2 | 1.66 | 0.77 |
| 25:BC:129:LEU:HD22 | 25:BC:134:ILE:HG22 | 1.67 | 0.76 |
| 26:BD:25:THR:HG21 | 26:BD:193:VAL:HG22 | 1.67 | 0.76 |
| 42:BU:42:LYS:HG3 | 42:BU:57:ILE:HG21 | 1.67 | 0.76 |
| 7:AH:103:VAL:HG22 | 7:AH:124:ILE:HA | 1.65 | 0.76 |
| 23:BB:62:U:H3' | 23:BB:63:A:C8 | 2.19 | 0.76 |
| 23:BB:38:A:O2' | 27:BE:43:THR:HA | 1.85 | 0.76 |
| 32:BK:24:VAL:HA | 32:BK:39:ILE:HD12 | 1.67 | 0.76 |
| 1:CA:1160:G:H4' | 20:CB:130:LYS:HB2 | 1.65 | 0.76 |
| 15:CP:25:ARG:H | 15:CP:25:ARG:HD3 | 1.50 | 0.76 |
| 23:DB:1166:G:H2' | 23:DB:1167:C:C6 | 2.21 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DE:58:LYS:HE2 | 27:DE:60:TRP:HD1 | 1.50 | 0.76 |
| 39:DR:7:SER:HB2 | 39:DR:22:LEU:HB3 | 1.68 | 0.76 |
| 28:BF:110:ILE:HA | 28:BF:111:ARG:CZ | 2.15 | 0.76 |
| 8:CI:27:ILE:HD12 | 8:CI:34:LEU:HD22 | 1.67 | 0.76 |
| 14:CO:35:ILE:HD11 | 14:CO:58:MET:HG3 | 1.66 | 0.76 |
| 23:DB:161:A:H3' | 23:DB:162:U:H5'' | 1.67 | 0.76 |
| 1:AA:243:A:H4' | 1:AA:244:U:H5' | 1.67 | 0.76 |
| 27:BE:157:LEU:HG | 27:BE:169:VAL:HG11 | 1.68 | 0.76 |
| 40:BS:70:LYS:HD3 | 40:BS:110:ARG:HA | 1.67 | 0.76 |
| 2:CC:77:GLY:HA3 | 2:CC:81:GLU:HB3 | 1.68 | 0.76 |
| 23:DB:354:A:H2' | 23:DB:355:U:C6 | 2.20 | 0.76 |
| 23:DB:2305:U:H5'' | 28:DF:130:GLY:HA3 | 1.68 | 0.76 |
| 30:DH:31:VAL:O | 30:DH:33:GLN:N | 2.18 | 0.76 |
| 45:BY:54:VAL:HB | 45:BY:56:VAL:HG23 | 1.67 | 0.76 |
| 6:CG:21:LEU:H | 6:CG:21:LEU:HD23 | 1.49 | 0.76 |
| 30:DH:133:GLN:HB3 | 30:DH:139:PHE:HA | 1.67 | 0.76 |
| 31:DJ:29:ALA:HA | 31:DJ:32:LEU:HD12 | 1.67 | 0.76 |
| 20:AB:163:ILE:HG23 | 20:AB:164:ASP:H | 1.49 | 0.76 |
| 23:BB:1082:U:N3 | 23:BB:1086:A:C2 | 2.53 | 0.76 |
| 23:BB:1469:A:H2' | 23:BB:1470:A:C8 | 2.21 | 0.76 |
| 39:BR:2:TYR:HB2 | 39:BR:42:ALA:HB2 | 1.66 | 0.76 |
| 24:BV:75:GLN:HG2 | 24:BV:92:VAL:HG23 | 1.66 | 0.76 |
| 1:CA:1306:A:H61 | 1:CA:1331:G:H1' | 1.50 | 0.76 |
| 1:CA:238:A:H2' | 1:CA:239:U:H5'' | 1.67 | 0.76 |
| 6:CG:14:ASP:HB3 | 6:CG:19:SER:H | 1.51 | 0.76 |
| 23:DB:1019:U:H2' | 23:DB:1020:A:C8 | 2.20 | 0.76 |
| 23:DB:1283:G:N2 | 23:DB:1286:A:H5' | 2.01 | 0.76 |
| 23:DB:3:U:H2' | 23:DB:4:U:C6 | 2.20 | 0.76 |
| 23:DB:62:U:H3' | 23:DB:63:A:C8 | 2.21 | 0.76 |
| 31:DJ:112:GLY:H | 31:DJ:113:PRO:CD | 1.97 | 0.76 |
| 15:AP:3:THR:HG22 | 15:AP:66:THR:HB | 1.68 | 0.76 |
| 23:BB:1166:G:H2' | 23:BB:1167:C:C6 | 2.20 | 0.76 |
| 1:CA:243:A:H4' | 1:CA:244:U:H5' | 1.66 | 0.76 |
| 3:CD:13:ARG:HA | 3:CD:37:PRO:HB3 | 1.67 | 0.76 |
| 8:CI:46:VAL:HA | 8:CI:49:GLN:HG3 | 1.68 | 0.76 |
| 10:CK:106:ILE:HG13 | 10:CK:107:THR:H | 1.51 | 0.76 |
| 48:D1:49:LYS:HG2 | 48:D1:50:GLU:H | 1.51 | 0.76 |
| 37:DP:1:SER:HA | 37:DP:4:ILE:HB | 1.68 | 0.76 |
| 24:DV:79:ARG:HA | 24:DV:86:LEU:HA | 1.68 | 0.76 |
| 23:BB:2653:U:H3' | 23:BB:2654:A:H2' | 1.67 | 0.76 |
| 31:BJ:112:GLY:H | 31:BJ:113:PRO:CD | 1.98 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:423:G:H2' | 1:CA:424:G:O4' | 1.85 | 0.76 |
| 15:CP:52:LEU:HD21 | 15:CP:75:ILE:HG12 | 1.67 | 0.76 |
| 23:DB:1437:C:H2' | 23:DB:1438:U:H6 | 1.49 | 0.76 |
| 32:DK:35:VAL:HG23 | 32:DK:36:GLY:N | 2.01 | 0.76 |
| 23:DB:1248:G:H2' | 38:DQ:2:ARG:HA | 1.67 | 0.76 |
| 2:CC:26:LYS:HG3 | 2:CC:27:GLU:HG3 | 1.68 | 0.76 |
| 19:CT:85:LEU:HD23 | 19:CT:86:ALA:H | 1.51 | 0.76 |
| 23:DB:2021:C:OP1 | 47:D0:8:THR:HG21 | 1.86 | 0.76 |
| 34:DM:78:LEU:HD12 | 34:DM:78:LEU:H | 1.51 | 0.76 |
| 1:AA:410:G:OP2 | 3:AD:25:ARG:HD2 | 1.85 | 0.76 |
| 3:AD:24:VAL:HA | 3:AD:27:ILE:HD11 | 1.66 | 0.76 |
| 21:AU:10:PRO:HB2 | 2:CC:71:ARG:HE | 1.49 | 0.76 |
| 6:CG:2:ARG:HH11 | 6:CG:2:ARG:HB3 | 1.51 | 0.76 |
| 10:CK:22:ILE:HD13 | 10:CK:85:VAL:HG22 | 1.68 | 0.76 |
| 48:D1:33:LEU:HB3 | 48:D1:51:ALA:HB3 | 1.67 | 0.76 |
| 28:DF:168:LEU:HD13 | 28:DF:169:LEU:H | 1.51 | 0.76 |
| 43:DW:37:VAL:HG12 | 43:DW:38:ARG:H | 1.50 | 0.76 |
| 12:AM:2:ARG:HB2 | 12:AM:56:ARG:HH22 | 1.49 | 0.75 |
| 23:BB:2143:C:H2' | 23:BB:2144:G:O4' | 1.87 | 0.75 |
| 25:BC:91:ALA:HB2 | 25:BC:105:ALA:HB2 | 1.68 | 0.75 |
| 43:BW:24:ARG:HD3 | 43:BW:65:LYS:HG2 | 1.68 | 0.75 |
| 23:DB:1099:G:P | 52:DI:4:VAL:H | 2.09 | 0.75 |
| 1:AA:238:A:H2' | 1:AA:239:U:H5'' | 1.65 | 0.75 |
| 23:BB:2328:A:H2' | 23:BB:2329:U:C6 | 2.21 | 0.75 |
| 23:BB:90:U:H3' | 23:BB:91:A:C5' | 2.16 | 0.75 |
| 28:BF:168:LEU:HD13 | 28:BF:169:LEU:H | 1.52 | 0.75 |
| 38:BQ:8:ILE:H | 38:BQ:8:ILE:HD12 | 1.49 | 0.75 |
| 1:CA:437:U:H2' | 1:CA:438:U:O4' | 1.86 | 0.75 |
| 34:DM:21:ALA:HB1 | 34:DM:100:LYS:HE2 | 1.68 | 0.75 |
| 1:AA:1133:G:H2' | 1:AA:1134:G:O4' | 1.87 | 0.75 |
| 8:AI:33:SER:HB3 | 8:AI:36:GLN:HB2 | 1.68 | 0.75 |
| 23:BB:2269:G:H4' | 43:BW:19:ARG:HH12 | 1.50 | 0.75 |
| 1:CA:264:C:H4' | 16:CQ:64:ARG:HD2 | 1.67 | 0.75 |
| 23:DB:742:A:H2' | 23:DB:743:A:C8 | 2.21 | 0.75 |
| 34:DM:11:LYS:HD3 | 34:DM:86:LYS:HG2 | 1.68 | 0.75 |
| 37:DP:13:LYS:HD3 | 37:DP:76:HIS:HA | 1.67 | 0.75 |
| 1:AA:1306:A:H61 | 1:AA:1331:G:H1' | 1.50 | 0.75 |
| 27:BE:130:LYS:HB2 | 27:BE:133:LEU:HG | 1.67 | 0.75 |
| 30:BH:31:VAL:O | 30:BH:33:GLN:N | 2.20 | 0.75 |
| 30:BH:73:ASN:HB3 | 30:BH:141:LYS:HZ1 | 1.52 | 0.75 |
| 39:BR:24:LYS:HA | 39:BR:94:THR:HG23 | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CE:44:ARG:HA | 4:CE:71:ILE:O | 1.87 | 0.75 |
| 23:DB:2010:G:H5'' | 40:DS:42:LYS:HB2 | 1.68 | 0.75 |
| 23:DB:2619:C:H5' | 26:DD:157:LYS:HD3 | 1.69 | 0.75 |
| 28:DF:65:LEU:N | 28:DF:88:VAL:HG22 | 1.99 | 0.75 |
| 32:BK:38:ILE:HD13 | 32:BK:61:VAL:HG12 | 1.66 | 0.75 |
| 34:BM:78:LEU:HD12 | 34:BM:78:LEU:H | 1.50 | 0.75 |
| 1:CA:812:G:O2' | 1:CA:813:U:H6 | 1.70 | 0.75 |
| 3:CD:24:VAL:HA | 3:CD:27:ILE:HD11 | 1.68 | 0.75 |
| 23:DB:1469:A:H2' | 23:DB:1470:A:C8 | 2.21 | 0.75 |
| 42:DU:84:PHE:O | 42:DU:85:ARG:HB2 | 1.86 | 0.75 |
| 2:AC:119:ILE:HG21 | 2:AC:197:VAL:HG11 | 1.69 | 0.75 |
| 36:BO:49:VAL:HG11 | 36:BO:82:ALA:HA | 1.69 | 0.75 |
| 43:BW:66:VAL:HA | 43:BW:81:ILE:HG22 | 1.69 | 0.75 |
| 23:DB:287:G:H2' | 23:DB:288:U:C6 | 2.21 | 0.75 |
| 52:DI:9:LYS:HG2 | 52:DI:57:VAL:HG13 | 1.69 | 0.75 |
| 22:DA:2:G:H2' | 22:DA:3:C:C6 | 2.21 | 0.75 |
| 1:AA:269:C:H2' | 1:AA:270:A:C8 | 2.22 | 0.75 |
| 1:AA:674:G:H2' | 1:AA:675:A:H8 | 1.52 | 0.75 |
| 23:BB:2258:C:H5' | 23:BB:2259:U:H5 | 1.52 | 0.75 |
| 28:BF:65:LEU:N | 28:BF:88:VAL:HG22 | 1.99 | 0.75 |
| 39:BR:60:LYS:H | 39:BR:100:GLY:HA3 | 1.50 | 0.75 |
| 41:BT:28:ASN:HA | 41:BT:91:GLN:HE22 | 1.52 | 0.75 |
| 9:CJ:10:LEU:HD11 | 9:CJ:25:ILE:HD12 | 1.68 | 0.75 |
| 23:DB:2653:U:H3' | 23:DB:2654:A:H2' | 1.69 | 0.75 |
| 27:DE:157:LEU:HG | 27:DE:169:VAL:HG11 | 1.69 | 0.75 |
| 37:DP:20:ARG:HE | 37:DP:91:VAL:HG21 | 1.50 | 0.75 |
| 42:DU:42:LYS:HG3 | 42:DU:57:ILE:HG21 | 1.67 | 0.75 |
| 1:AA:423:G:H2' | 1:AA:424:G:O4' | 1.86 | 0.75 |
| 6:AG:2:ARG:HB3 | 6:AG:3:ARG:HH11 | 1.50 | 0.75 |
| 1:AA:1348:U:H4' | 8:AI:121:ARG:HG3 | 1.69 | 0.75 |
| 29:BG:167:VAL:HG23 | 29:BG:168:VAL:H | 1.51 | 0.75 |
| 39:BR:7:SER:HB2 | 39:BR:22:LEU:HB3 | 1.69 | 0.75 |
| 43:BW:37:VAL:HG12 | 43:BW:38:ARG:H | 1.51 | 0.75 |
| 23:DB:2756:U:H1' | 23:DB:2757:A:H5'' | 1.67 | 0.75 |
| 23:DB:877:A:N6 | 23:DB:898:C:H2' | 2.01 | 0.75 |
| 52:DI:72:THR:HG21 | 52:DI:112:LYS:HA | 1.69 | 0.75 |
| 32:DK:38:ILE:HD13 | 32:DK:61:VAL:HG12 | 1.67 | 0.75 |
| 33:DL:109:LYS:HG2 | 33:DL:126:ARG:HB2 | 1.67 | 0.75 |
| 23:BB:1283:G:N2 | 23:BB:1286:A:H5' | 2.01 | 0.74 |
| 23:BB:161:A:H3' | 23:BB:162:U:H5'' | 1.68 | 0.74 |
| 28:BF:177:ARG:CZ | 28:BF:177:ARG:HA | 2.16 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:979:C:H1' | 1:CA:1317:C:H41 | 1.51 | 0.74 |
| 1:CA:946:A:H2' | 1:CA:947:G:C8 | 2.22 | 0.74 |
| 20:CB:163:ILE:HG23 | 20:CB:164:ASP:H | 1.52 | 0.74 |
| 21:CU:16:ARG:NE | 21:CU:16:ARG:HA | 2.01 | 0.74 |
| 23:DB:1168:G:H2' | 23:DB:1169:A:C8 | 2.22 | 0.74 |
| 23:DB:404:A:H4' | 23:DB:405:U:H5' | 1.69 | 0.74 |
| 28:DF:177:ARG:CZ | 28:DF:177:ARG:HA | 2.16 | 0.74 |
| 25:BC:156:SER:O | 25:BC:194:VAL:HG11 | 1.87 | 0.74 |
| 38:BQ:107:ALA:HB1 | 39:BR:48:LYS:HE2 | 1.67 | 0.74 |
| 1:CA:108:G:H5' | 1:CA:109:A:H5'' | 1.69 | 0.74 |
| 13:CN:68:ARG:HH12 | 13:CN:70:HIS:HB2 | 1.53 | 0.74 |
| 23:DB:856:G:H1' | 43:DW:23:LYS:HB3 | 1.68 | 0.74 |
| 37:DP:7:LEU:H | 37:DP:7:LEU:HD12 | 1.50 | 0.74 |
| 23:BB:2882:A:H4' | 35:BN:97:ILE:HD11 | 1.67 | 0.74 |
| 52:BI:27:LEU:HD12 | 52:BI:32:VAL:HG11 | 1.69 | 0.74 |
| 38:BQ:65:ASN:HD21 | 38:BQ:69:ARG:HH11 | 1.33 | 0.74 |
| 40:BS:66:ILE:HD13 | 40:BS:66:ILE:H | 1.51 | 0.74 |
| 41:BT:76:ARG:NH2 | 41:BT:77:ARG:HB2 | 2.01 | 0.74 |
| 41:BT:82:LYS:HD3 | 41:BT:84:TYR:HE1 | 1.51 | 0.74 |
| 8:AI:99:LYS:HE3 | 9:CJ:80:THR:HA | 1.68 | 0.74 |
| 34:DM:63:ILE:HG23 | 34:DM:105:MET:HG3 | 1.68 | 0.74 |
| 1:AA:1144:G:N2 | 1:AA:1146:A:H62 | 1.84 | 0.74 |
| 1:AA:979:C:H1' | 1:AA:1317:C:H41 | 1.52 | 0.74 |
| 20:AB:59:ILE:H | 20:AB:59:ILE:HD12 | 1.52 | 0.74 |
| 4:AE:105:ILE:HG13 | 4:AE:123:LEU:HA | 1.69 | 0.74 |
| 9:AJ:36:VAL:HG22 | 9:AJ:76:ILE:HG22 | 1.68 | 0.74 |
| 30:BH:116:ARG:HD2 | 30:BH:133:GLN:HB3 | 1.69 | 0.74 |
| 38:BQ:57:ARG:HH11 | 38:BQ:57:ARG:HB3 | 1.52 | 0.74 |
| 9:CJ:36:VAL:HG22 | 9:CJ:76:ILE:HG22 | 1.67 | 0.74 |
| 23:DB:2354:C:H4' | 43:DW:31:LEU:HD23 | 1.67 | 0.74 |
| 23:DB:2901:C:H2' | 23:DB:2902:C:C6 | 2.23 | 0.74 |
| 23:DB:90:U:H3' | 23:DB:91:A:C5' | 2.16 | 0.74 |
| 23:DB:2579:C:O2' | 26:DD:136:ASN:HA | 1.88 | 0.74 |
| 27:DE:130:LYS:HB2 | 27:DE:133:LEU:HG | 1.67 | 0.74 |
| 38:DQ:86:SER:HB3 | 39:DR:51:VAL:HA | 1.68 | 0.74 |
| 41:DT:28:ASN:HA | 41:DT:91:GLN:HE22 | 1.52 | 0.74 |
| 1:AA:1472:U:H2' | 1:AA:1473:G:C8 | 2.23 | 0.74 |
| 2:AC:77:GLY:HA3 | 2:AC:81:GLU:HB3 | 1.69 | 0.74 |
| 3:AD:13:ARG:HA | 3:AD:37:PRO:HB3 | 1.69 | 0.74 |
| 23:BB:2153:C:H2' | 23:BB:2154:A:C8 | 2.23 | 0.74 |
| 23:BB:2185:U:H2' | 23:BB:2186:G:C8 | 2.23 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:591:U:H1' | 50:B3:1:PRO:N | 2.03 | 0.74 |
| 29:BG:26:LYS:HB3 | 29:BG:26:LYS:HZ2 | 1.52 | 0.74 |
| 23:DB:1082:U:N3 | 23:DB:1086:A:C2 | 2.55 | 0.74 |
| 29:DG:148:ARG:HA | 29:DG:161:VAL:HB | 1.70 | 0.74 |
| 29:DG:167:VAL:HG23 | 29:DG:168:VAL:H | 1.51 | 0.74 |
| 52:DI:105:LEU:HD13 | 52:DI:129:GLU:HG2 | 1.68 | 0.74 |
| 40:DS:28:LYS:HD2 | 40:DS:29:VAL:H | 1.52 | 0.74 |
| 2:AC:57:GLU:HB2 | 2:AC:64:ARG:HB2 | 1.68 | 0.74 |
| 10:AK:22:ILE:HG21 | 10:AK:95:THR:HG21 | 1.68 | 0.74 |
| 10:AK:91:GLY:HA2 | 10:AK:94:SER:HB3 | 1.70 | 0.74 |
| 17:AR:38:ILE:H | 17:AR:38:ILE:HD13 | 1.51 | 0.74 |
| 51:B4:16:ILE:HG12 | 51:B4:25:VAL:HG22 | 1.68 | 0.74 |
| 23:BB:2333:A:H4' | 23:BB:2334:U:H5'' | 1.68 | 0.74 |
| 33:BL:109:LYS:HG2 | 33:BL:126:ARG:HB2 | 1.68 | 0.74 |
| 34:BM:63:ILE:HG23 | 34:BM:105:MET:HG3 | 1.69 | 0.74 |
| 1:CA:269:C:H2' | 1:CA:270:A:C8 | 2.23 | 0.74 |
| 1:CA:674:G:H2' | 1:CA:675:A:H8 | 1.50 | 0.74 |
| 4:CE:105:ILE:HG13 | 4:CE:123:LEU:HA | 1.70 | 0.74 |
| 23:DB:2352:A:C6 | 43:DW:30:VAL:HG11 | 2.21 | 0.74 |
| 23:DB:2376:A:H1' | 36:DO:111:ARG:HH22 | 1.52 | 0.74 |
| 29:DG:126:THR:HB | 29:DG:129:GLU:HG3 | 1.68 | 0.74 |
| 31:DJ:77:HIS:HD2 | 31:DJ:84:ILE:H | 1.36 | 0.74 |
| 24:DV:63:ILE:HB | 24:DV:70:ILE:HD11 | 1.70 | 0.74 |
| 45:DY:54:VAL:HB | 45:DY:56:VAL:HG23 | 1.68 | 0.74 |
| 19:AT:38:ILE:HD11 | 19:AT:82:ILE:HG22 | 1.68 | 0.74 |
| 22:BA:75:G:H1 | 22:BA:102:G:H22 | 1.34 | 0.74 |
| 23:BB:608:A:H2' | 23:BB:609:A:C8 | 2.22 | 0.74 |
| 25:BC:35:LYS:HG2 | 25:BC:36:ASN:H | 1.52 | 0.74 |
| 26:BD:51:THR:HG22 | 26:BD:52:THR:H | 1.51 | 0.74 |
| 23:DB:2748:A:H1' | 29:DG:66:THR:HB | 1.69 | 0.74 |
| 20:AB:202:ASN:ND2 | 20:AB:204:ASP:H | 1.84 | 0.74 |
| 9:AJ:51:VAL:HG23 | 13:AN:80:ARG:HB2 | 1.69 | 0.74 |
| 43:BW:39:GLN:HG3 | 43:BW:42:THR:HB | 1.70 | 0.74 |
| 45:BY:23:LEU:HD13 | 45:BY:28:LEU:HB2 | 1.70 | 0.74 |
| 20:CB:61:SER:HB2 | 20:CB:62:ARG:HH11 | 1.52 | 0.74 |
| 9:CJ:51:VAL:HG23 | 13:CN:80:ARG:HB2 | 1.69 | 0.74 |
| 10:CK:20:ALA:HB2 | 10:CK:81:LEU:HD12 | 1.70 | 0.74 |
| 10:CK:22:ILE:HG21 | 10:CK:95:THR:HG21 | 1.69 | 0.74 |
| 17:CR:38:ILE:H | 17:CR:38:ILE:HD13 | 1.51 | 0.74 |
| 19:CT:43:LYS:HE2 | 19:CT:44:ALA:H | 1.50 | 0.74 |
| 23:DB:1301:A:O2' | 23:DB:1302:A:H3' | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:224:U:O4 | 23:DB:420:C:H5' | 1.88 | 0.74 |
| 30:DH:54:LEU:HD23 | 30:DH:58:LEU:HD12 | 1.70 | 0.74 |
| 42:DU:81:ARG:HH21 | 42:DU:81:ARG:N | 1.86 | 0.74 |
| 43:DW:51:GLY:CA | 43:DW:59:PHE:HB2 | 2.17 | 0.74 |
| 15:AP:25:ARG:HD3 | 15:AP:25:ARG:H | 1.53 | 0.74 |
| 25:BC:64:VAL:O | 25:BC:65:ASP:HB3 | 1.88 | 0.74 |
| 1:CA:410:G:OP2 | 3:CD:25:ARG:HD2 | 1.88 | 0.74 |
| 19:CT:47:GLN:HG2 | 19:CT:82:ILE:HD12 | 1.70 | 0.74 |
| 23:DB:1097:U:H2' | 23:DB:1098:A:O4' | 1.87 | 0.74 |
| 23:DB:571:U:H3' | 39:DR:80:ARG:NH1 | 2.03 | 0.74 |
| 26:DD:25:THR:HG21 | 26:DD:193:VAL:HG22 | 1.68 | 0.74 |
| 26:DD:51:THR:HG22 | 26:DD:52:THR:H | 1.53 | 0.74 |
| 23:BB:2834:G:H1' | 23:BB:2883:A:N6 | 2.02 | 0.74 |
| 23:BB:404:A:H4' | 23:BB:405:U:H5' | 1.68 | 0.74 |
| 28:BF:126:ASN:HB3 | 28:BF:156:THR:HA | 1.70 | 0.74 |
| 52:BI:77:VAL:HA | 52:BI:80:LYS:HE2 | 1.70 | 0.74 |
| 31:BJ:29:ALA:HA | 31:BJ:32:LEU:HD12 | 1.69 | 0.74 |
| 29:DG:148:ARG:HD3 | 29:DG:152:ARG:CZ | 2.17 | 0.74 |
| 23:DB:1454:C:H5' | 35:DN:63:ARG:HE | 1.53 | 0.74 |
| 38:DQ:27:ARG:HG2 | 38:DQ:37:ALA:HB2 | 1.69 | 0.74 |
| 45:DY:6:ILE:HA | 45:DY:56:VAL:HG22 | 1.70 | 0.74 |
| 23:BB:1287:A:OP1 | 35:BN:104:ALA:HB3 | 1.88 | 0.73 |
| 23:BB:1451:C:H4' | 23:BB:1452:G:H5' | 1.68 | 0.73 |
| 23:BB:479:A:N3 | 23:BB:481:G:H5'' | 2.03 | 0.73 |
| 35:BN:33:ILE:HG22 | 35:BN:114:GLU:HB2 | 1.69 | 0.73 |
| 6:CG:74:VAL:HA | 6:CG:87:PRO:HA | 1.70 | 0.73 |
| 23:DB:2393:U:H5'' | 33:DL:62:PRO:HG3 | 1.70 | 0.73 |
| 31:DJ:6:ALA:HB3 | 31:DJ:45:THR:HG21 | 1.70 | 0.73 |
| 3:AD:137:SER:HB2 | 3:AD:138:PRO:HD2 | 1.70 | 0.73 |
| 47:B0:32:THR:OG1 | 47:B0:50:GLY:HA2 | 1.88 | 0.73 |
| 23:BB:1019:U:H2' | 23:BB:1020:A:C8 | 2.23 | 0.73 |
| 28:BF:48:LEU:H | 28:BF:48:LEU:HD23 | 1.53 | 0.73 |
| 29:BG:37:ASN:HD22 | 29:BG:40:VAL:HB | 1.53 | 0.73 |
| 31:BJ:124:VAL:HG23 | 31:BJ:125:TYR:H | 1.52 | 0.73 |
| 35:BN:116:VAL:O | 35:BN:117:ASP:HB3 | 1.88 | 0.73 |
| 37:BP:91:VAL:HG23 | 37:BP:92:ARG:H | 1.52 | 0.73 |
| 42:BU:84:PHE:O | 42:BU:85:ARG:HB2 | 1.88 | 0.73 |
| 2:CC:57:GLU:HB2 | 2:CC:64:ARG:HB2 | 1.69 | 0.73 |
| 23:DB:143:C:H2' | 23:DB:144:A:H8 | 1.52 | 0.73 |
| 23:DB:1868:C:H2' | 23:DB:1869:G:O4' | 1.88 | 0.73 |
| 23:DB:2769:U:H2' | 23:DB:2770:G:C8 | 2.23 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:743:A:O2' | 23:DB:744:U:H5' | 1.88 | 0.73 |
| 28:DF:48:LEU:HD23 | 28:DF:48:LEU:H | 1.52 | 0.73 |
| 35:DN:33:ILE:HG22 | 35:DN:114:GLU:HB2 | 1.69 | 0.73 |
| 38:DQ:8:ILE:HD12 | 38:DQ:8:ILE:H | 1.51 | 0.73 |
| 24:DV:9:ARG:HH22 | 24:DV:12:GLN:HA | 1.54 | 0.73 |
| 1:AA:1472:U:H2' | 1:AA:1473:G:H8 | 1.51 | 0.73 |
| 1:AA:842:U:H3' | 1:AA:843:U:H4' | 1.68 | 0.73 |
| 4:AE:44:ARG:HA | 4:AE:71:ILE:O | 1.88 | 0.73 |
| 8:AI:46:VAL:HA | 8:AI:49:GLN:HG3 | 1.70 | 0.73 |
| 9:AJ:10:LEU:HD11 | 9:AJ:25:ILE:HD12 | 1.68 | 0.73 |
| 1:AA:1220:G:H3' | 18:AS:36:ARG:HH21 | 1.53 | 0.73 |
| 23:BB:2109:U:H2' | 23:BB:2110:G:H5' | 1.70 | 0.73 |
| 23:BB:616:A:H3' | 23:BB:617:G:H8 | 1.53 | 0.73 |
| 26:BD:114:LYS:NZ | 26:BD:116:LYS:HZ2 | 1.83 | 0.73 |
| 1:CA:1323:G:H2' | 1:CA:1324:A:H8 | 1.54 | 0.73 |
| 19:CT:38:ILE:HD11 | 19:CT:82:ILE:HG22 | 1.68 | 0.73 |
| 23:DB:1925:C:H2' | 23:DB:1926:U:H5'' | 1.68 | 0.73 |
| 25:DC:156:SER:O | 25:DC:194:VAL:HG11 | 1.89 | 0.73 |
| 28:DF:72:SER:HA | 28:DF:80:GLN:H | 1.53 | 0.73 |
| 23:DB:171:U:H2' | 23:DB:172:A:C8 | 2.23 | 0.73 |
| 23:DB:2258:C:H5' | 23:DB:2259:U:H5 | 1.54 | 0.73 |
| 23:DB:2333:A:H4' | 23:DB:2334:U:H5'' | 1.69 | 0.73 |
| 28:DF:62:GLN:NE2 | 28:DF:90:LEU:HD13 | 2.03 | 0.73 |
| 38:DQ:65:ASN:HB2 | 38:DQ:75:TYR:HB2 | 1.70 | 0.73 |
| 43:DW:49:ASN:HB3 | 43:DW:81:ILE:HD11 | 1.69 | 0.73 |
| 43:DW:66:VAL:HA | 43:DW:81:ILE:HG22 | 1.70 | 0.73 |
| 46:DZ:64:ILE:HD12 | 46:DZ:64:ILE:H | 1.51 | 0.73 |
| 23:BB:2241:A:H2' | 23:BB:2242:G:C8 | 2.22 | 0.73 |
| 34:BM:34:LYS:HE2 | 34:BM:99:GLY:HA2 | 1.70 | 0.73 |
| 23:BB:532:A:H3' | 38:BQ:27:ARG:HH12 | 1.53 | 0.73 |
| 42:BU:81:ARG:N | 42:BU:81:ARG:HH21 | 1.87 | 0.73 |
| 13:CN:52:ARG:HH11 | 13:CN:58:ARG:HH21 | 1.37 | 0.73 |
| 23:DB:580:U:H2' | 23:DB:581:C:H6 | 1.54 | 0.73 |
| 25:DC:64:VAL:O | 25:DC:65:ASP:HB3 | 1.86 | 0.73 |
| 30:DH:94:ILE:O | 30:DH:122:LEU:HB2 | 1.88 | 0.73 |
| 13:AN:52:ARG:HH11 | 13:AN:58:ARG:HH21 | 1.36 | 0.73 |
| 21:AU:43:GLU:HG3 | 21:AU:44:ARG:HH21 | 1.54 | 0.73 |
| 23:BB:362:A:H3' | 23:BB:363:G:H8 | 1.54 | 0.73 |
| 30:BH:81:ALA:HA | 30:BH:146:VAL:HA | 1.70 | 0.73 |
| 1:CA:842:U:H3' | 1:CA:843:U:H4' | 1.69 | 0.73 |
| 13:CN:50:LEU:H | 13:CN:51:PRO:HD2 | 1.53 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:547:A:H2' | 23:BB:548:G:H5' | 1.71 | 0.73 |
| 24:BV:9:ARG:HH22 | 24:BV:12:GLN:HA | 1.54 | 0.73 |
| 46:BZ:64:ILE:H | 46:BZ:64:ILE:HD12 | 1.53 | 0.73 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:C8 | 2.23 | 0.73 |
| 23:DB:1080:A:H2' | 23:DB:1081:U:H6 | 1.52 | 0.73 |
| 23:DB:38:A:O2' | 27:DE:43:THR:HA | 1.89 | 0.73 |
| 25:DC:91:ALA:HB2 | 25:DC:105:ALA:HB2 | 1.71 | 0.73 |
| 32:DK:19:VAL:HG12 | 32:DK:41:ILE:HG12 | 1.70 | 0.73 |
| 38:DQ:43:GLN:NE2 | 39:DR:77:PHE:HB3 | 2.03 | 0.73 |
| 40:DS:70:LYS:HD3 | 40:DS:110:ARG:HA | 1.69 | 0.73 |
| 14:AO:7:THR:O | 14:AO:10:ILE:HG22 | 1.88 | 0.73 |
| 12:AM:92:ARG:HH12 | 18:AS:79:TYR:HD2 | 1.37 | 0.73 |
| 23:BB:125:A:H3' | 23:BB:126:A:H5'' | 1.71 | 0.73 |
| 23:BB:2292:U:H2' | 23:BB:2293:G:H8 | 1.52 | 0.73 |
| 28:BF:72:SER:HA | 28:BF:80:GLN:H | 1.52 | 0.73 |
| 34:BM:40:ARG:HB2 | 34:BM:93:VAL:HG22 | 1.70 | 0.73 |
| 1:CA:1026:G:H2' | 1:CA:1027:C:H6 | 1.54 | 0.73 |
| 1:CA:957:U:H4' | 18:CS:78:THR:HB | 1.70 | 0.73 |
| 20:CB:19:THR:HA | 20:CB:37:VAL:HA | 1.70 | 0.73 |
| 20:CB:61:SER:HB2 | 20:CB:62:ARG:NH1 | 2.03 | 0.73 |
| 23:DB:580:U:H2' | 23:DB:581:C:C6 | 2.24 | 0.73 |
| 23:DB:836:G:H2' | 23:DB:837:C:C6 | 2.23 | 0.73 |
| 28:DF:8:LYS:HA | 28:DF:12:VAL:HG21 | 1.71 | 0.73 |
| 29:DG:37:ASN:HD22 | 29:DG:40:VAL:HB | 1.53 | 0.73 |
| 23:DB:2264:C:H41 | 43:DW:11:ASN:HD21 | 1.36 | 0.73 |
| 44:DX:3:ALA:HA | 44:DX:6:LEU:HD23 | 1.71 | 0.73 |
| 19:AT:47:GLN:HG2 | 19:AT:82:ILE:HD12 | 1.70 | 0.73 |
| 26:BD:24:VAL:HG21 | 26:BD:188:LEU:HB3 | 1.70 | 0.73 |
| 32:BK:15:GLY:HA3 | 32:BK:52:VAL:HG23 | 1.70 | 0.73 |
| 35:BN:72:ASP:HB3 | 35:BN:75:ILE:HG12 | 1.69 | 0.73 |
| 38:BQ:27:ARG:HG2 | 38:BQ:37:ALA:HB2 | 1.71 | 0.73 |
| 40:BS:15:GLN:HA | 40:BS:18:ARG:HG2 | 1.71 | 0.73 |
| 24:BV:79:ARG:HA | 24:BV:86:LEU:HA | 1.69 | 0.73 |
| 43:BW:23:LYS:HD2 | 43:BW:24:ARG:HB3 | 1.69 | 0.73 |
| 45:BY:6:ILE:HA | 45:BY:56:VAL:HG22 | 1.71 | 0.73 |
| 12:CM:19:THR:HA | 12:CM:24:VAL:HG23 | 1.69 | 0.73 |
| 14:CO:7:THR:O | 14:CO:10:ILE:HG22 | 1.88 | 0.73 |
| 23:DB:1098:A:H2' | 52:DI:4:VAL:N | 2.02 | 0.73 |
| 28:DF:126:ASN:HB3 | 28:DF:156:THR:HA | 1.70 | 0.73 |
| 29:DG:157:LYS:HB3 | 29:DG:159:LYS:HG3 | 1.71 | 0.73 |
| 38:DQ:65:ASN:HD21 | 38:DQ:69:ARG:HH11 | 1.35 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:84:U:O2 | 1:AA:84:U:H2' | 1.88 | 0.73 |
| 21:AU:36:PHE:CB | 21:AU:40:PRO:HD3 | 2.19 | 0.73 |
| 28:BF:62:GLN:NE2 | 28:BF:90:LEU:HD13 | 2.04 | 0.73 |
| 29:BG:148:ARG:HD3 | 29:BG:152:ARG:CZ | 2.19 | 0.73 |
| 40:BS:28:LYS:HD2 | 40:BS:29:VAL:H | 1.53 | 0.73 |
| 40:BS:30:SER:HA | 40:BS:33:LEU:HD12 | 1.71 | 0.73 |
| 1:CA:1320:C:H41 | 18:CS:36:ARG:HG2 | 1.54 | 0.73 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.24 | 0.73 |
| 9:CJ:12:ALA:HB2 | 9:CJ:96:VAL:HG12 | 1.69 | 0.73 |
| 12:CM:89:ARG:HH22 | 12:CM:94:LEU:HD12 | 1.54 | 0.73 |
| 23:DB:2243:U:H2' | 23:DB:2244:U:C6 | 2.24 | 0.73 |
| 23:DB:30:G:H2' | 23:DB:31:C:C6 | 2.24 | 0.73 |
| 30:DH:67:ALA:O | 30:DH:70:GLU:HG3 | 1.89 | 0.73 |
| 52:DI:55:PRO:HD3 | 52:DI:74:PRO:HD3 | 1.69 | 0.73 |
| 31:DJ:124:VAL:HG23 | 31:DJ:125:TYR:H | 1.54 | 0.73 |
| 34:DM:40:ARG:HB2 | 34:DM:93:VAL:HG22 | 1.69 | 0.73 |
| 35:DN:116:VAL:O | 35:DN:117:ASP:HB3 | 1.87 | 0.73 |
| 6:AG:3:ARG:HD3 | 6:AG:3:ARG:N | 2.03 | 0.72 |
| 8:AI:126:PHE:HE1 | 8:AI:129:ARG:HD3 | 1.54 | 0.72 |
| 48:B1:49:LYS:HG2 | 48:B1:50:GLU:H | 1.53 | 0.72 |
| 28:BF:128:SER:HB3 | 28:BF:154:THR:HG23 | 1.70 | 0.72 |
| 32:BK:99:ILE:HB | 32:BK:118:LEU:HD22 | 1.71 | 0.72 |
| 37:BP:1:SER:HA | 37:BP:4:ILE:HB | 1.69 | 0.72 |
| 4:CE:104:ILE:HG23 | 4:CE:111:ARG:HH12 | 1.53 | 0.72 |
| 6:CG:110:ARG:HD2 | 6:CG:122:GLU:HB2 | 1.70 | 0.72 |
| 11:CL:37:TYR:HB2 | 11:CL:51:VAL:HB | 1.71 | 0.72 |
| 23:DB:140:C:OP1 | 41:DT:2:ILE:HG23 | 1.88 | 0.72 |
| 25:DC:129:LEU:HD23 | 25:DC:130:PRO:HD2 | 1.71 | 0.72 |
| 40:DS:66:ILE:H | 40:DS:66:ILE:HD13 | 1.54 | 0.72 |
| 20:AB:61:SER:HB2 | 20:AB:62:ARG:HH11 | 1.53 | 0.72 |
| 6:AG:110:ARG:HD2 | 6:AG:122:GLU:HB2 | 1.69 | 0.72 |
| 23:BB:2867:G:H2' | 23:BB:2867:G:N3 | 2.04 | 0.72 |
| 1:CA:337:G:H2' | 1:CA:338:A:C8 | 2.24 | 0.72 |
| 20:CB:15:PHE:HA | 20:CB:42:LEU:HD21 | 1.71 | 0.72 |
| 36:DO:49:VAL:HG11 | 36:DO:82:ALA:HA | 1.71 | 0.72 |
| 41:DT:82:LYS:HD3 | 41:DT:84:TYR:HE1 | 1.52 | 0.72 |
| 5:AF:64:VAL:HG12 | 5:AF:65:GLU:H | 1.52 | 0.72 |
| 7:AH:74:ILE:HG13 | 7:AH:128:VAL:HG22 | 1.72 | 0.72 |
| 21:AU:16:ARG:HE | 21:AU:16:ARG:CA | 2.01 | 0.72 |
| 27:BE:108:ILE:HG13 | 33:BL:2:ARG:NH2 | 2.04 | 0.72 |
| 34:BM:66:ARG:CZ | 34:BM:101:VAL:HG11 | 2.18 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:812:C:H4' | 38:BQ:12:ARG:HH22 | 1.54 | 0.72 |
| 41:BT:73:ARG:HA | 41:BT:73:ARG:HH21 | 1.54 | 0.72 |
| 43:BW:51:GLY:CA | 43:BW:59:PHE:HB2 | 2.20 | 0.72 |
| 1:CA:859:G:H2' | 1:CA:860:A:C8 | 2.23 | 0.72 |
| 9:CJ:8:ILE:HG13 | 9:CJ:100:ILE:HG22 | 1.71 | 0.72 |
| 13:CN:63:CYS:HB2 | 13:CN:79:SER:HB3 | 1.71 | 0.72 |
| 25:DC:196:ASN:ND2 | 25:DC:199:HIS:HB2 | 2.04 | 0.72 |
| 29:DG:166:GLU:HG2 | 29:DG:168:VAL:HG23 | 1.71 | 0.72 |
| 34:DM:34:LYS:HE2 | 34:DM:99:GLY:HA2 | 1.70 | 0.72 |
| 35:DN:17:ARG:HA | 35:DN:20:MET:HB3 | 1.70 | 0.72 |
| 38:DQ:68:ALA:HB1 | 38:DQ:73:ILE:HG23 | 1.71 | 0.72 |
| 24:DV:62:THR:HA | 24:DV:71:LYS:HA | 1.71 | 0.72 |
| 24:DV:44:HIS:CE1 | 24:DV:86:LEU:H | 2.07 | 0.72 |
| 1:AA:1118:U:H2' | 1:AA:1119:C:C6 | 2.24 | 0.72 |
| 1:AA:1320:C:H41 | 18:AS:36:ARG:HG2 | 1.53 | 0.72 |
| 2:AC:149:LYS:HB3 | 2:AC:200:TRP:HB2 | 1.71 | 0.72 |
| 2:AC:156:LEU:HD12 | 2:AC:163:ARG:HD2 | 1.70 | 0.72 |
| 12:AM:67:ASP:O | 12:AM:71:GLU:HB2 | 1.89 | 0.72 |
| 13:AN:30:ILE:HB | 13:AN:44:VAL:HG11 | 1.71 | 0.72 |
| 18:AS:30:LEU:HB2 | 18:AS:48:ILE:HG23 | 1.72 | 0.72 |
| 23:BB:329:G:H22 | 42:BU:16:LYS:HE3 | 1.54 | 0.72 |
| 27:BE:58:LYS:HE2 | 27:BE:60:TRP:HD1 | 1.53 | 0.72 |
| 30:BH:73:ASN:HB3 | 30:BH:141:LYS:NZ | 2.04 | 0.72 |
| 32:BK:35:VAL:HG23 | 32:BK:36:GLY:N | 2.03 | 0.72 |
| 1:CA:1472:U:H2' | 1:CA:1473:G:C8 | 2.25 | 0.72 |
| 37:DP:91:VAL:HG23 | 37:DP:92:ARG:H | 1.53 | 0.72 |
| 38:DQ:107:ALA:HB1 | 39:DR:48:LYS:HE2 | 1.71 | 0.72 |
| 23:DB:992:C:H4' | 39:DR:74:ILE:HD13 | 1.71 | 0.72 |
| 24:DV:62:THR:HG22 | 24:DV:71:LYS:HG2 | 1.71 | 0.72 |
| 23:DB:2386:A:C2 | 43:DW:38:ARG:HB3 | 2.24 | 0.72 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.24 | 0.72 |
| 20:AB:120:SER:HA | 20:AB:125:PHE:CG | 2.25 | 0.72 |
| 23:BB:1105:U:H2' | 23:BB:1106:G:C8 | 2.24 | 0.72 |
| 23:BB:1301:A:O2' | 23:BB:1302:A:H3' | 1.89 | 0.72 |
| 23:BB:191:A:H2' | 23:BB:192:C:C6 | 2.24 | 0.72 |
| 23:BB:856:G:C1' | 43:BW:23:LYS:HB3 | 2.20 | 0.72 |
| 20:CB:66:ILE:HD13 | 20:CB:159:ALA:HB3 | 1.71 | 0.72 |
| 21:CU:36:PHE:CB | 21:CU:40:PRO:HD3 | 2.19 | 0.72 |
| 23:DB:1168:G:H2' | 23:DB:1169:A:H8 | 1.53 | 0.72 |
| 23:DB:2292:U:H2' | 23:DB:2293:G:H8 | 1.52 | 0.72 |
| 23:DB:616:A:H3' | 23:DB:617:G:H8 | 1.54 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:855:G:N2 | 43:DW:23:LYS:HG2 | 2.05 | 0.72 |
| 23:DB:878:A:N3 | 23:DB:878:A:H2' | 2.04 | 0.72 |
| 26:DD:69:ALA:HA | 26:DD:73:VAL:HB | 1.72 | 0.72 |
| 28:DF:110:ILE:HA | 28:DF:111:ARG:CZ | 2.18 | 0.72 |
| 30:DH:63:ALA:HA | 30:DH:66:ASN:HD22 | 1.52 | 0.72 |
| 42:DU:24:VAL:HA | 42:DU:35:VAL:HA | 1.72 | 0.72 |
| 1:AA:1292:G:H2' | 1:AA:1293:C:C6 | 2.25 | 0.72 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.24 | 0.72 |
| 9:AJ:8:ILE:HG13 | 9:AJ:100:ILE:HG22 | 1.72 | 0.72 |
| 10:AK:20:ALA:HB2 | 10:AK:81:LEU:HD12 | 1.71 | 0.72 |
| 12:AM:10:ASP:HA | 12:AM:44:ILE:HD13 | 1.70 | 0.72 |
| 23:BB:2353:G:H1' | 43:BW:30:VAL:CG1 | 2.18 | 0.72 |
| 23:BB:743:A:O2' | 23:BB:744:U:H5' | 1.89 | 0.72 |
| 26:BD:69:ALA:HA | 26:BD:73:VAL:HB | 1.71 | 0.72 |
| 32:BK:17:ARG:HB3 | 32:BK:45:GLU:HG3 | 1.71 | 0.72 |
| 1:CA:193:C:H2' | 1:CA:194:C:C6 | 2.25 | 0.72 |
| 20:CB:99:MET:HA | 20:CB:106:VAL:HG21 | 1.72 | 0.72 |
| 2:CC:149:LYS:HB3 | 2:CC:200:TRP:HB2 | 1.72 | 0.72 |
| 1:CA:1348:U:H4' | 8:CI:121:ARG:HG3 | 1.70 | 0.72 |
| 23:DB:28:A:H61 | 23:DB:512:G:H1' | 1.55 | 0.72 |
| 52:DI:20:SER:HB3 | 52:DI:21:PRO:HD3 | 1.69 | 0.72 |
| 32:DK:15:GLY:HA3 | 32:DK:52:VAL:HG23 | 1.70 | 0.72 |
| 37:DP:85:VAL:HG21 | 37:DP:88:ARG:HH11 | 1.52 | 0.72 |
| 48:B1:46:VAL:HG22 | 48:B1:47:ILE:H | 1.52 | 0.72 |
| 23:BB:2591:C:H2' | 23:BB:2592:G:C8 | 2.25 | 0.72 |
| 25:BC:129:LEU:HD23 | 25:BC:130:PRO:HD2 | 1.71 | 0.72 |
| 1:CA:279:A:H5'' | 1:CA:280:C:H3' | 1.71 | 0.72 |
| 23:DB:1412:U:H2' | 23:DB:1413:A:H8 | 1.55 | 0.72 |
| 30:DH:83:LYS:HG3 | 30:DH:149:GLU:HG2 | 1.69 | 0.72 |
| 32:DK:99:ILE:HB | 32:DK:118:LEU:HD22 | 1.71 | 0.72 |
| 2:AC:16:PRO:HG2 | 2:AC:53:ARG:HH12 | 1.54 | 0.72 |
| 23:BB:2794:C:H2' | 23:BB:2795:C:C6 | 2.24 | 0.72 |
| 25:BC:81:GLU:HB2 | 25:BC:90:ILE:HG22 | 1.70 | 0.72 |
| 1:CA:1004:A:H3' | 1:CA:1024:G:H22 | 1.53 | 0.72 |
| 20:CB:59:ILE:HD12 | 20:CB:59:ILE:H | 1.54 | 0.72 |
| 23:DB:1060:U:C4 | 23:DB:1088:A:N6 | 2.58 | 0.72 |
| 23:DB:2241:A:H2' | 23:DB:2242:G:C8 | 2.25 | 0.72 |
| 23:DB:2800:A:N3 | 23:DB:2801:G:H1' | 2.05 | 0.72 |
| 23:DB:2834:G:H1' | 23:DB:2883:A:N6 | 2.04 | 0.72 |
| 30:DH:122:LEU:HD11 | 30:DH:130:VAL:HG21 | 1.70 | 0.72 |
| 40:DS:30:SER:HA | 40:DS:33:LEU:HD12 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AI:25:GLY:HA2 | 8:AI:60:LEU:O | 1.90 | 0.72 |
| 23:BB:141:G:O6 | 41:BT:2:ILE:HD12 | 1.90 | 0.72 |
| 23:BB:2331:G:H21 | 23:BB:2336:A:H8 | 1.37 | 0.72 |
| 23:BB:2886:A:H3' | 23:BB:2887:A:H8 | 1.55 | 0.72 |
| 23:BB:28:A:H61 | 23:BB:512:G:H1' | 1.54 | 0.72 |
| 34:BM:19:GLY:HA2 | 34:BM:98:PRO:HD2 | 1.72 | 0.72 |
| 1:CA:1133:G:H2' | 1:CA:1134:G:O4' | 1.89 | 0.72 |
| 23:DB:1099:G:O4' | 52:DI:3:LYS:C | 2.27 | 0.72 |
| 23:DB:1274:A:N3 | 23:DB:1297:C:H1' | 2.05 | 0.72 |
| 23:DB:191:A:H2' | 23:DB:192:C:C6 | 2.24 | 0.72 |
| 25:DC:129:LEU:HD22 | 25:DC:134:ILE:HG22 | 1.70 | 0.72 |
| 28:DF:126:ASN:HA | 28:DF:157:THR:HG22 | 1.72 | 0.72 |
| 38:DQ:91:ARG:HH12 | 39:DR:10:LYS:HB3 | 1.55 | 0.72 |
| 7:AH:17:GLN:HG2 | 7:AH:62:LEU:HD23 | 1.70 | 0.72 |
| 23:BB:2091:C:H1' | 46:BZ:34:HIS:CD2 | 2.25 | 0.72 |
| 23:BB:571:U:H3' | 39:BR:80:ARG:NH1 | 2.05 | 0.72 |
| 24:BV:21:ARG:HE | 24:BV:87:GLN:HB3 | 1.55 | 0.72 |
| 43:BW:49:ASN:HB3 | 43:BW:81:ILE:HD11 | 1.72 | 0.72 |
| 43:BW:43:LYS:HD2 | 43:BW:79:ILE:HD11 | 1.71 | 0.72 |
| 1:CA:1292:G:H2' | 1:CA:1293:C:C6 | 2.25 | 0.72 |
| 1:CA:462:G:H5' | 1:CA:463:U:OP2 | 1.90 | 0.72 |
| 2:CC:104:GLU:HG2 | 2:CC:105:VAL:H | 1.53 | 0.72 |
| 4:CE:76:ASN:HB2 | 4:CE:81:GLN:NE2 | 2.05 | 0.72 |
| 20:AB:66:ILE:HD13 | 20:AB:159:ALA:HB3 | 1.72 | 0.71 |
| 6:AG:87:PRO:HG2 | 6:AG:151:ALA:HB2 | 1.69 | 0.71 |
| 15:AP:28:ARG:CD | 15:AP:29:ASN:H | 2.03 | 0.71 |
| 48:B1:32:LYS:HA | 48:B1:51:ALA:O | 1.90 | 0.71 |
| 23:BB:1868:C:H2' | 23:BB:1869:G:O4' | 1.89 | 0.71 |
| 28:BF:8:LYS:HA | 28:BF:12:VAL:HG21 | 1.72 | 0.71 |
| 52:BI:106:GLN:O | 52:BI:110:GLN:HG3 | 1.90 | 0.71 |
| 32:BK:19:VAL:HG12 | 32:BK:41:ILE:HG12 | 1.73 | 0.71 |
| 24:BV:63:ILE:HB | 24:BV:70:ILE:HD11 | 1.72 | 0.71 |
| 8:CI:33:SER:HB3 | 8:CI:36:GLN:HB2 | 1.72 | 0.71 |
| 23:DB:1464:G:H2' | 23:DB:1465:G:H8 | 1.53 | 0.71 |
| 35:DN:83:LEU:HA | 35:DN:86:ARG:HG3 | 1.70 | 0.71 |
| 41:DT:73:ARG:HH21 | 41:DT:73:ARG:HA | 1.55 | 0.71 |
| 38:BQ:104:ALA:HA | 39:BR:46:GLU:CD | 2.10 | 0.71 |
| 38:BQ:68:ALA:HB1 | 38:BQ:73:ILE:HG23 | 1.71 | 0.71 |
| 31:DJ:112:GLY:N | 31:DJ:113:PRO:HD2 | 2.04 | 0.71 |
| 34:DM:19:GLY:HA2 | 34:DM:98:PRO:HD2 | 1.73 | 0.71 |
| 1:AA:337:G:H2' | 1:AA:338:A:C8 | 2.26 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:408:A:OP1 | 3:AD:111:ALA:HB3 | 1.90 | 0.71 |
| 1:AA:764:C:H2' | 1:AA:765:G:H5' | 1.71 | 0.71 |
| 13:AN:68:ARG:HH12 | 13:AN:70:HIS:HB2 | 1.53 | 0.71 |
| 23:BB:1056:G:H1' | 23:BB:1103:A:N6 | 2.06 | 0.71 |
| 23:BB:1354:A:H2' | 23:BB:1355:G:O4' | 1.90 | 0.71 |
| 23:BB:181:A:H2' | 23:BB:182:A:C8 | 2.24 | 0.71 |
| 23:BB:2146:C:H1' | 23:BB:2147:A:H5' | 1.71 | 0.71 |
| 23:BB:2153:C:H2' | 23:BB:2154:A:H8 | 1.53 | 0.71 |
| 23:BB:2749:A:H3' | 23:BB:2750:A:H5'' | 1.71 | 0.71 |
| 23:BB:62:U:H3' | 23:BB:63:A:H8 | 1.54 | 0.71 |
| 29:BG:166:GLU:HG2 | 29:BG:168:VAL:HG23 | 1.71 | 0.71 |
| 52:BI:20:SER:HB3 | 52:BI:21:PRO:HD3 | 1.71 | 0.71 |
| 37:BP:88:ARG:HB2 | 37:BP:112:ARG:NH1 | 2.03 | 0.71 |
| 41:BT:32:LEU:H | 41:BT:83:ALA:HB3 | 1.55 | 0.71 |
| 24:BV:62:THR:HA | 24:BV:71:LYS:HA | 1.72 | 0.71 |
| 1:CA:1142:G:H2' | 1:CA:1143:G:O4' | 1.90 | 0.71 |
| 1:CA:882:C:O2' | 1:CA:883:C:H5' | 1.91 | 0.71 |
| 1:CA:408:A:OP1 | 3:CD:111:ALA:HB3 | 1.90 | 0.71 |
| 23:DB:2591:C:H2' | 23:DB:2592:G:C8 | 2.25 | 0.71 |
| 23:DB:2867:G:N3 | 23:DB:2867:G:H2' | 2.04 | 0.71 |
| 25:DC:43:ASN:ND2 | 25:DC:44:ASN:H | 1.88 | 0.71 |
| 23:DB:1080:A:O2' | 52:DI:126:ARG:HD2 | 1.90 | 0.71 |
| 40:DS:24:ILE:HG22 | 40:DS:71:VAL:HG11 | 1.72 | 0.71 |
| 2:AC:63:ILE:HD12 | 2:AC:98:ALA:HB2 | 1.71 | 0.71 |
| 13:AN:50:LEU:H | 13:AN:51:PRO:HD2 | 1.53 | 0.71 |
| 21:AU:9:GLU:HG2 | 2:CC:108:PRO:HG3 | 1.73 | 0.71 |
| 23:BB:580:U:H2' | 23:BB:581:C:C6 | 2.24 | 0.71 |
| 23:BB:742:A:H2' | 23:BB:743:A:C8 | 2.24 | 0.71 |
| 23:BB:836:G:H2' | 23:BB:837:C:C6 | 2.25 | 0.71 |
| 23:BB:2880:C:O4' | 35:BN:91:ALA:HB3 | 1.91 | 0.71 |
| 1:CA:797:C:OP1 | 10:CK:125:LYS:HE3 | 1.91 | 0.71 |
| 6:CG:115:MET:HA | 6:CG:118:ARG:HD2 | 1.72 | 0.71 |
| 22:DA:32:U:H4' | 22:DA:52:A:H62 | 1.55 | 0.71 |
| 22:DA:98:G:N1 | 24:DV:14:LYS:HB2 | 2.04 | 0.71 |
| 31:DJ:17:VAL:HG22 | 31:DJ:55:ILE:HD11 | 1.69 | 0.71 |
| 41:DT:76:ARG:NH2 | 41:DT:77:ARG:HB2 | 2.05 | 0.71 |
| 3:AD:196:GLU:O | 3:AD:199:ILE:HG13 | 1.90 | 0.71 |
| 8:AI:26:LYS:H | 8:AI:61:ASP:CB | 2.03 | 0.71 |
| 16:AQ:20:ILE:HD13 | 16:AQ:47:ASP:HB3 | 1.73 | 0.71 |
| 19:AT:43:LYS:HE2 | 19:AT:44:ALA:H | 1.55 | 0.71 |
| 23:BB:918:A:H2' | 23:BB:919:U:H5' | 1.70 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BC:202:ARG:HH11 | 25:BC:213:ARG:HE | 1.36 | 0.71 |
| 28:BF:126:ASN:HA | 28:BF:157:THR:HG22 | 1.73 | 0.71 |
| 36:BO:51:ALA:HB3 | 36:BO:78:VAL:HG22 | 1.72 | 0.71 |
| 1:CA:1472:U:H2' | 1:CA:1473:G:H8 | 1.53 | 0.71 |
| 1:CA:764:C:H2' | 1:CA:765:G:H5' | 1.72 | 0.71 |
| 23:DB:1440:U:H2' | 23:DB:1441:G:H8 | 1.55 | 0.71 |
| 27:DE:58:LYS:HE2 | 27:DE:60:TRP:CD1 | 2.26 | 0.71 |
| 42:DU:26:ASN:HD21 | 42:DU:34:ILE:HD12 | 1.54 | 0.71 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.24 | 0.71 |
| 20:AB:205:ALA:HB3 | 20:AB:208:ALA:HB3 | 1.72 | 0.71 |
| 23:BB:1060:U:C4 | 23:BB:1088:A:N6 | 2.58 | 0.71 |
| 23:BB:27:G:N2 | 23:BB:512:G:H2' | 2.05 | 0.71 |
| 23:BB:590:A:H2' | 23:BB:591:U:C6 | 2.26 | 0.71 |
| 29:BG:157:LYS:HB3 | 29:BG:159:LYS:HG3 | 1.72 | 0.71 |
| 52:BI:122:GLU:O | 52:BI:126:ARG:HG3 | 1.91 | 0.71 |
| 23:DB:1447:C:H2' | 23:DB:1448:G:H8 | 1.56 | 0.71 |
| 38:DQ:63:ARG:HH22 | 38:DQ:96:ASP:CA | 2.02 | 0.71 |
| 23:DB:329:G:H22 | 42:DU:16:LYS:HE3 | 1.53 | 0.71 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:H8 | 1.55 | 0.71 |
| 1:AA:559:A:H4' | 1:AA:560:A:H3' | 1.73 | 0.71 |
| 1:AA:812:G:O2' | 1:AA:813:U:H6 | 1.72 | 0.71 |
| 20:AB:19:THR:HA | 20:AB:37:VAL:HA | 1.72 | 0.71 |
| 2:AC:148:ILE:HA | 2:AC:200:TRP:O | 1.90 | 0.71 |
| 4:AE:36:THR:HG21 | 4:AE:63:MET:HG2 | 1.72 | 0.71 |
| 9:AJ:12:ALA:HB2 | 9:AJ:96:VAL:HG12 | 1.70 | 0.71 |
| 23:BB:773:U:H5' | 23:BB:774:G:OP2 | 1.91 | 0.71 |
| 28:BF:34:THR:HG22 | 28:BF:89:THR:HG22 | 1.72 | 0.71 |
| 28:BF:34:THR:HA | 28:BF:89:THR:HA | 1.72 | 0.71 |
| 31:BJ:77:HIS:CD2 | 31:BJ:84:ILE:H | 2.08 | 0.71 |
| 35:BN:83:LEU:HA | 35:BN:86:ARG:HG3 | 1.71 | 0.71 |
| 9:CJ:57:VAL:HG22 | 9:CJ:58:ASN:H | 1.56 | 0.71 |
| 13:CN:30:ILE:HB | 13:CN:44:VAL:HG11 | 1.71 | 0.71 |
| 23:DB:1354:A:H2' | 23:DB:1355:G:O4' | 1.91 | 0.71 |
| 23:DB:2071:A:H2' | 23:DB:2072:C:C6 | 2.25 | 0.71 |
| 23:DB:919:U:H2' | 23:DB:920:A:C8 | 2.25 | 0.71 |
| 25:DC:81:GLU:HB2 | 25:DC:90:ILE:HG22 | 1.71 | 0.71 |
| 24:DV:51:GLN:NE2 | 24:DV:79:ARG:HH22 | 1.89 | 0.71 |
| 23:DB:200:U:H5'' | 46:DZ:22:LEU:O | 1.90 | 0.71 |
| 1:AA:1477:U:H2' | 1:AA:1478:U:C6 | 2.26 | 0.71 |
| 1:AA:677:U:H2' | 1:AA:678:U:C6 | 2.26 | 0.71 |
| 6:AG:14:ASP:HB3 | 6:AG:19:SER:H | 1.54 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:957:U:H4' | 18:AS:78:THR:HB | 1.71 | 0.71 |
| 29:BG:71:LEU:HA | 29:BG:74:MET:SD | 2.31 | 0.71 |
| 46:BZ:59:ILE:HG22 | 46:BZ:64:ILE:HA | 1.72 | 0.71 |
| 1:CA:764:C:C2' | 1:CA:765:G:H5' | 2.21 | 0.71 |
| 10:CK:91:GLY:HA2 | 10:CK:94:SER:HB3 | 1.72 | 0.71 |
| 21:CU:43:GLU:HG3 | 21:CU:44:ARG:HH21 | 1.56 | 0.71 |
| 23:DB:742:A:H2' | 23:DB:743:A:H8 | 1.54 | 0.71 |
| 31:DJ:93:ILE:O | 31:DJ:97:PRO:HG3 | 1.91 | 0.71 |
| 36:DO:11:ALA:CB | 36:DO:96:GLY:H | 2.03 | 0.71 |
| 20:AB:61:SER:HB2 | 20:AB:62:ARG:NH1 | 2.05 | 0.71 |
| 21:AU:42:THR:O | 21:AU:46:ARG:HG3 | 1.91 | 0.71 |
| 23:BB:224:U:O4 | 23:BB:420:C:H5' | 1.91 | 0.71 |
| 29:BG:43:LYS:HB2 | 29:BG:50:THR:HB | 1.71 | 0.71 |
| 1:CA:1118:U:H2' | 1:CA:1119:C:C6 | 2.25 | 0.71 |
| 34:DM:66:ARG:CZ | 34:DM:101:VAL:HG11 | 2.20 | 0.71 |
| 43:DW:23:LYS:HD2 | 43:DW:24:ARG:HB3 | 1.72 | 0.71 |
| 46:DZ:59:ILE:HG22 | 46:DZ:64:ILE:HA | 1.73 | 0.71 |
| 1:AA:1072:G:N2 | 20:AB:105:THR:HG21 | 2.06 | 0.71 |
| 23:BB:2071:A:H2' | 23:BB:2072:C:C6 | 2.25 | 0.71 |
| 23:BB:2872:A:O2' | 23:BB:2873:A:H5'' | 1.91 | 0.71 |
| 28:BF:126:ASN:HA | 28:BF:157:THR:H | 1.55 | 0.71 |
| 31:BJ:93:ILE:O | 31:BJ:97:PRO:HG3 | 1.90 | 0.71 |
| 23:DB:1857:G:H1' | 23:DB:1885:A:H61 | 1.56 | 0.71 |
| 23:DB:1949:G:H2' | 23:DB:1950:G:C8 | 2.25 | 0.71 |
| 23:DB:2328:A:H2' | 23:DB:2329:U:C6 | 2.25 | 0.71 |
| 23:DB:362:A:H3' | 23:DB:363:G:H8 | 1.56 | 0.71 |
| 23:DB:62:U:H3' | 23:DB:63:A:H8 | 1.55 | 0.71 |
| 20:AB:53:LEU:HA | 20:AB:56:LEU:HD13 | 1.73 | 0.70 |
| 23:BB:1001:A:H2' | 23:BB:1002:G:O4' | 1.91 | 0.70 |
| 23:BB:171:U:H2' | 23:BB:172:A:C8 | 2.26 | 0.70 |
| 23:BB:30:G:H2' | 23:BB:31:C:C6 | 2.25 | 0.70 |
| 44:BX:3:ALA:HA | 44:BX:6:LEU:HD23 | 1.73 | 0.70 |
| 1:CA:1132:C:H2' | 1:CA:1133:G:H8 | 1.55 | 0.70 |
| 1:CA:522:C:H41 | 11:CL:49:ARG:HH22 | 1.39 | 0.70 |
| 1:CA:617:G:H4' | 15:CP:46:LYS:HE2 | 1.73 | 0.70 |
| 1:CA:695:A:H61 | 1:CA:797:C:H1' | 1.56 | 0.70 |
| 8:CI:93:LEU:HD13 | 8:CI:97:LEU:HD11 | 1.71 | 0.70 |
| 23:DB:1001:A:H2' | 23:DB:1002:G:O4' | 1.91 | 0.70 |
| 23:DB:2438:U:O2' | 23:DB:2439:A:H5'' | 1.91 | 0.70 |
| 30:DH:27:ARG:NH1 | 46:DZ:60:ASP:HA | 2.06 | 0.70 |
| 23:DB:1287:A:OP1 | 35:DN:104:ALA:HB3 | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DT:15:HIS:H | 41:DT:32:LEU:HA | 1.55 | 0.70 |
| 1:AA:1142:G:H2' | 1:AA:1143:G:O4' | 1.91 | 0.70 |
| 1:AA:437:U:H2' | 1:AA:438:U:O4' | 1.90 | 0.70 |
| 1:AA:764:C:C2' | 1:AA:765:G:H5' | 2.22 | 0.70 |
| 2:AC:112:ALA:HB1 | 2:AC:184:ASN:HB2 | 1.72 | 0.70 |
| 8:AI:93:LEU:HD13 | 8:AI:97:LEU:HD11 | 1.73 | 0.70 |
| 1:AA:108:G:C6 | 19:AT:9:ARG:HG2 | 2.26 | 0.70 |
| 23:BB:1437:C:H2' | 23:BB:1438:U:H6 | 1.54 | 0.70 |
| 23:BB:2297:A:N6 | 23:BB:2319:G:H1' | 2.06 | 0.70 |
| 31:BJ:29:ALA:HA | 31:BJ:32:LEU:HB2 | 1.73 | 0.70 |
| 20:CB:137:THR:O | 20:CB:141:GLU:HG3 | 1.92 | 0.70 |
| 12:CM:90:HIS:HA | 12:CM:108:ARG:NH2 | 2.06 | 0.70 |
| 12:CM:86:ARG:HG3 | 12:CM:96:VAL:HG11 | 1.73 | 0.70 |
| 15:CP:57:ILE:O | 15:CP:61:VAL:HG23 | 1.90 | 0.70 |
| 23:DB:27:G:N2 | 23:DB:512:G:H2' | 2.06 | 0.70 |
| 23:DB:849:A:H2' | 23:DB:850:U:C6 | 2.26 | 0.70 |
| 28:DF:126:ASN:HA | 28:DF:157:THR:H | 1.56 | 0.70 |
| 28:DF:128:SER:HB3 | 28:DF:154:THR:HG23 | 1.73 | 0.70 |
| 41:DT:11:LEU:HD21 | 41:DT:46:ALA:HB1 | 1.71 | 0.70 |
| 23:DB:96:C:H4' | 44:DX:41:HIS:ND1 | 2.06 | 0.70 |
| 1:AA:475:C:H2' | 1:AA:476:U:C6 | 2.25 | 0.70 |
| 1:AA:90:C:H2' | 1:AA:91:U:C5 | 2.27 | 0.70 |
| 7:AH:44:PHE:HA | 7:AH:70:VAL:HG11 | 1.72 | 0.70 |
| 48:B1:9:LYS:H | 48:B1:9:LYS:HD3 | 1.57 | 0.70 |
| 23:BB:287:G:H2' | 23:BB:288:U:C6 | 2.25 | 0.70 |
| 36:BO:24:THR:HG22 | 36:BO:42:PRO:HD3 | 1.72 | 0.70 |
| 1:CA:235:C:H2' | 1:CA:236:A:C8 | 2.27 | 0.70 |
| 20:CB:53:LEU:HA | 20:CB:56:LEU:HD13 | 1.72 | 0.70 |
| 2:CC:112:ALA:HB1 | 2:CC:184:ASN:HB2 | 1.73 | 0.70 |
| 8:CI:64:ILE:H | 8:CI:64:ILE:HD12 | 1.57 | 0.70 |
| 13:CN:30:ILE:HG22 | 13:CN:41:TRP:HB2 | 1.74 | 0.70 |
| 23:DB:2720:U:H5'' | 37:DP:52:ARG:HH21 | 1.55 | 0.70 |
| 25:DC:202:ARG:HH11 | 25:DC:213:ARG:HE | 1.38 | 0.70 |
| 25:DC:32:LEU:O | 25:DC:63:ILE:HG12 | 1.90 | 0.70 |
| 20:AB:99:MET:HA | 20:AB:106:VAL:HG21 | 1.72 | 0.70 |
| 18:AS:62:THR:HB | 18:AS:64:GLU:OE1 | 1.92 | 0.70 |
| 23:BB:2021:C:OP1 | 47:B0:8:THR:HG21 | 1.91 | 0.70 |
| 25:BC:43:ASN:ND2 | 25:BC:44:ASN:H | 1.89 | 0.70 |
| 30:BH:73:ASN:HD22 | 30:BH:74:ALA:N | 1.87 | 0.70 |
| 34:BM:59:ARG:NH1 | 34:BM:60:GLN:HB3 | 2.07 | 0.70 |
| 37:BP:45:VAL:H | 37:BP:60:VAL:HB | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:63:ILE:HD12 | 2:CC:98:ALA:HB2 | 1.72 | 0.70 |
| 3:CD:197:HIS:O | 3:CD:200:VAL:HG22 | 1.91 | 0.70 |
| 3:CD:47:LEU:HB2 | 3:CD:51:GLY:HA3 | 1.72 | 0.70 |
| 10:CK:33:ILE:HG13 | 10:CK:73:VAL:HG21 | 1.72 | 0.70 |
| 13:CN:86:ALA:HB1 | 13:CN:91:GLU:HB2 | 1.73 | 0.70 |
| 26:DD:124:ARG:HA | 26:DD:165:MET:HE3 | 1.73 | 0.70 |
| 29:DG:84:LYS:HB3 | 29:DG:132:LEU:O | 1.91 | 0.70 |
| 4:AE:76:ASN:HB2 | 4:AE:81:GLN:NE2 | 2.07 | 0.70 |
| 22:BA:32:U:H4' | 22:BA:52:A:H62 | 1.55 | 0.70 |
| 23:BB:1412:U:H2' | 23:BB:1413:A:H8 | 1.56 | 0.70 |
| 23:BB:1464:G:H2' | 23:BB:1465:G:H8 | 1.55 | 0.70 |
| 32:BK:102:PRO:HA | 32:BK:120:PRO:HB3 | 1.74 | 0.70 |
| 47:D0:32:THR:OG1 | 47:D0:50:GLY:HA2 | 1.90 | 0.70 |
| 48:D1:46:VAL:HG22 | 48:D1:47:ILE:H | 1.53 | 0.70 |
| 23:DB:2872:A:O2' | 23:DB:2873:A:H5'' | 1.92 | 0.70 |
| 25:DC:35:LYS:HG2 | 25:DC:36:ASN:H | 1.54 | 0.70 |
| 29:DG:71:LEU:HA | 29:DG:74:MET:SD | 2.31 | 0.70 |
| 40:DS:26:GLY:N | 40:DS:71:VAL:HG13 | 2.06 | 0.70 |
| 3:AD:58:GLN:O | 3:AD:62:ARG:HG2 | 1.92 | 0.70 |
| 16:AQ:30:HIS:CE1 | 16:AQ:32:ILE:HG22 | 2.27 | 0.70 |
| 16:AQ:74:LEU:HD22 | 16:AQ:75:VAL:N | 2.06 | 0.70 |
| 23:BB:1454:C:H5' | 35:BN:63:ARG:HE | 1.55 | 0.70 |
| 23:BB:2557:G:H2' | 23:BB:2558:C:C6 | 2.27 | 0.70 |
| 30:BH:90:LEU:HD11 | 30:BH:146:VAL:HG11 | 1.71 | 0.70 |
| 44:BX:8:GLU:O | 44:BX:12:GLU:HB2 | 1.92 | 0.70 |
| 2:CC:156:LEU:HD12 | 2:CC:163:ARG:HD2 | 1.72 | 0.70 |
| 21:CU:42:THR:O | 21:CU:46:ARG:HG3 | 1.92 | 0.70 |
| 23:DB:2109:U:H2' | 23:DB:2110:G:H5'' | 1.73 | 0.70 |
| 23:DB:215:G:H4' | 23:DB:216:A:H4' | 1.74 | 0.70 |
| 23:DB:2794:C:H2' | 23:DB:2795:C:C6 | 2.26 | 0.70 |
| 20:AB:76:SER:HA | 20:AB:92:ASN:HB2 | 1.73 | 0.70 |
| 8:AI:64:ILE:HD12 | 8:AI:64:ILE:H | 1.57 | 0.70 |
| 16:AQ:59:GLU:O | 16:AQ:75:VAL:HG22 | 1.91 | 0.70 |
| 23:BB:1447:C:H2' | 23:BB:1448:G:H8 | 1.56 | 0.70 |
| 23:BB:1461:C:H2' | 23:BB:1462:C:H6 | 1.56 | 0.70 |
| 23:BB:2512:C:H2' | 23:BB:2513:A:O4' | 1.91 | 0.70 |
| 41:BT:12:ARG:HA | 44:BX:29:ARG:HH22 | 1.57 | 0.70 |
| 24:BV:62:THR:HG22 | 24:BV:71:LYS:HG2 | 1.73 | 0.70 |
| 1:CA:974:A:H4' | 1:CA:975:A:H5' | 1.74 | 0.70 |
| 1:CA:522:C:H41 | 11:CL:49:ARG:NH2 | 1.90 | 0.70 |
| 23:DB:2645:G:H3' | 23:DB:2646:C:H5' | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:871:U:H2' | 23:DB:872:U:H6 | 1.56 | 0.70 |
| 27:DE:192:ALA:HA | 27:DE:195:GLN:HE21 | 1.56 | 0.70 |
| 24:DV:21:ARG:HE | 24:DV:87:GLN:HB3 | 1.56 | 0.70 |
| 1:AA:964:A:H2' | 1:AA:965:U:H5'' | 1.72 | 0.70 |
| 23:BB:1056:G:H1' | 23:BB:1103:A:H62 | 1.56 | 0.70 |
| 23:BB:1287:A:H3' | 23:BB:1288:G:N2 | 2.07 | 0.70 |
| 23:BB:2645:G:H3' | 23:BB:2646:C:H5' | 1.74 | 0.70 |
| 30:BH:132:PHE:H | 30:BH:142:VAL:HG23 | 1.56 | 0.70 |
| 20:CB:60:ALA:HA | 20:CB:64:GLY:HA3 | 1.73 | 0.70 |
| 20:CB:76:SER:HA | 20:CB:92:ASN:HB2 | 1.74 | 0.70 |
| 23:DB:1592:C:H2' | 23:DB:1593:A:H8 | 1.57 | 0.70 |
| 23:DB:2366:A:H4' | 43:DW:61:LYS:HE2 | 1.73 | 0.70 |
| 23:DB:591:U:H1' | 50:D3:1:PRO:N | 2.06 | 0.70 |
| 28:DF:34:THR:HA | 28:DF:89:THR:HA | 1.74 | 0.70 |
| 27:DE:117:ARG:HH12 | 33:DL:2:ARG:HB2 | 1.57 | 0.70 |
| 41:DT:32:LEU:H | 41:DT:83:ALA:HB3 | 1.56 | 0.70 |
| 1:AA:974:A:H4' | 1:AA:975:A:H5' | 1.74 | 0.70 |
| 20:AB:15:PHE:HA | 20:AB:42:LEU:HD21 | 1.72 | 0.70 |
| 12:AM:86:ARG:HG3 | 12:AM:96:VAL:HG11 | 1.74 | 0.70 |
| 16:AQ:45:VAL:HG12 | 16:AQ:46:HIS:H | 1.55 | 0.70 |
| 23:BB:643:A:N3 | 48:B1:43:ARG:HD2 | 2.07 | 0.70 |
| 23:BB:1440:U:H2' | 23:BB:1441:G:H8 | 1.57 | 0.70 |
| 23:BB:2800:A:N3 | 23:BB:2801:G:H1' | 2.07 | 0.70 |
| 23:BB:2060:A:H2' | 27:BE:63:LYS:HE2 | 1.72 | 0.70 |
| 31:BJ:18:VAL:HG22 | 31:BJ:19:ASP:H | 1.57 | 0.70 |
| 33:BL:112:LEU:HG | 33:BL:113:ALA:H | 1.56 | 0.70 |
| 3:CD:137:SER:HB2 | 3:CD:138:PRO:HD2 | 1.73 | 0.70 |
| 23:DB:1535:A:O2' | 23:DB:1536:C:H5' | 1.92 | 0.70 |
| 23:DB:27:G:H1' | 23:DB:513:A:N6 | 2.07 | 0.70 |
| 23:DB:458:G:N2 | 23:DB:469:G:H2' | 2.07 | 0.70 |
| 23:DB:807:U:H2' | 23:DB:808:G:H8 | 1.56 | 0.70 |
| 42:DU:38:ILE:HG23 | 42:DU:39:ASN:N | 2.05 | 0.70 |
| 44:DX:23:ARG:HD2 | 44:DX:27:ASN:HD21 | 1.57 | 0.70 |
| 15:AP:52:LEU:HD21 | 15:AP:75:ILE:HG12 | 1.71 | 0.70 |
| 23:BB:1178:C:H2' | 23:BB:1179:G:H8 | 1.55 | 0.70 |
| 37:BP:85:VAL:HG21 | 37:BP:88:ARG:HH11 | 1.55 | 0.70 |
| 3:CD:196:GLU:O | 3:CD:199:ILE:HG13 | 1.91 | 0.70 |
| 5:CF:26:THR:HA | 5:CF:29:ILE:HD12 | 1.73 | 0.70 |
| 7:CH:44:PHE:HA | 7:CH:70:VAL:HG11 | 1.72 | 0.70 |
| 11:CL:122:LYS:HD2 | 11:CL:123:ALA:N | 2.06 | 0.70 |
| 16:CQ:45:VAL:HG12 | 16:CQ:46:HIS:H | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:773:U:H5' | 23:DB:774:G:OP2 | 1.92 | 0.70 |
| 30:DH:48:GLU:HB2 | 30:DH:51:ARG:NH2 | 2.06 | 0.70 |
| 31:DJ:117:ALA:HA | 31:DJ:120:ARG:HD2 | 1.74 | 0.70 |
| 31:DJ:77:HIS:CD2 | 31:DJ:84:ILE:H | 2.10 | 0.70 |
| 39:DR:16:GLU:H | 39:DR:101:ILE:HG13 | 1.57 | 0.70 |
| 39:DR:14:VAL:HG22 | 39:DR:15:SER:N | 2.07 | 0.70 |
| 1:AA:920:U:H2' | 1:AA:921:U:C6 | 2.27 | 0.69 |
| 20:AB:60:ALA:HA | 20:AB:64:GLY:HA3 | 1.74 | 0.69 |
| 23:BB:2751:G:N3 | 23:BB:2751:G:H2' | 2.07 | 0.69 |
| 23:BB:919:U:H2' | 23:BB:920:A:C8 | 2.27 | 0.69 |
| 28:BF:62:GLN:NE2 | 28:BF:90:LEU:HA | 2.07 | 0.69 |
| 30:BH:68:ARG:NH1 | 30:BH:110:VAL:HG12 | 2.07 | 0.69 |
| 35:BN:17:ARG:HA | 35:BN:20:MET:HB3 | 1.72 | 0.69 |
| 41:BT:15:HIS:H | 41:BT:32:LEU:HA | 1.57 | 0.69 |
| 6:CG:66:GLU:HA | 6:CG:69:ARG:HD2 | 1.74 | 0.69 |
| 11:CL:51:VAL:HG12 | 11:CL:52:CYS:H | 1.57 | 0.69 |
| 11:CL:66:ILE:HG21 | 11:CL:71:HIS:HB3 | 1.72 | 0.69 |
| 12:CM:92:ARG:HH12 | 18:CS:79:TYR:HD2 | 1.40 | 0.69 |
| 23:DB:1993:U:H4' | 26:DD:133:THR:CG2 | 2.22 | 0.69 |
| 36:DO:24:THR:HG22 | 36:DO:42:PRO:HD3 | 1.73 | 0.69 |
| 1:AA:193:C:H2' | 1:AA:194:C:C6 | 2.26 | 0.69 |
| 2:AC:171:ARG:HB2 | 2:AC:171:ARG:HH11 | 1.57 | 0.69 |
| 3:AD:153:ARG:HG3 | 3:AD:154:VAL:N | 2.08 | 0.69 |
| 3:AD:29:THR:HB | 3:AD:30:LYS:NZ | 2.06 | 0.69 |
| 4:AE:32:PHE:O | 4:AE:51:LYS:HB2 | 1.91 | 0.69 |
| 23:BB:1274:A:N3 | 23:BB:1297:C:H1' | 2.06 | 0.69 |
| 23:BB:215:G:H4' | 23:BB:216:A:H4' | 1.74 | 0.69 |
| 23:BB:580:U:H2' | 23:BB:581:C:H6 | 1.57 | 0.69 |
| 23:BB:2619:C:H5' | 26:BD:157:LYS:HD3 | 1.72 | 0.69 |
| 42:BU:24:VAL:HA | 42:BU:35:VAL:HA | 1.73 | 0.69 |
| 42:BU:86:PHE:HB2 | 42:BU:92:VAL:HB | 1.73 | 0.69 |
| 20:CB:205:ALA:HB3 | 20:CB:208:ALA:HB3 | 1.73 | 0.69 |
| 23:DB:350:G:H2' | 23:DB:351:C:O4' | 1.92 | 0.69 |
| 23:DB:45:G:H5' | 23:DB:46:G:H5' | 1.73 | 0.69 |
| 23:DB:571:U:H3' | 39:DR:80:ARG:HH12 | 1.57 | 0.69 |
| 26:DD:13:ARG:HD2 | 37:DP:55:HIS:ND1 | 2.07 | 0.69 |
| 30:DH:88:GLY:HA3 | 30:DH:125:THR:OG1 | 1.93 | 0.69 |
| 31:DJ:18:VAL:HG22 | 31:DJ:19:ASP:H | 1.55 | 0.69 |
| 31:DJ:45:THR:H | 31:DJ:46:PRO:HD3 | 1.56 | 0.69 |
| 1:AA:1026:G:H2' | 1:AA:1027:C:H6 | 1.55 | 0.69 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:239:U:H4' | 1:AA:239:U:OP1 | 1.90 | 0.69 |
| 2:AC:104:GLU:HG2 | 2:AC:105:VAL:H | 1.56 | 0.69 |
| 5:AF:26:THR:HA | 5:AF:29:ILE:HD12 | 1.74 | 0.69 |
| 7:AH:63:LYS:HD2 | 7:AH:70:VAL:HG21 | 1.74 | 0.69 |
| 9:AJ:57:VAL:HG22 | 9:AJ:58:ASN:H | 1.56 | 0.69 |
| 12:AM:90:HIS:HA | 12:AM:108:ARG:NH2 | 2.08 | 0.69 |
| 13:AN:30:ILE:HG22 | 13:AN:41:TRP:HB2 | 1.73 | 0.69 |
| 23:BB:1038:G:H2' | 23:BB:1039:A:C8 | 2.28 | 0.69 |
| 23:BB:1857:G:HO2' | 23:BB:1858:A:H8 | 1.39 | 0.69 |
| 33:BL:57:LEU:O | 33:BL:61:LEU:HD13 | 1.93 | 0.69 |
| 2:CC:148:ILE:HA | 2:CC:200:TRP:O | 1.92 | 0.69 |
| 7:CH:124:ILE:HG22 | 7:CH:125:ILE:H | 1.55 | 0.69 |
| 12:CM:67:ASP:O | 12:CM:71:GLU:HB2 | 1.92 | 0.69 |
| 23:DB:142:A:H2' | 23:DB:143:C:C6 | 2.26 | 0.69 |
| 23:DB:2732:G:H5' | 23:DB:2733:A:O4' | 1.92 | 0.69 |
| 52:DI:85:ILE:HD13 | 52:DI:137:LEU:HD21 | 1.73 | 0.69 |
| 41:DT:12:ARG:HA | 44:DX:29:ARG:HH22 | 1.58 | 0.69 |
| 1:AA:449:G:H2' | 1:AA:450:G:C8 | 2.28 | 0.69 |
| 1:AA:859:G:H2' | 1:AA:860:A:C8 | 2.25 | 0.69 |
| 11:AL:66:ILE:HG21 | 11:AL:71:HIS:HB3 | 1.72 | 0.69 |
| 51:B4:2:LYS:HE3 | 51:B4:4:ARG:HH21 | 1.58 | 0.69 |
| 22:BA:29:A:H3' | 22:BA:30:C:H6 | 1.58 | 0.69 |
| 34:BM:4:PRO:HG3 | 34:BM:68:PHE:HE2 | 1.58 | 0.69 |
| 37:BP:29:VAL:HG12 | 37:BP:80:VAL:HA | 1.74 | 0.69 |
| 39:BR:16:GLU:H | 39:BR:101:ILE:HG13 | 1.57 | 0.69 |
| 4:CE:36:THR:HG21 | 4:CE:63:MET:HG2 | 1.73 | 0.69 |
| 11:CL:86:VAL:HG11 | 11:CL:89:LEU:HD23 | 1.74 | 0.69 |
| 12:CM:28:ARG:NH2 | 12:CM:62:PHE:HB2 | 2.08 | 0.69 |
| 18:CS:62:THR:HB | 18:CS:64:GLU:OE1 | 1.90 | 0.69 |
| 51:D4:2:LYS:HE3 | 51:D4:4:ARG:HH21 | 1.56 | 0.69 |
| 29:DG:85:LYS:HB2 | 29:DG:164:ALA:HB3 | 1.75 | 0.69 |
| 40:DS:15:GLN:HA | 40:DS:18:ARG:HG2 | 1.74 | 0.69 |
| 1:AA:462:G:H5' | 1:AA:463:U:OP2 | 1.93 | 0.69 |
| 1:AA:797:C:OP1 | 10:AK:125:LYS:HE3 | 1.92 | 0.69 |
| 20:AB:199:ILE:HD13 | 20:AB:212:TYR:HE2 | 1.58 | 0.69 |
| 1:AA:522:C:H41 | 11:AL:49:ARG:HH22 | 1.40 | 0.69 |
| 13:AN:63:CYS:HB2 | 13:AN:79:SER:HB3 | 1.74 | 0.69 |
| 1:AA:617:G:H4' | 15:AP:46:LYS:HE2 | 1.73 | 0.69 |
| 23:BB:620:G:N3 | 23:BB:620:G:H5' | 2.08 | 0.69 |
| 1:CA:964:A:H2' | 1:CA:965:U:H5'' | 1.74 | 0.69 |
| 4:CE:84:VAL:HG11 | 4:CE:146:MET:HB3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2512:C:H2' | 23:DB:2513:A:O4' | 1.92 | 0.69 |
| 29:DG:53:PRO:HG3 | 29:DG:61:TRP:HA | 1.75 | 0.69 |
| 32:DK:54:LYS:H | 32:DK:54:LYS:HD2 | 1.57 | 0.69 |
| 37:DP:45:VAL:H | 37:DP:60:VAL:HB | 1.56 | 0.69 |
| 38:DQ:26:ALA:HA | 38:DQ:29:ARG:HG2 | 1.75 | 0.69 |
| 38:DQ:81:GLY:HA2 | 38:DQ:84:LYS:HB3 | 1.74 | 0.69 |
| 1:AA:1004:A:H3' | 1:AA:1024:G:H22 | 1.56 | 0.69 |
| 26:BD:113:SER:CB | 26:BD:168:GLU:H | 2.06 | 0.69 |
| 26:BD:172:VAL:HG11 | 26:BD:175:LEU:HD12 | 1.74 | 0.69 |
| 26:BD:62:LYS:HD2 | 26:BD:62:LYS:H | 1.57 | 0.69 |
| 28:BF:30:VAL:HG21 | 28:BF:96:TRP:HE1 | 1.57 | 0.69 |
| 1:CA:229:U:H2' | 1:CA:230:G:H8 | 1.58 | 0.69 |
| 8:CI:25:GLY:HA2 | 8:CI:60:LEU:O | 1.93 | 0.69 |
| 23:DB:1911:U:H2' | 23:DB:1918:A:C2 | 2.28 | 0.69 |
| 23:DB:2097:A:H2' | 23:DB:2098:U:C6 | 2.28 | 0.69 |
| 23:DB:2722:G:H4' | 35:DN:4:ARG:HB2 | 1.73 | 0.69 |
| 23:DB:721:A:H2' | 23:DB:722:A:C8 | 2.27 | 0.69 |
| 30:DH:96:THR:HG23 | 30:DH:97:ARG:H | 1.56 | 0.69 |
| 52:DI:105:LEU:HD11 | 52:DI:139:VAL:HG21 | 1.72 | 0.69 |
| 1:AA:1060:U:C4' | 9:AJ:54:SER:HB2 | 2.23 | 0.69 |
| 1:AA:522:C:H41 | 11:AL:49:ARG:NH2 | 1.89 | 0.69 |
| 6:AG:66:GLU:HA | 6:AG:69:ARG:HD2 | 1.75 | 0.69 |
| 23:BB:1486:U:H2' | 23:BB:1487:U:C6 | 2.28 | 0.69 |
| 23:BB:458:G:N2 | 23:BB:469:G:H2' | 2.07 | 0.69 |
| 27:BE:192:ALA:HA | 27:BE:195:GLN:HE21 | 1.56 | 0.69 |
| 29:BG:85:LYS:HB2 | 29:BG:164:ALA:HB3 | 1.75 | 0.69 |
| 43:BW:35:ILE:HA | 43:BW:57:THR:HG23 | 1.73 | 0.69 |
| 3:CD:58:GLN:O | 3:CD:62:ARG:HG2 | 1.92 | 0.69 |
| 23:DB:1098:A:H2' | 52:DI:4:VAL:CA | 2.21 | 0.69 |
| 23:DB:140:C:H5' | 23:DB:141:G:N7 | 2.08 | 0.69 |
| 23:DB:1827:U:O2' | 23:DB:1828:G:H5' | 1.93 | 0.69 |
| 23:DB:674:G:H1' | 27:DE:69:ARG:HE | 1.57 | 0.69 |
| 32:DK:20:MET:O | 32:DK:41:ILE:HG13 | 1.93 | 0.69 |
| 1:AA:532:A:H62 | 2:AC:191:THR:CB | 2.05 | 0.69 |
| 11:AL:51:VAL:HG12 | 11:AL:52:CYS:H | 1.57 | 0.69 |
| 1:CA:920:U:H2' | 1:CA:921:U:C6 | 2.27 | 0.69 |
| 2:CC:119:ILE:HG21 | 2:CC:197:VAL:HG11 | 1.72 | 0.69 |
| 23:DB:1654:A:H2' | 23:DB:1655:A:H8 | 1.58 | 0.69 |
| 23:DB:3:U:H2' | 23:DB:4:U:H6 | 1.57 | 0.69 |
| 6:AG:115:MET:HA | 6:AG:118:ARG:HD2 | 1.74 | 0.69 |
| 23:BB:1935:G:H1' | 23:BB:1964:G:N2 | 2.08 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:871:U:H2' | 23:BB:872:U:H6 | 1.57 | 0.69 |
| 40:BS:24:ILE:HG22 | 40:BS:71:VAL:HG11 | 1.73 | 0.69 |
| 1:CA:475:C:H2' | 1:CA:476:U:C6 | 2.28 | 0.69 |
| 20:CB:88:GLN:OE1 | 20:CB:221:ARG:HB3 | 1.93 | 0.69 |
| 8:CI:126:PHE:HE1 | 8:CI:129:ARG:HD3 | 1.57 | 0.69 |
| 30:DH:53:GLU:OE2 | 30:DH:54:LEU:HG | 1.93 | 0.69 |
| 37:DP:29:VAL:HG12 | 37:DP:80:VAL:HA | 1.75 | 0.69 |
| 41:DT:8:LEU:HD13 | 41:DT:49:LYS:HD2 | 1.75 | 0.69 |
| 1:AA:1026:G:H2' | 1:AA:1027:C:C6 | 2.28 | 0.69 |
| 1:AA:662:U:H2' | 1:AA:663:A:C8 | 2.27 | 0.69 |
| 20:AB:69:VAL:HB | 20:AB:162:VAL:HG23 | 1.73 | 0.69 |
| 3:AD:122:ILE:O | 3:AD:128:VAL:HG23 | 1.93 | 0.69 |
| 21:AU:16:ARG:HA | 21:AU:16:ARG:NE | 2.00 | 0.69 |
| 23:BB:2438:U:O2' | 23:BB:2439:A:H5'' | 1.93 | 0.69 |
| 33:BL:116:VAL:HG13 | 33:BL:117:THR:H | 1.58 | 0.69 |
| 37:BP:19:PHE:O | 37:BP:20:ARG:HB2 | 1.92 | 0.69 |
| 39:BR:20:VAL:HG12 | 39:BR:21:ARG:H | 1.58 | 0.69 |
| 20:CB:69:VAL:HB | 20:CB:162:VAL:HG23 | 1.74 | 0.69 |
| 25:DC:145:MET:HB2 | 25:DC:152:GLN:HE22 | 1.58 | 0.69 |
| 28:DF:62:GLN:NE2 | 28:DF:90:LEU:HA | 2.08 | 0.69 |
| 31:DJ:20:ALA:HB1 | 31:DJ:23:LYS:HB2 | 1.73 | 0.69 |
| 31:DJ:29:ALA:HA | 31:DJ:32:LEU:HB2 | 1.75 | 0.69 |
| 39:DR:71:LYS:HG2 | 39:DR:73:LYS:NZ | 2.08 | 0.69 |
| 23:DB:973:A:H5'' | 39:DR:81:LYS:HD2 | 1.75 | 0.69 |
| 42:DU:34:ILE:HG12 | 42:DU:63:ALA:HB2 | 1.75 | 0.69 |
| 45:DY:23:LEU:HD13 | 45:DY:28:LEU:HB2 | 1.74 | 0.69 |
| 20:AB:145:ASN:N | 20:AB:145:ASN:HD22 | 1.88 | 0.69 |
| 11:AL:86:VAL:HG11 | 11:AL:89:LEU:HD23 | 1.74 | 0.69 |
| 23:BB:2866:U:H4' | 23:BB:2867:G:H4' | 1.75 | 0.69 |
| 28:BF:102:LEU:HD22 | 28:BF:103:ILE:N | 2.08 | 0.69 |
| 31:BJ:6:ALA:HB3 | 31:BJ:45:THR:HG21 | 1.75 | 0.69 |
| 1:CA:337:G:H2' | 1:CA:338:A:H8 | 1.58 | 0.69 |
| 1:CA:677:U:H2' | 1:CA:678:U:C6 | 2.27 | 0.69 |
| 8:CI:26:LYS:H | 8:CI:61:ASP:CB | 2.05 | 0.69 |
| 8:CI:71:ILE:H | 8:CI:71:ILE:HD12 | 1.56 | 0.69 |
| 15:CP:28:ARG:HD2 | 15:CP:29:ASN:N | 2.08 | 0.69 |
| 23:DB:18:U:H2' | 23:DB:19:A:C8 | 2.28 | 0.69 |
| 23:DB:479:A:N3 | 23:DB:481:G:H5'' | 2.07 | 0.69 |
| 7:AH:124:ILE:HG22 | 7:AH:125:ILE:H | 1.57 | 0.68 |
| 16:AQ:77:VAL:HG11 | 16:AQ:80:LYS:HB3 | 1.75 | 0.68 |
| 23:BB:1060:U:O2 | 23:BB:1088:A:N7 | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1788:C:O2' | 23:BB:1789:A:H5' | 1.92 | 0.68 |
| 23:BB:1857:G:H1' | 23:BB:1885:A:H61 | 1.56 | 0.68 |
| 23:BB:729:G:OP1 | 25:BC:12:ARG:HB2 | 1.93 | 0.68 |
| 38:BQ:26:ALA:HA | 38:BQ:29:ARG:HG2 | 1.76 | 0.68 |
| 1:CA:195:A:H1' | 1:CA:222:C:O2' | 1.93 | 0.68 |
| 1:CA:449:G:H2' | 1:CA:450:G:C8 | 2.28 | 0.68 |
| 7:CH:74:ILE:HG13 | 7:CH:128:VAL:HG22 | 1.74 | 0.68 |
| 8:CI:51:LEU:HD13 | 8:CI:56:MET:HG2 | 1.75 | 0.68 |
| 9:CJ:7:ARG:O | 9:CJ:100:ILE:HA | 1.93 | 0.68 |
| 16:CQ:77:VAL:HG11 | 16:CQ:80:LYS:HB3 | 1.74 | 0.68 |
| 48:D1:9:LYS:H | 48:D1:9:LYS:HD3 | 1.58 | 0.68 |
| 23:DB:278:A:H1' | 23:DB:362:A:C2 | 2.28 | 0.68 |
| 43:DW:24:ARG:HD3 | 43:DW:65:LYS:HG2 | 1.73 | 0.68 |
| 23:BB:721:A:H2' | 23:BB:722:A:C8 | 2.28 | 0.68 |
| 25:BC:4:LYS:HD2 | 25:BC:5:CYS:N | 2.09 | 0.68 |
| 52:BI:10:LEU:HD13 | 52:BI:12:VAL:HG13 | 1.74 | 0.68 |
| 35:BN:19:ALA:HA | 35:BN:22:ARG:HB3 | 1.75 | 0.68 |
| 23:BB:200:U:H5'' | 46:BZ:22:LEU:O | 1.92 | 0.68 |
| 1:CA:1026:G:H2' | 1:CA:1027:C:C6 | 2.27 | 0.68 |
| 2:CC:2:GLN:H | 2:CC:2:GLN:NE2 | 1.92 | 0.68 |
| 1:CA:1220:G:H3' | 18:CS:36:ARG:HH21 | 1.56 | 0.68 |
| 23:DB:2893:A:H5'' | 23:DB:2894:G:H5' | 1.74 | 0.68 |
| 29:DG:43:LYS:HB2 | 29:DG:50:THR:HB | 1.73 | 0.68 |
| 31:DJ:55:ILE:HB | 31:DJ:123:LYS:HB2 | 1.74 | 0.68 |
| 34:DM:10:ARG:HE | 34:DM:89:VAL:HG21 | 1.58 | 0.68 |
| 34:DM:59:ARG:NH1 | 34:DM:60:GLN:HB3 | 2.08 | 0.68 |
| 35:DN:19:ALA:HA | 35:DN:22:ARG:HB3 | 1.76 | 0.68 |
| 2:AC:51:VAL:HA | 2:AC:69:THR:HA | 1.75 | 0.68 |
| 4:AE:85:LYS:HG3 | 4:AE:93:VAL:O | 1.92 | 0.68 |
| 7:AH:11:THR:HG22 | 7:AH:14:ARG:HH22 | 1.59 | 0.68 |
| 23:BB:163:C:H2' | 23:BB:164:C:O4' | 1.93 | 0.68 |
| 23:BB:192:C:H2' | 23:BB:193:U:H5' | 1.73 | 0.68 |
| 23:BB:222:A:N6 | 23:BB:232:G:H1' | 2.09 | 0.68 |
| 25:BC:14:HIS:O | 25:BC:203:VAL:HG11 | 1.93 | 0.68 |
| 27:BE:181:ILE:HG13 | 33:BL:2:ARG:HB3 | 1.75 | 0.68 |
| 30:BH:96:THR:HB | 30:BH:112:LYS:HB2 | 1.75 | 0.68 |
| 31:BJ:112:GLY:N | 31:BJ:113:PRO:HD2 | 2.04 | 0.68 |
| 31:BJ:117:ALA:HA | 31:BJ:120:ARG:HD2 | 1.75 | 0.68 |
| 31:BJ:57:LEU:HD11 | 31:BJ:129:GLU:H | 1.57 | 0.68 |
| 36:BO:67:ASN:H | 36:BO:70:ALA:HB3 | 1.58 | 0.68 |
| 23:BB:1248:G:H2' | 38:BQ:2:ARG:HA | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:8:LEU:HD13 | 41:BT:49:LYS:HD2 | 1.75 | 0.68 |
| 42:BU:34:ILE:HG12 | 42:BU:63:ALA:HB2 | 1.75 | 0.68 |
| 16:CQ:30:HIS:CE1 | 16:CQ:32:ILE:HG22 | 2.27 | 0.68 |
| 16:CQ:83:LEU:H | 16:CQ:83:LEU:HD22 | 1.57 | 0.68 |
| 39:DR:20:VAL:HG12 | 39:DR:21:ARG:H | 1.57 | 0.68 |
| 40:DS:52:GLU:HA | 40:DS:55:ILE:HG22 | 1.76 | 0.68 |
| 1:AA:532:A:H62 | 2:AC:191:THR:HB | 1.58 | 0.68 |
| 20:AB:88:GLN:OE1 | 20:AB:221:ARG:HB3 | 1.92 | 0.68 |
| 1:AA:935:A:H61 | 6:AG:2:ARG:HD2 | 1.57 | 0.68 |
| 49:B2:30:VAL:HA | 49:B2:33:ARG:NH2 | 2.08 | 0.68 |
| 23:BB:129:C:H2' | 23:BB:130:C:H6 | 1.58 | 0.68 |
| 23:BB:27:G:H1' | 23:BB:513:A:N6 | 2.09 | 0.68 |
| 23:BB:807:U:H2' | 23:BB:808:G:H8 | 1.59 | 0.68 |
| 38:BQ:81:GLY:HA2 | 38:BQ:84:LYS:HB3 | 1.73 | 0.68 |
| 39:BR:71:LYS:HG2 | 39:BR:73:LYS:NZ | 2.08 | 0.68 |
| 1:CA:176:C:H2' | 1:CA:177:G:N3 | 2.07 | 0.68 |
| 1:CA:17:U:H2' | 1:CA:18:C:H6 | 1.57 | 0.68 |
| 2:CC:16:PRO:HG2 | 2:CC:53:ARG:HH12 | 1.58 | 0.68 |
| 12:CM:10:ASP:HA | 12:CM:44:ILE:HD13 | 1.73 | 0.68 |
| 23:DB:1778:U:H2' | 23:DB:1784:A:H62 | 1.57 | 0.68 |
| 23:DB:2199:A:H5' | 23:DB:2200:C:OP2 | 1.93 | 0.68 |
| 32:DK:102:PRO:HA | 32:DK:120:PRO:HB3 | 1.74 | 0.68 |
| 1:AA:1306:A:N6 | 1:AA:1331:G:H1' | 2.08 | 0.68 |
| 1:AA:1288:A:N1 | 1:AA:1371:G:H1' | 2.08 | 0.68 |
| 13:AN:52:ARG:NH1 | 13:AN:58:ARG:HH21 | 1.92 | 0.68 |
| 15:AP:34:GLU:CD | 15:AP:60:TRP:HE1 | 1.97 | 0.68 |
| 18:AS:38:THR:HA | 18:AS:69:LYS:HA | 1.75 | 0.68 |
| 25:BC:76:VAL:HA | 25:BC:113:ASP:O | 1.93 | 0.68 |
| 27:BE:58:LYS:HE2 | 27:BE:60:TRP:CD1 | 2.28 | 0.68 |
| 28:BF:78:ILE:HA | 28:BF:82:TYR:CD1 | 2.29 | 0.68 |
| 1:CA:451:A:H5' | 15:CP:70:ARG:HH22 | 1.58 | 0.68 |
| 14:CO:28:VAL:HG11 | 14:CO:80:LEU:HD21 | 1.75 | 0.68 |
| 23:DB:1386:C:H2' | 23:DB:1387:A:C8 | 2.29 | 0.68 |
| 23:DB:775:G:H4' | 23:DB:776:G:H5' | 1.75 | 0.68 |
| 28:DF:78:ILE:HA | 28:DF:82:TYR:CD1 | 2.29 | 0.68 |
| 31:DJ:25:LEU:HD13 | 31:DJ:26:GLY:N | 2.08 | 0.68 |
| 36:DO:67:ASN:H | 36:DO:70:ALA:HB3 | 1.57 | 0.68 |
| 38:DQ:34:ALA:O | 38:DQ:37:ALA:HB3 | 1.93 | 0.68 |
| 1:AA:176:C:H2' | 1:AA:177:G:N3 | 2.09 | 0.68 |
| 25:BC:74:PRO:HG2 | 25:BC:96:LYS:HG3 | 1.76 | 0.68 |
| 31:BJ:20:ALA:HB1 | 31:BJ:23:LYS:HB2 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BJ:55:ILE:HB | 31:BJ:123:LYS:HB2 | 1.75 | 0.68 |
| 38:BQ:97:ILE:HG13 | 38:BQ:105:PHE:HB2 | 1.74 | 0.68 |
| 20:CB:145:ASN:N | 20:CB:145:ASN:HD22 | 1.90 | 0.68 |
| 2:CC:149:LYS:HA | 2:CC:168:ARG:HB2 | 1.76 | 0.68 |
| 23:DB:2461:A:H2' | 23:DB:2462:C:C6 | 2.29 | 0.68 |
| 23:DB:352:A:H3' | 23:DB:353:C:H6 | 1.59 | 0.68 |
| 27:DE:108:ILE:HD11 | 27:DE:181:ILE:HB | 1.75 | 0.68 |
| 30:DH:2:GLN:O | 30:DH:3:VAL:HG22 | 1.94 | 0.68 |
| 30:DH:94:ILE:HG13 | 30:DH:98:ASP:HB3 | 1.75 | 0.68 |
| 19:AT:61:ALA:HA | 19:AT:67:HIS:H | 1.58 | 0.68 |
| 23:BB:1028:A:H2' | 23:BB:1029:A:C8 | 2.29 | 0.68 |
| 23:BB:1041:G:H2' | 23:BB:1042:G:C8 | 2.29 | 0.68 |
| 29:BG:84:LYS:HB3 | 29:BG:132:LEU:O | 1.94 | 0.68 |
| 40:BS:73:LYS:HE3 | 40:BS:74:ILE:H | 1.58 | 0.68 |
| 40:BS:81:SER:HA | 40:BS:99:ARG:HA | 1.76 | 0.68 |
| 1:CA:559:A:H4' | 1:CA:560:A:H3' | 1.76 | 0.68 |
| 1:CA:89:U:H2' | 1:CA:90:C:C6 | 2.28 | 0.68 |
| 2:CC:51:VAL:HA | 2:CC:69:THR:HA | 1.74 | 0.68 |
| 1:CA:108:G:C6 | 19:CT:9:ARG:HG2 | 2.29 | 0.68 |
| 23:DB:858:G:H21 | 23:DB:2268:A:H3' | 1.59 | 0.68 |
| 25:DC:14:HIS:O | 25:DC:203:VAL:HG11 | 1.93 | 0.68 |
| 25:DC:74:PRO:HG2 | 25:DC:96:LYS:HG3 | 1.76 | 0.68 |
| 37:DP:3:ILE:HD13 | 37:DP:7:LEU:HD11 | 1.74 | 0.68 |
| 23:DB:499:U:H5' | 42:DU:44:HIS:HE1 | 1.58 | 0.68 |
| 44:DX:31:GLN:HG2 | 44:DX:37:LEU:HB2 | 1.75 | 0.68 |
| 45:DY:8:GLN:CG | 45:DY:31:ILE:HA | 2.19 | 0.68 |
| 20:AB:9:LEU:H | 20:AB:9:LEU:HD12 | 1.57 | 0.68 |
| 4:AE:84:VAL:HG11 | 4:AE:146:MET:HB3 | 1.74 | 0.68 |
| 1:AA:108:G:O6 | 19:AT:9:ARG:HG2 | 1.93 | 0.68 |
| 23:BB:2732:G:H5' | 23:BB:2733:A:O4' | 1.93 | 0.68 |
| 24:BV:40:ILE:H | 24:BV:40:ILE:HD13 | 1.59 | 0.68 |
| 1:CA:1134:G:C2 | 1:CA:1135:U:H1' | 2.29 | 0.68 |
| 1:CA:1238:A:H5' | 1:CA:1336:C:H41 | 1.59 | 0.68 |
| 1:CA:1505:G:H4' | 1:CA:1506:U:H5'' | 1.73 | 0.68 |
| 1:CA:97:G:H2' | 1:CA:98:A:O4' | 1.94 | 0.68 |
| 19:CT:61:ALA:HA | 19:CT:67:HIS:H | 1.59 | 0.68 |
| 47:D0:38:LEU:HB3 | 47:D0:41:HIS:NE2 | 2.09 | 0.68 |
| 23:DB:171:U:H2' | 23:DB:172:A:H8 | 1.57 | 0.68 |
| 23:DB:2153:C:H2' | 23:DB:2154:A:C8 | 2.29 | 0.68 |
| 52:DI:73:PRO:HG2 | 52:DI:78:LEU:HD21 | 1.74 | 0.68 |
| 1:AA:1513:A:H2' | 1:AA:1514:G:C8 | 2.29 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1021:A:H61 | 23:BB:1142:A:N6 | 1.92 | 0.68 |
| 23:BB:2340:A:H2' | 23:BB:2341:G:H8 | 1.59 | 0.68 |
| 28:BF:134:GLN:NE2 | 28:BF:136:ILE:HD13 | 2.08 | 0.68 |
| 37:BP:13:LYS:HD3 | 37:BP:76:HIS:HA | 1.75 | 0.68 |
| 23:BB:2365:G:H4' | 43:BW:59:PHE:HE1 | 1.57 | 0.68 |
| 1:CA:344:A:H4' | 1:CA:345:C:OP2 | 1.93 | 0.68 |
| 5:CF:64:VAL:HG12 | 5:CF:65:GLU:H | 1.57 | 0.68 |
| 26:DD:24:VAL:HG21 | 26:DD:188:LEU:HB3 | 1.75 | 0.68 |
| 37:DP:61:ARG:HD3 | 37:DP:70:GLU:HG3 | 1.76 | 0.68 |
| 42:DU:86:PHE:HB2 | 42:DU:92:VAL:HB | 1.73 | 0.68 |
| 23:BB:1353:A:H2' | 23:BB:1354:A:C8 | 2.29 | 0.68 |
| 23:BB:2064:C:H2' | 23:BB:2065:C:C6 | 2.29 | 0.68 |
| 25:BC:16:VAL:H | 25:BC:203:VAL:HG12 | 1.59 | 0.68 |
| 29:BG:140:ILE:HA | 29:BG:143:VAL:HG22 | 1.76 | 0.68 |
| 31:BJ:17:VAL:HG22 | 31:BJ:55:ILE:HD11 | 1.76 | 0.68 |
| 34:BM:10:ARG:HE | 34:BM:89:VAL:HG21 | 1.59 | 0.68 |
| 40:BS:52:GLU:HA | 40:BS:55:ILE:HG22 | 1.76 | 0.68 |
| 41:BT:38:ALA:HB3 | 41:BT:81:LYS:NZ | 2.09 | 0.68 |
| 43:BW:24:ARG:HA | 43:BW:66:VAL:H | 1.59 | 0.68 |
| 1:CA:1234:C:O2' | 1:CA:1235:U:H5' | 1.94 | 0.68 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:H8 | 1.59 | 0.68 |
| 1:CA:1414:U:H2' | 1:CA:1415:G:H8 | 1.60 | 0.68 |
| 1:CA:239:U:OP1 | 1:CA:239:U:H4' | 1.92 | 0.68 |
| 6:CG:91:ARG:HB3 | 6:CG:92:PRO:HD2 | 1.76 | 0.68 |
| 11:CL:49:ARG:HG2 | 11:CL:89:LEU:HD21 | 1.75 | 0.68 |
| 16:CQ:16:MET:CB | 16:CQ:19:SER:HB2 | 2.23 | 0.68 |
| 18:CS:31:ARG:HA | 18:CS:49:ALA:HB3 | 1.76 | 0.68 |
| 25:DC:76:VAL:HA | 25:DC:113:ASP:O | 1.94 | 0.68 |
| 29:DG:103:ASN:HD21 | 29:DG:111:PRO:HB3 | 1.58 | 0.68 |
| 34:DM:4:PRO:HG3 | 34:DM:68:PHE:HE2 | 1.59 | 0.68 |
| 1:AA:1486:G:H2' | 1:AA:1487:G:O4' | 1.94 | 0.67 |
| 1:AA:279:A:H5'' | 1:AA:280:C:H3' | 1.74 | 0.67 |
| 1:AA:451:A:H5' | 15:AP:70:ARG:HH22 | 1.59 | 0.67 |
| 3:AD:47:LEU:HB2 | 3:AD:51:GLY:HA3 | 1.77 | 0.67 |
| 11:AL:106:VAL:HG23 | 11:AL:116:TYR:HB3 | 1.76 | 0.67 |
| 13:AN:86:ALA:HB1 | 13:AN:91:GLU:HB2 | 1.74 | 0.67 |
| 23:BB:1102:C:O2' | 23:BB:1103:A:H5' | 1.94 | 0.67 |
| 23:BB:1447:C:H2' | 23:BB:1448:G:C8 | 2.29 | 0.67 |
| 23:BB:2658:C:H5' | 29:BG:159:LYS:HZ2 | 1.59 | 0.67 |
| 23:BB:742:A:H2' | 23:BB:743:A:H8 | 1.59 | 0.67 |
| 31:BJ:89:PHE:HE1 | 31:BJ:93:ILE:HD13 | 1.57 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:BM:64:TRP:HB2 | 34:BM:104:GLU:HB2 | 1.76 | 0.67 |
| 24:BV:44:HIS:CE1 | 24:BV:86:LEU:H | 2.08 | 0.67 |
| 43:BW:23:LYS:HD2 | 43:BW:24:ARG:H | 1.59 | 0.67 |
| 1:CA:1306:A:N6 | 1:CA:1331:G:H1' | 2.09 | 0.67 |
| 1:CA:1513:A:H2' | 1:CA:1514:G:C8 | 2.29 | 0.67 |
| 1:CA:810:C:O2' | 1:CA:811:C:H5' | 1.93 | 0.67 |
| 1:CA:973:G:H3' | 1:CA:974:A:H5'' | 1.76 | 0.67 |
| 3:CD:56:GLU:HG2 | 3:CD:198:LEU:HD12 | 1.77 | 0.67 |
| 12:CM:70:ARG:O | 12:CM:74:MET:HG2 | 1.94 | 0.67 |
| 23:DB:143:C:H2' | 23:DB:144:A:C8 | 2.28 | 0.67 |
| 23:DB:1592:C:H2' | 23:DB:1593:A:C8 | 2.29 | 0.67 |
| 23:DB:277:G:H4' | 23:DB:278:A:C5 | 2.29 | 0.67 |
| 23:DB:2866:U:H4' | 23:DB:2867:G:H4' | 1.75 | 0.67 |
| 26:DD:37:VAL:HG23 | 26:DD:91:THR:HA | 1.76 | 0.67 |
| 36:DO:88:LYS:HD2 | 36:DO:89:ASP:N | 2.09 | 0.67 |
| 24:DV:20:LEU:HB3 | 24:DV:25:LYS:O | 1.94 | 0.67 |
| 1:AA:195:A:H1' | 1:AA:222:C:O2' | 1.94 | 0.67 |
| 1:AA:80:A:H3' | 1:AA:81:A:H8 | 1.57 | 0.67 |
| 2:AC:2:GLN:H | 2:AC:2:GLN:NE2 | 1.92 | 0.67 |
| 16:AQ:16:MET:CB | 16:AQ:19:SER:HB2 | 2.24 | 0.67 |
| 21:AU:38:GLU:C | 21:AU:40:PRO:HD2 | 2.14 | 0.67 |
| 23:BB:145:C:H2' | 23:BB:146:A:H8 | 1.59 | 0.67 |
| 23:BB:152:A:H2' | 23:BB:153:U:C6 | 2.30 | 0.67 |
| 27:BE:47:LYS:HB3 | 27:BE:51:GLU:HB2 | 1.75 | 0.67 |
| 31:BJ:37:ARG:HE | 31:BJ:110:PRO:HG3 | 1.59 | 0.67 |
| 31:BJ:43:GLU:O | 31:BJ:45:THR:N | 2.27 | 0.67 |
| 20:CB:199:ILE:HD13 | 20:CB:212:TYR:HE2 | 1.59 | 0.67 |
| 21:AU:10:PRO:HG3 | 2:CC:71:ARG:HH21 | 1.59 | 0.67 |
| 1:CA:1060:U:C4' | 9:CJ:54:SER:HB2 | 2.24 | 0.67 |
| 21:CU:38:GLU:C | 21:CU:40:PRO:HD2 | 2.14 | 0.67 |
| 23:DB:729:G:H2' | 23:DB:1775:U:H1' | 1.76 | 0.67 |
| 23:DB:1866:A:H2' | 23:DB:1867:G:O4' | 1.94 | 0.67 |
| 23:DB:2108:A:N3 | 23:DB:2108:A:H2' | 2.09 | 0.67 |
| 23:DB:222:A:N6 | 23:DB:232:G:H1' | 2.09 | 0.67 |
| 23:DB:2400:G:O2' | 23:DB:2401:U:H5' | 1.94 | 0.67 |
| 23:DB:2886:A:H3' | 23:DB:2887:A:H8 | 1.59 | 0.67 |
| 33:DL:116:VAL:HG13 | 33:DL:117:THR:H | 1.57 | 0.67 |
| 39:DR:60:LYS:H | 39:DR:100:GLY:CA | 2.07 | 0.67 |
| 1:AA:763:G:H2' | 1:AA:764:C:H6 | 1.59 | 0.67 |
| 11:AL:37:TYR:HB2 | 11:AL:51:VAL:HB | 1.75 | 0.67 |
| 15:AP:28:ARG:HD2 | 15:AP:29:ASN:N | 2.06 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1314:C:H3' | 18:AS:5:LYS:HZ2 | 1.59 | 0.67 |
| 23:BB:246:C:C2' | 23:BB:247:G:H5' | 2.24 | 0.67 |
| 23:BB:460:A:H2' | 23:BB:461:C:O4' | 1.94 | 0.67 |
| 23:BB:545:U:H3 | 23:BB:548:G:P | 2.17 | 0.67 |
| 31:BJ:45:THR:H | 31:BJ:46:PRO:HD3 | 1.59 | 0.67 |
| 41:BT:11:LEU:HD21 | 41:BT:46:ALA:HB1 | 1.75 | 0.67 |
| 1:CA:376:G:H5'' | 15:CP:5:ARG:HB2 | 1.76 | 0.67 |
| 3:CD:153:ARG:HG3 | 3:CD:154:VAL:N | 2.07 | 0.67 |
| 8:CI:29:ILE:HA | 8:CI:64:ILE:O | 1.95 | 0.67 |
| 23:DB:152:A:H2' | 23:DB:153:U:C6 | 2.30 | 0.67 |
| 23:DB:181:A:H2' | 23:DB:182:A:C8 | 2.30 | 0.67 |
| 23:DB:2336:A:H61 | 43:DW:40:ARG:CD | 2.07 | 0.67 |
| 23:DB:729:G:OP1 | 25:DC:12:ARG:HB2 | 1.95 | 0.67 |
| 26:DD:172:VAL:HG11 | 26:DD:175:LEU:HD12 | 1.76 | 0.67 |
| 38:DQ:63:ARG:HA | 38:DQ:66:ALA:HB3 | 1.75 | 0.67 |
| 1:AA:1132:C:H2' | 1:AA:1133:G:H8 | 1.58 | 0.67 |
| 1:AA:973:G:H3' | 1:AA:974:A:H5'' | 1.75 | 0.67 |
| 1:AA:98:A:H2' | 1:AA:99:C:O4' | 1.94 | 0.67 |
| 1:AA:1148:U:H5' | 8:AI:6:TYR:OH | 1.94 | 0.67 |
| 23:BB:2292:U:H2' | 23:BB:2293:G:C8 | 2.29 | 0.67 |
| 29:BG:89:VAL:HB | 29:BG:159:LYS:HA | 1.76 | 0.67 |
| 22:DA:75:G:H1' | 24:DV:29:ILE:HG12 | 1.76 | 0.67 |
| 35:DN:49:GLU:OE2 | 35:DN:95:THR:HG22 | 1.94 | 0.67 |
| 37:DP:5:LYS:HE2 | 37:DP:5:LYS:HA | 1.75 | 0.67 |
| 3:AD:36:ALA:HA | 3:AD:41:GLY:HA3 | 1.75 | 0.67 |
| 8:AI:71:ILE:HD12 | 8:AI:71:ILE:H | 1.59 | 0.67 |
| 23:BB:322:A:H3' | 27:BE:163:ASN:HD21 | 1.59 | 0.67 |
| 23:BB:634:C:H2' | 23:BB:635:C:H6 | 1.60 | 0.67 |
| 23:BB:729:G:H2' | 23:BB:1775:U:H1' | 1.75 | 0.67 |
| 25:BC:16:VAL:HB | 25:BC:203:VAL:HB | 1.77 | 0.67 |
| 29:BG:103:ASN:HD21 | 29:BG:111:PRO:HB3 | 1.58 | 0.67 |
| 23:BB:571:U:H3' | 39:BR:80:ARG:HH12 | 1.59 | 0.67 |
| 1:CA:108:G:O6 | 19:CT:9:ARG:HG2 | 1.95 | 0.67 |
| 16:CQ:20:ILE:HD13 | 16:CQ:47:ASP:HB3 | 1.76 | 0.67 |
| 23:DB:1447:C:H2' | 23:DB:1448:G:C8 | 2.29 | 0.67 |
| 23:DB:1486:U:H2' | 23:DB:1487:U:C6 | 2.28 | 0.67 |
| 23:DB:2039:U:H2' | 23:DB:2040:G:C8 | 2.29 | 0.67 |
| 43:DW:43:LYS:HD2 | 43:DW:79:ILE:HD11 | 1.76 | 0.67 |
| 1:AA:1297:G:H1' | 1:AA:1298:U:H5 | 1.60 | 0.67 |
| 1:AA:1323:G:H2' | 1:AA:1324:A:H8 | 1.55 | 0.67 |
| 12:AM:28:ARG:NH2 | 12:AM:62:PHE:HB2 | 2.09 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AU:9:GLU:HG2 | 2:CC:108:PRO:CG | 2.24 | 0.67 |
| 25:BC:180:MET:HB3 | 25:BC:267:VAL:HB | 1.77 | 0.67 |
| 27:BE:188:MET:HG2 | 27:BE:193:VAL:HG22 | 1.75 | 0.67 |
| 1:CA:1314:C:H3' | 18:CS:5:LYS:HZ2 | 1.58 | 0.67 |
| 23:DB:145:C:H2' | 23:DB:146:A:H8 | 1.59 | 0.67 |
| 23:DB:95:A:H4' | 44:DX:38:GLN:O | 1.94 | 0.67 |
| 31:DJ:57:LEU:HD11 | 31:DJ:129:GLU:H | 1.58 | 0.67 |
| 31:DJ:32:LEU:O | 31:DJ:36:LEU:HD23 | 1.95 | 0.67 |
| 32:DK:71:ARG:HD2 | 32:DK:105:ARG:NE | 2.07 | 0.67 |
| 37:DP:19:PHE:O | 37:DP:20:ARG:HB2 | 1.93 | 0.67 |
| 1:AA:337:G:H2' | 1:AA:338:A:H8 | 1.60 | 0.67 |
| 1:AA:882:C:O2' | 1:AA:883:C:H5' | 1.93 | 0.67 |
| 12:AM:64:VAL:HA | 12:AM:68:LEU:HD11 | 1.75 | 0.67 |
| 18:AS:41:PRO:O | 18:AS:44:ILE:HG22 | 1.95 | 0.67 |
| 23:BB:1050:A:H2' | 23:BB:1051:G:H8 | 1.59 | 0.67 |
| 23:BB:125:A:H3' | 23:BB:126:A:C5' | 2.24 | 0.67 |
| 23:BB:1911:U:H2' | 23:BB:1918:A:C2 | 2.30 | 0.67 |
| 23:BB:2425:A:H5' | 23:BB:2427:C:O4' | 1.94 | 0.67 |
| 23:BB:575:A:O2' | 23:BB:576:U:H5' | 1.94 | 0.67 |
| 26:BD:124:ARG:HA | 26:BD:165:MET:HE3 | 1.77 | 0.67 |
| 6:CG:23:ALA:O | 6:CG:26:VAL:HG22 | 1.95 | 0.67 |
| 18:CS:38:THR:HA | 18:CS:69:LYS:HA | 1.77 | 0.67 |
| 23:DB:1287:A:H3' | 23:DB:1288:G:N2 | 2.09 | 0.67 |
| 25:DC:127:ASN:O | 25:DC:190:THR:HA | 1.95 | 0.67 |
| 26:DD:141:ARG:O | 26:DD:141:ARG:HG3 | 1.95 | 0.67 |
| 26:DD:62:LYS:HD2 | 26:DD:62:LYS:H | 1.60 | 0.67 |
| 23:DB:2298:A:OP1 | 28:DF:70:ARG:HD3 | 1.94 | 0.67 |
| 23:DB:812:C:H4' | 38:DQ:12:ARG:HH22 | 1.59 | 0.67 |
| 40:DS:81:SER:HA | 40:DS:99:ARG:HA | 1.76 | 0.67 |
| 46:DZ:6:GLN:HE22 | 46:DZ:50:ARG:N | 1.90 | 0.67 |
| 1:AA:1258:G:H2' | 1:AA:1259:C:C6 | 2.30 | 0.67 |
| 14:AO:28:VAL:HG11 | 14:AO:80:LEU:HD21 | 1.77 | 0.67 |
| 23:BB:1654:A:H2' | 23:BB:1655:A:H8 | 1.59 | 0.67 |
| 23:BB:280:U:H2' | 23:BB:281:C:C6 | 2.29 | 0.67 |
| 30:BH:127:GLU:HA | 30:BH:144:VAL:O | 1.94 | 0.67 |
| 30:BH:116:ARG:NE | 30:BH:139:PHE:HB2 | 2.10 | 0.67 |
| 36:BO:11:ALA:CB | 36:BO:96:GLY:H | 2.06 | 0.67 |
| 20:CB:113:LEU:HD13 | 20:CB:147:LEU:HB2 | 1.75 | 0.67 |
| 2:CC:171:ARG:HH11 | 2:CC:171:ARG:HB2 | 1.58 | 0.67 |
| 13:CN:68:ARG:NH1 | 13:CN:71:GLY:H | 1.92 | 0.67 |
| 50:D3:41:ARG:HA | 50:D3:44:ARG:HH21 | 1.58 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1461:C:H2' | 23:DB:1462:C:H6 | 1.58 | 0.67 |
| 23:DB:2808:G:HO2' | 23:DB:2809:A:H8 | 1.43 | 0.67 |
| 23:DB:634:C:H2' | 23:DB:635:C:H6 | 1.59 | 0.67 |
| 23:DB:636:G:H3' | 33:DL:128:THR:HG21 | 1.75 | 0.67 |
| 28:DF:16:MET:O | 28:DF:20:ASN:HA | 1.95 | 0.67 |
| 23:DB:2312:U:O2 | 28:DF:38:GLY:HA3 | 1.95 | 0.67 |
| 1:AA:344:A:H4' | 1:AA:345:C:OP2 | 1.94 | 0.67 |
| 1:AA:373:A:H2' | 1:AA:374:A:H8 | 1.59 | 0.67 |
| 1:AA:539:A:H2' | 1:AA:540:G:C8 | 2.30 | 0.67 |
| 20:AB:113:LEU:HD13 | 20:AB:147:LEU:HB2 | 1.76 | 0.67 |
| 2:AC:149:LYS:HA | 2:AC:168:ARG:HB2 | 1.77 | 0.67 |
| 12:AM:89:ARG:HG3 | 12:AM:96:VAL:HG13 | 1.76 | 0.67 |
| 23:BB:1032:A:H1' | 51:B4:23:ILE:HD13 | 1.77 | 0.67 |
| 23:BB:18:U:H2' | 23:BB:19:A:C8 | 2.30 | 0.67 |
| 26:BD:107:VAL:HG13 | 26:BD:203:VAL:HG23 | 1.76 | 0.67 |
| 38:BQ:63:ARG:HA | 38:BQ:66:ALA:HB3 | 1.76 | 0.67 |
| 24:BV:51:GLN:NE2 | 24:BV:79:ARG:HH22 | 1.92 | 0.67 |
| 1:CA:865:A:H2 | 1:CA:918:A:H4' | 1.60 | 0.67 |
| 23:DB:163:C:H2' | 23:DB:164:C:O4' | 1.94 | 0.67 |
| 23:DB:528:A:C2 | 23:DB:2042:A:H2' | 2.30 | 0.67 |
| 26:DD:5:VAL:N | 26:DD:32:ASN:HD21 | 1.90 | 0.67 |
| 26:DD:33:ARG:NE | 26:DD:74:GLU:HB3 | 2.10 | 0.67 |
| 35:DN:24:MET:HE1 | 35:DN:40:LYS:HD2 | 1.77 | 0.67 |
| 35:DN:34:ILE:HB | 35:DN:113:ILE:HG22 | 1.77 | 0.67 |
| 42:DU:81:ARG:H | 42:DU:81:ARG:NH2 | 1.93 | 0.67 |
| 1:AA:1513:A:H2' | 1:AA:1514:G:H8 | 1.58 | 0.67 |
| 6:AG:72:VAL:HG12 | 6:AG:89:GLU:HB3 | 1.76 | 0.67 |
| 9:AJ:7:ARG:O | 9:AJ:100:ILE:HA | 1.95 | 0.67 |
| 23:BB:1000:A:H2' | 23:BB:1001:A:C8 | 2.30 | 0.67 |
| 23:BB:1440:U:H2' | 23:BB:1441:G:C8 | 2.30 | 0.67 |
| 23:BB:718:A:H2' | 23:BB:719:C:H5' | 1.77 | 0.67 |
| 23:BB:849:A:H2' | 23:BB:850:U:C6 | 2.30 | 0.67 |
| 25:BC:196:ASN:ND2 | 25:BC:199:HIS:HB2 | 2.10 | 0.67 |
| 27:BE:108:ILE:HD11 | 27:BE:181:ILE:HB | 1.76 | 0.67 |
| 28:BF:135:ILE:HD11 | 28:BF:137:PHE:HB3 | 1.77 | 0.67 |
| 32:BK:54:LYS:H | 32:BK:54:LYS:HD2 | 1.58 | 0.67 |
| 38:BQ:104:ALA:HA | 39:BR:46:GLU:OE1 | 1.93 | 0.67 |
| 43:BW:47:GLY:HA3 | 43:BW:80:SER:HA | 1.77 | 0.67 |
| 1:CA:157:U:O2' | 1:CA:158:G:H5' | 1.94 | 0.67 |
| 48:D1:32:LYS:HA | 48:D1:51:ALA:O | 1.95 | 0.67 |
| 23:DB:1060:U:O2 | 23:DB:1088:A:N7 | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DN:78:LYS:HG3 | 35:DN:83:LEU:HG | 1.76 | 0.67 |
| 44:DX:1:MET:HB3 | 44:DX:4:LYS:HB3 | 1.77 | 0.67 |
| 1:AA:235:C:H2' | 1:AA:236:A:C8 | 2.29 | 0.66 |
| 23:BB:858:G:H21 | 23:BB:2268:A:H3' | 1.59 | 0.66 |
| 23:BB:547:A:H3' | 23:BB:548:G:C8 | 2.25 | 0.66 |
| 1:CA:229:U:H2' | 1:CA:230:G:C8 | 2.30 | 0.66 |
| 8:CI:87:MET:HA | 8:CI:93:LEU:HD11 | 1.77 | 0.66 |
| 23:DB:309:A:H4' | 42:DU:15:GLY:CA | 2.25 | 0.66 |
| 23:DB:361:G:O2' | 23:DB:362:A:H5' | 1.94 | 0.66 |
| 25:DC:36:ASN:HD21 | 25:DC:85:ASN:ND2 | 1.93 | 0.66 |
| 27:DE:127:GLU:HB2 | 27:DE:133:LEU:HD13 | 1.77 | 0.66 |
| 33:DL:101:ILE:HG22 | 33:DL:105:ILE:HG13 | 1.77 | 0.66 |
| 23:DB:329:G:H1 | 42:DU:16:LYS:HG2 | 1.60 | 0.66 |
| 1:AA:157:U:O2' | 1:AA:158:G:H5' | 1.95 | 0.66 |
| 1:AA:17:U:H2' | 1:AA:18:C:H6 | 1.60 | 0.66 |
| 12:AM:2:ARG:H | 12:AM:2:ARG:HD3 | 1.58 | 0.66 |
| 23:BB:2243:U:H2' | 23:BB:2244:U:C6 | 2.31 | 0.66 |
| 23:BB:2400:G:O2' | 23:BB:2401:U:H5' | 1.95 | 0.66 |
| 28:BF:101:ARG:HA | 28:BF:105:ILE:HD13 | 1.76 | 0.66 |
| 30:BH:133:GLN:HB2 | 30:BH:139:PHE:HA | 1.77 | 0.66 |
| 30:BH:90:LEU:HD21 | 30:BH:146:VAL:HG11 | 1.76 | 0.66 |
| 32:BK:70:ARG:HB3 | 32:BK:76:VAL:HG22 | 1.77 | 0.66 |
| 41:BT:54:GLU:HG3 | 41:BT:90:GLY:H | 1.57 | 0.66 |
| 1:CA:1388:C:H2' | 1:CA:1389:C:H6 | 1.60 | 0.66 |
| 1:CA:21:G:H2' | 1:CA:22:G:C8 | 2.30 | 0.66 |
| 1:CA:415:A:H3' | 1:CA:416:G:H8 | 1.60 | 0.66 |
| 1:CA:706:A:H4' | 10:CK:30:ILE:HD11 | 1.77 | 0.66 |
| 15:CP:34:GLU:CD | 15:CP:60:TRP:HE1 | 1.99 | 0.66 |
| 23:DB:246:C:C2' | 23:DB:247:G:H5' | 2.26 | 0.66 |
| 23:DB:545:U:C5 | 23:DB:547:A:H5'' | 2.31 | 0.66 |
| 23:DB:620:G:N3 | 23:DB:620:G:H5' | 2.10 | 0.66 |
| 30:DH:48:GLU:HA | 30:DH:51:ARG:HE | 1.60 | 0.66 |
| 31:DJ:56:VAL:HG12 | 31:DJ:57:LEU:H | 1.60 | 0.66 |
| 32:DK:17:ARG:HB3 | 32:DK:45:GLU:HG3 | 1.75 | 0.66 |
| 34:DM:66:ARG:NE | 34:DM:101:VAL:HG11 | 2.09 | 0.66 |
| 40:DS:32:ALA:O | 40:DS:35:ILE:HB | 1.95 | 0.66 |
| 41:DT:54:GLU:HG3 | 41:DT:90:GLY:H | 1.58 | 0.66 |
| 43:DW:77:LYS:O | 43:DW:78:PHE:HB2 | 1.95 | 0.66 |
| 1:AA:21:G:H2' | 1:AA:22:G:C8 | 2.31 | 0.66 |
| 1:AA:841:C:O5' | 1:AA:842:U:H5'' | 1.95 | 0.66 |
| 6:AG:91:ARG:HB3 | 6:AG:92:PRO:HD2 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:B0:38:LEU:HB3 | 47:B0:41:HIS:NE2 | 2.11 | 0.66 |
| 23:BB:1812:U:H2' | 23:BB:1813:G:H8 | 1.61 | 0.66 |
| 23:BB:528:A:C2 | 23:BB:2042:A:H2' | 2.29 | 0.66 |
| 23:BB:222:A:H61 | 23:BB:232:G:H1' | 1.57 | 0.66 |
| 23:BB:2443:C:H2' | 23:BB:2444:G:H8 | 1.59 | 0.66 |
| 26:BD:14:ILE:HA | 37:BP:11:GLN:HE22 | 1.60 | 0.66 |
| 32:BK:68:GLY:HA3 | 32:BK:78:ARG:HB3 | 1.77 | 0.66 |
| 33:BL:79:LEU:HD23 | 33:BL:82:LEU:HD11 | 1.76 | 0.66 |
| 38:BQ:34:ALA:O | 38:BQ:37:ALA:HB3 | 1.95 | 0.66 |
| 42:BU:87:GLU:OE2 | 42:BU:88:ASP:HB3 | 1.95 | 0.66 |
| 1:CA:6:G:N3 | 1:CA:6:G:H3' | 2.09 | 0.66 |
| 6:CG:72:VAL:HG12 | 6:CG:89:GLU:HB3 | 1.78 | 0.66 |
| 1:CA:1382:C:H4' | 6:CG:78:ARG:CZ | 2.25 | 0.66 |
| 10:CK:83:VAL:HG21 | 10:CK:109:ILE:HG12 | 1.76 | 0.66 |
| 13:CN:52:ARG:NH1 | 13:CN:58:ARG:HH21 | 1.92 | 0.66 |
| 23:DB:1464:G:H2' | 23:DB:1465:G:C8 | 2.31 | 0.66 |
| 23:DB:2591:C:H2' | 23:DB:2592:G:H8 | 1.60 | 0.66 |
| 23:DB:812:C:H4' | 38:DQ:12:ARG:HH12 | 1.60 | 0.66 |
| 28:DF:30:VAL:HG21 | 28:DF:96:TRP:HE1 | 1.59 | 0.66 |
| 36:DO:51:ALA:HB3 | 36:DO:78:VAL:HG22 | 1.76 | 0.66 |
| 40:DS:17:VAL:C | 40:DS:19:LEU:H | 1.99 | 0.66 |
| 24:DV:40:ILE:HD13 | 24:DV:40:ILE:H | 1.60 | 0.66 |
| 1:AA:1152:A:H2' | 1:AA:1153:G:H8 | 1.61 | 0.66 |
| 1:AA:1432:G:H5'' | 37:BP:105:LYS:CG | 2.25 | 0.66 |
| 20:AB:119:GLN:O | 20:AB:124:THR:HG23 | 1.96 | 0.66 |
| 20:AB:209:VAL:HG23 | 20:AB:210:THR:H | 1.61 | 0.66 |
| 7:AH:6:ILE:HD11 | 7:AH:31:LEU:HD23 | 1.78 | 0.66 |
| 7:AH:51:GLU:HG2 | 7:AH:52:GLY:H | 1.61 | 0.66 |
| 1:AA:1343:G:H1' | 8:AI:122:ARG:NH1 | 2.10 | 0.66 |
| 11:AL:122:LYS:HD2 | 11:AL:123:ALA:N | 2.10 | 0.66 |
| 23:BB:1486:U:H2' | 23:BB:1487:U:H6 | 1.60 | 0.66 |
| 23:BB:1676:A:H2' | 23:BB:1677:A:O4' | 1.95 | 0.66 |
| 23:BB:1866:A:H2' | 23:BB:1867:G:O4' | 1.96 | 0.66 |
| 23:BB:2461:A:H2' | 23:BB:2462:C:C6 | 2.30 | 0.66 |
| 23:BB:499:U:H5' | 42:BU:44:HIS:HE1 | 1.60 | 0.66 |
| 26:BD:68:PHE:HB3 | 26:BD:73:VAL:HA | 1.77 | 0.66 |
| 27:BE:189:THR:O | 27:BE:193:VAL:HG23 | 1.96 | 0.66 |
| 34:BM:78:LEU:O | 34:BM:80:VAL:HG12 | 1.95 | 0.66 |
| 38:BQ:91:ARG:NH2 | 39:BR:11:GLN:H | 1.94 | 0.66 |
| 1:CA:1288:A:N1 | 1:CA:1371:G:H1' | 2.10 | 0.66 |
| 20:CB:212:TYR:HA | 20:CB:215:ALA:HB3 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:D1:26:LYS:HB2 | 48:D1:52:LYS:HZ2 | 1.61 | 0.66 |
| 23:DB:414:C:H2' | 23:DB:415:A:C8 | 2.30 | 0.66 |
| 27:DE:47:LYS:HB3 | 27:DE:51:GLU:HB2 | 1.78 | 0.66 |
| 30:DH:63:ALA:HA | 30:DH:66:ASN:ND2 | 2.10 | 0.66 |
| 38:DQ:104:ALA:HA | 39:DR:46:GLU:CD | 2.16 | 0.66 |
| 1:AA:129:A:H1' | 1:AA:130:A:C8 | 2.31 | 0.66 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:H8 | 1.61 | 0.66 |
| 1:AA:865:A:H2 | 1:AA:918:A:H4' | 1.59 | 0.66 |
| 10:AK:33:ILE:HG13 | 10:AK:73:VAL:HG21 | 1.77 | 0.66 |
| 23:BB:2039:U:H2' | 23:BB:2040:G:C8 | 2.28 | 0.66 |
| 23:BB:2376:A:H61 | 36:BO:94:ARG:HD3 | 1.60 | 0.66 |
| 23:BB:634:C:H2' | 23:BB:635:C:C6 | 2.30 | 0.66 |
| 25:BC:131:MET:HE2 | 25:BC:143:VAL:HG13 | 1.75 | 0.66 |
| 27:BE:127:GLU:HB2 | 27:BE:133:LEU:HD13 | 1.78 | 0.66 |
| 32:BK:71:ARG:HD2 | 32:BK:105:ARG:NE | 2.08 | 0.66 |
| 44:BX:23:ARG:HD2 | 44:BX:27:ASN:HD21 | 1.60 | 0.66 |
| 1:CA:1078:U:H4' | 4:CE:137:ARG:HH12 | 1.57 | 0.66 |
| 1:CA:1080:A:H2' | 1:CA:1081:A:H5' | 1.78 | 0.66 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:C8 | 2.29 | 0.66 |
| 20:CB:68:PHE:HA | 20:CB:161:PHE:O | 1.96 | 0.66 |
| 15:CP:28:ARG:CD | 15:CP:29:ASN:H | 2.05 | 0.66 |
| 23:DB:2471:A:O2' | 23:DB:2472:G:H8 | 1.78 | 0.66 |
| 28:DF:107:VAL:HG11 | 28:DF:175:PRO:HG3 | 1.77 | 0.66 |
| 28:DF:135:ILE:HD11 | 28:DF:137:PHE:HB3 | 1.76 | 0.66 |
| 37:DP:4:ILE:C | 37:DP:6:GLN:H | 1.99 | 0.66 |
| 42:DU:10:VAL:O | 42:DU:21:ARG:HA | 1.96 | 0.66 |
| 1:AA:473:U:H2' | 1:AA:474:G:C8 | 2.31 | 0.66 |
| 22:BA:6:G:H2' | 22:BA:7:G:H8 | 1.60 | 0.66 |
| 23:BB:2649:C:H2' | 23:BB:2650:U:H6 | 1.61 | 0.66 |
| 23:BB:45:G:H5' | 23:BB:46:G:H5' | 1.78 | 0.66 |
| 23:BB:857:G:O2' | 43:BW:19:ARG:HD2 | 1.96 | 0.66 |
| 39:BR:60:LYS:H | 39:BR:100:GLY:CA | 2.08 | 0.66 |
| 39:BR:39:LEU:HA | 39:BR:53:PHE:HA | 1.78 | 0.66 |
| 38:BQ:43:GLN:NE2 | 39:BR:77:PHE:HB3 | 2.11 | 0.66 |
| 23:BB:138:U:C1' | 41:BT:1:MET:H2 | 2.08 | 0.66 |
| 24:BV:80:HIS:CD2 | 24:BV:83:LYS:H | 2.13 | 0.66 |
| 1:CA:1342:C:H2' | 1:CA:1343:G:C8 | 2.30 | 0.66 |
| 1:CA:208:U:H2' | 1:CA:210:C:C4 | 2.30 | 0.66 |
| 3:CD:96:ARG:HB3 | 3:CD:98:ASP:OD2 | 1.95 | 0.66 |
| 4:CE:32:PHE:O | 4:CE:51:LYS:HB2 | 1.94 | 0.66 |
| 23:DB:1124:G:H1' | 51:D4:38:GLY:OXT | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:192:C:H2' | 23:DB:193:U:H5' | 1.78 | 0.66 |
| 23:DB:460:A:H2' | 23:DB:461:C:O4' | 1.96 | 0.66 |
| 23:DB:575:A:O2' | 23:DB:576:U:H5' | 1.95 | 0.66 |
| 30:DH:133:GLN:NE2 | 30:DH:139:PHE:HB3 | 2.10 | 0.66 |
| 39:DR:78:ARG:HB3 | 39:DR:83:TYR:HB3 | 1.77 | 0.66 |
| 43:DW:35:ILE:HA | 43:DW:57:THR:HG23 | 1.76 | 0.66 |
| 46:DZ:6:GLN:NE2 | 46:DZ:50:ARG:H | 1.90 | 0.66 |
| 1:AA:1080:A:H2' | 1:AA:1081:A:H5' | 1.78 | 0.66 |
| 1:AA:6:G:H3' | 1:AA:6:G:N3 | 2.09 | 0.66 |
| 1:AA:86:G:H1' | 1:AA:87:C:C5 | 2.30 | 0.66 |
| 8:AI:10:ARG:HA | 8:AI:77:ALA:HB1 | 1.76 | 0.66 |
| 8:AI:87:MET:HA | 8:AI:93:LEU:HD11 | 1.77 | 0.66 |
| 50:B3:54:LEU:O | 50:B3:58:ILE:HG13 | 1.96 | 0.66 |
| 23:BB:1387:A:C4' | 23:BB:1469:A:H1' | 2.26 | 0.66 |
| 23:BB:1993:U:H4' | 26:BD:133:THR:HG21 | 1.75 | 0.66 |
| 35:BN:101:GLY:HA2 | 35:BN:110:MET:H | 1.58 | 0.66 |
| 37:BP:45:VAL:N | 37:BP:60:VAL:HB | 2.10 | 0.66 |
| 1:CA:1095:U:H2' | 1:CA:1096:C:C6 | 2.30 | 0.66 |
| 1:CA:1417:G:H22 | 1:CA:1482:G:H2' | 1.60 | 0.66 |
| 1:CA:266:G:O2' | 1:CA:267:C:H3' | 1.96 | 0.66 |
| 1:CA:384:G:H2' | 1:CA:385:C:C6 | 2.30 | 0.66 |
| 23:DB:1440:U:H2' | 23:DB:1441:G:C8 | 2.30 | 0.66 |
| 23:DB:162:U:H4' | 23:DB:163:C:OP1 | 1.96 | 0.66 |
| 23:DB:1676:A:H2' | 23:DB:1677:A:O4' | 1.94 | 0.66 |
| 23:DB:2292:U:H2' | 23:DB:2293:G:C8 | 2.29 | 0.66 |
| 23:DB:2340:A:H2' | 23:DB:2341:G:H8 | 1.59 | 0.66 |
| 23:DB:2352:A:H2' | 23:DB:2353:G:O4' | 1.95 | 0.66 |
| 23:DB:634:C:H2' | 23:DB:635:C:C6 | 2.31 | 0.66 |
| 23:DB:784:G:N1 | 25:DC:227:VAL:HG11 | 2.10 | 0.66 |
| 27:DE:58:LYS:O | 27:DE:60:TRP:N | 2.29 | 0.66 |
| 31:DJ:43:GLU:O | 31:DJ:45:THR:N | 2.29 | 0.66 |
| 33:DL:56:PRO:HD2 | 33:DL:59:ARG:HG3 | 1.78 | 0.66 |
| 34:DM:78:LEU:O | 34:DM:80:VAL:HG12 | 1.95 | 0.66 |
| 42:DU:82:VAL:HG13 | 42:DU:93:ARG:HB3 | 1.78 | 0.66 |
| 43:DW:24:ARG:HA | 43:DW:66:VAL:H | 1.61 | 0.66 |
| 1:AA:1141:C:H2' | 1:AA:1142:G:H8 | 1.61 | 0.66 |
| 1:AA:384:G:H2' | 1:AA:385:C:C6 | 2.31 | 0.66 |
| 10:AK:108:ASN:ND2 | 21:AU:6:ARG:HB2 | 2.11 | 0.66 |
| 23:BB:1939:U:H6 | 23:BB:1939:U:H5' | 1.59 | 0.66 |
| 23:BB:279:A:C2 | 23:BB:362:A:H4' | 2.30 | 0.66 |
| 26:BD:5:VAL:N | 26:BD:32:ASN:HD21 | 1.90 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BD:37:VAL:HG23 | 26:BD:91:THR:HA | 1.76 | 0.66 |
| 27:BE:97:ASN:HD21 | 27:BE:100:MET:HG3 | 1.59 | 0.66 |
| 27:BE:69:ARG:O | 27:BE:70:SER:HB3 | 1.94 | 0.66 |
| 33:BL:101:ILE:HG22 | 33:BL:105:ILE:HG13 | 1.76 | 0.66 |
| 37:BP:20:ARG:HB3 | 37:BP:23:ASP:OD2 | 1.96 | 0.66 |
| 1:CA:673:A:H2' | 1:CA:674:G:C8 | 2.31 | 0.66 |
| 8:CI:10:ARG:HA | 8:CI:77:ALA:HB1 | 1.76 | 0.66 |
| 22:DA:56:G:H4' | 22:DA:57:A:H5' | 1.78 | 0.66 |
| 23:DB:1684:G:H2' | 23:DB:1685:C:C6 | 2.31 | 0.66 |
| 23:DB:2144:G:N3 | 23:DB:2146:C:H5' | 2.11 | 0.66 |
| 28:DF:102:LEU:HD22 | 28:DF:103:ILE:N | 2.09 | 0.66 |
| 23:DB:974:G:OP2 | 39:DR:78:ARG:HD3 | 1.96 | 0.66 |
| 1:AA:1095:U:H2' | 1:AA:1096:C:C6 | 2.31 | 0.66 |
| 20:AB:212:TYR:HA | 20:AB:215:ALA:HB3 | 1.78 | 0.66 |
| 2:AC:48:LYS:N | 2:AC:48:LYS:HE2 | 2.09 | 0.66 |
| 12:AM:89:ARG:NH2 | 12:AM:94:LEU:HD12 | 2.11 | 0.66 |
| 23:BB:1947:C:H2' | 23:BB:1948:G:H8 | 1.59 | 0.66 |
| 23:BB:2473:U:H2' | 23:BB:2473:U:O2 | 1.96 | 0.66 |
| 32:BK:112:PHE:O | 32:BK:115:ILE:HG22 | 1.95 | 0.66 |
| 35:BN:34:ILE:HB | 35:BN:113:ILE:HG22 | 1.78 | 0.66 |
| 44:BX:1:MET:HB3 | 44:BX:4:LYS:HB3 | 1.78 | 0.66 |
| 1:CA:1152:A:H2' | 1:CA:1153:G:H8 | 1.61 | 0.66 |
| 1:CA:575:G:H4' | 1:CA:576:C:O5' | 1.96 | 0.66 |
| 4:CE:45:VAL:HG12 | 4:CE:116:VAL:HG23 | 1.78 | 0.66 |
| 16:CQ:74:LEU:HD22 | 16:CQ:75:VAL:N | 2.08 | 0.66 |
| 23:DB:1099:G:C5' | 52:DI:3:LYS:N | 2.59 | 0.66 |
| 23:DB:1412:U:H2' | 23:DB:1413:A:C8 | 2.30 | 0.66 |
| 23:DB:2073:C:H5'' | 25:DC:227:VAL:HG12 | 1.78 | 0.66 |
| 23:DB:222:A:H61 | 23:DB:232:G:H1' | 1.58 | 0.66 |
| 23:DB:28:A:N6 | 23:DB:512:G:H1' | 2.11 | 0.66 |
| 23:DB:445:C:O2' | 23:DB:446:G:H5' | 1.96 | 0.66 |
| 23:DB:65:U:H2' | 23:DB:66:C:H6 | 1.61 | 0.66 |
| 25:DC:16:VAL:HB | 25:DC:203:VAL:HB | 1.77 | 0.66 |
| 23:DB:2680:U:OP2 | 26:DD:114:LYS:HB3 | 1.95 | 0.66 |
| 28:DF:87:LYS:HG3 | 28:DF:88:VAL:H | 1.60 | 0.66 |
| 40:DS:4:ILE:HG22 | 40:DS:106:VAL:HG13 | 1.77 | 0.66 |
| 43:DW:23:LYS:HD2 | 43:DW:24:ARG:H | 1.61 | 0.66 |
| 20:AB:68:PHE:HA | 20:AB:161:PHE:O | 1.96 | 0.66 |
| 3:AD:197:HIS:O | 3:AD:200:VAL:HG22 | 1.96 | 0.66 |
| 12:AM:63:VAL:O | 12:AM:68:LEU:HD21 | 1.96 | 0.66 |
| 35:BN:99:LYS:HB2 | 47:B0:41:HIS:HB3 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1827:U:O2' | 23:BB:1828:G:H5' | 1.95 | 0.66 |
| 23:BB:2:G:H2' | 23:BB:3:U:C6 | 2.30 | 0.66 |
| 26:BD:182:ALA:O | 26:BD:184:ARG:HG2 | 1.95 | 0.66 |
| 27:BE:58:LYS:O | 27:BE:60:TRP:N | 2.29 | 0.66 |
| 28:BF:111:ARG:NH2 | 28:BF:113:PHE:HB2 | 2.10 | 0.66 |
| 38:BQ:94:LEU:HD21 | 39:BR:11:GLN:HB2 | 1.77 | 0.66 |
| 40:BS:26:GLY:N | 40:BS:71:VAL:HG13 | 2.09 | 0.66 |
| 1:CA:1343:G:H1' | 8:CI:122:ARG:NH1 | 2.10 | 0.66 |
| 12:CM:89:ARG:HG3 | 12:CM:96:VAL:HG13 | 1.77 | 0.66 |
| 16:CQ:75:VAL:HG23 | 16:CQ:76:ARG:HG2 | 1.77 | 0.66 |
| 23:DB:590:A:H2' | 23:DB:591:U:C6 | 2.31 | 0.66 |
| 23:DB:718:A:H2' | 23:DB:719:C:H5' | 1.77 | 0.66 |
| 25:DC:16:VAL:H | 25:DC:203:VAL:HG12 | 1.60 | 0.66 |
| 26:DD:107:VAL:H | 26:DD:205:PRO:HA | 1.61 | 0.66 |
| 27:DE:98:LYS:HZ2 | 27:DE:99:LYS:HG2 | 1.60 | 0.66 |
| 44:DX:8:GLU:O | 44:DX:12:GLU:HB2 | 1.96 | 0.66 |
| 1:AA:1382:C:H4' | 6:AG:78:ARG:CZ | 2.26 | 0.65 |
| 1:AA:335:C:H2' | 1:AA:336:A:H8 | 1.62 | 0.65 |
| 8:AI:29:ILE:HA | 8:AI:64:ILE:O | 1.96 | 0.65 |
| 23:BB:1386:C:H2' | 23:BB:1387:A:C8 | 2.30 | 0.65 |
| 23:BB:1535:A:O2' | 23:BB:1536:C:H5' | 1.96 | 0.65 |
| 23:BB:2213:U:O2 | 23:BB:2213:U:H2' | 1.94 | 0.65 |
| 23:BB:2591:C:H2' | 23:BB:2592:G:H8 | 1.60 | 0.65 |
| 26:BD:109:VAL:HG11 | 26:BD:193:VAL:HB | 1.78 | 0.65 |
| 29:BG:152:ARG:NH1 | 29:BG:162:ARG:HA | 2.11 | 0.65 |
| 52:BI:129:GLU:HB3 | 52:BI:133:ARG:NH1 | 2.09 | 0.65 |
| 36:BO:88:LYS:HD2 | 36:BO:89:ASP:N | 2.11 | 0.65 |
| 38:BQ:60:TRP:O | 38:BQ:64:ILE:HG12 | 1.96 | 0.65 |
| 42:BU:10:VAL:O | 42:BU:21:ARG:HA | 1.95 | 0.65 |
| 23:DB:1000:A:H2' | 23:DB:1001:A:C8 | 2.31 | 0.65 |
| 23:DB:1788:C:O2' | 23:DB:1789:A:H5' | 1.97 | 0.65 |
| 23:DB:2143:C:H3' | 23:DB:2144:G:H8 | 1.61 | 0.65 |
| 28:DF:31:GLU:O | 28:DF:32:LYS:HD3 | 1.97 | 0.65 |
| 20:AB:71:THR:CG2 | 20:AB:94:ARG:H | 2.10 | 0.65 |
| 12:AM:70:ARG:O | 12:AM:74:MET:HG2 | 1.94 | 0.65 |
| 49:B2:33:ARG:HH21 | 49:B2:33:ARG:CB | 2.09 | 0.65 |
| 23:BB:2457:U:H2' | 23:BB:2458:G:H5' | 1.77 | 0.65 |
| 23:BB:557:C:H2' | 23:BB:558:U:C6 | 2.31 | 0.65 |
| 25:BC:173:LEU:H | 25:BC:173:LEU:HD13 | 1.61 | 0.65 |
| 30:BH:2:GLN:O | 30:BH:3:VAL:HG22 | 1.95 | 0.65 |
| 36:BO:83:LEU:HD21 | 36:BO:114:GLY:HA3 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BR:78:ARG:HG3 | 39:BR:78:ARG:HH21 | 1.61 | 0.65 |
| 41:BT:2:ILE:N | 41:BT:2:ILE:HD13 | 2.11 | 0.65 |
| 42:BU:81:ARG:H | 42:BU:81:ARG:NH2 | 1.93 | 0.65 |
| 1:CA:1149:C:H2' | 1:CA:1150:A:H8 | 1.61 | 0.65 |
| 1:CA:1513:A:H2' | 1:CA:1514:G:H8 | 1.60 | 0.65 |
| 1:CA:825:A:H2' | 1:CA:826:C:H6 | 1.60 | 0.65 |
| 20:CB:209:VAL:HG23 | 20:CB:210:THR:H | 1.60 | 0.65 |
| 4:CE:152:VAL:HG21 | 7:CH:98:LEU:HB3 | 1.78 | 0.65 |
| 6:CG:56:SER:HB3 | 6:CG:59:GLU:HG3 | 1.77 | 0.65 |
| 23:DB:1098:A:OP2 | 52:DI:3:LYS:HG2 | 1.97 | 0.65 |
| 23:DB:1939:U:H5' | 23:DB:1939:U:H6 | 1.61 | 0.65 |
| 25:DC:180:MET:HB3 | 25:DC:267:VAL:HB | 1.78 | 0.65 |
| 23:DB:1203:U:O4' | 33:DL:3:LEU:HD12 | 1.96 | 0.65 |
| 6:AG:23:ALA:O | 6:AG:26:VAL:HG22 | 1.97 | 0.65 |
| 6:AG:49:LEU:HD21 | 6:AG:60:ALA:HB3 | 1.78 | 0.65 |
| 18:AS:30:LEU:HD12 | 18:AS:48:ILE:HG12 | 1.78 | 0.65 |
| 23:BB:1993:U:H4' | 26:BD:133:THR:HG22 | 1.79 | 0.65 |
| 23:BB:2086:U:H2' | 23:BB:2087:G:C8 | 2.31 | 0.65 |
| 23:BB:2199:A:H5' | 23:BB:2200:C:OP2 | 1.96 | 0.65 |
| 23:BB:2472:G:H2' | 23:BB:2475:C:H42 | 1.62 | 0.65 |
| 23:BB:532:A:H4' | 23:BB:533:G:C8 | 2.32 | 0.65 |
| 23:BB:718:A:H3' | 23:BB:719:C:H6 | 1.61 | 0.65 |
| 28:BF:107:VAL:HG11 | 28:BF:175:PRO:HG3 | 1.77 | 0.65 |
| 29:BG:53:PRO:HG3 | 29:BG:61:TRP:HA | 1.78 | 0.65 |
| 30:BH:27:ARG:HH11 | 46:BZ:64:ILE:HD11 | 1.61 | 0.65 |
| 45:BY:6:ILE:HA | 45:BY:56:VAL:HG13 | 1.78 | 0.65 |
| 1:CA:841:C:O5' | 1:CA:842:U:H5'' | 1.96 | 0.65 |
| 12:CM:64:VAL:HA | 12:CM:68:LEU:HD11 | 1.77 | 0.65 |
| 23:DB:2649:C:H2' | 23:DB:2650:U:H6 | 1.61 | 0.65 |
| 29:DG:140:ILE:HA | 29:DG:143:VAL:HG22 | 1.79 | 0.65 |
| 52:DI:1:ALA:HB1 | 52:DI:2:LYS:HD2 | 1.78 | 0.65 |
| 32:DK:60:ALA:HA | 32:DK:87:LEU:HD23 | 1.78 | 0.65 |
| 10:AK:83:VAL:HG21 | 10:AK:109:ILE:HG12 | 1.77 | 0.65 |
| 23:BB:2751:G:H5' | 29:BG:2:ARG:HD3 | 1.78 | 0.65 |
| 23:BB:28:A:N6 | 23:BB:512:G:H1' | 2.12 | 0.65 |
| 36:BO:7:ARG:HA | 36:BO:10:ARG:CZ | 2.25 | 0.65 |
| 37:BP:3:ILE:HD13 | 37:BP:7:LEU:HD11 | 1.77 | 0.65 |
| 23:BB:973:A:H5'' | 39:BR:81:LYS:HD2 | 1.79 | 0.65 |
| 24:BV:20:LEU:HB3 | 24:BV:25:LYS:O | 1.96 | 0.65 |
| 43:BW:18:LYS:H | 43:BW:35:ILE:HG23 | 1.61 | 0.65 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:C6 | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1297:G:H1' | 1:CA:1298:U:H5 | 1.61 | 0.65 |
| 20:CB:195:VAL:HG12 | 20:CB:197:PHE:H | 1.61 | 0.65 |
| 12:CM:63:VAL:O | 12:CM:68:LEU:HD21 | 1.97 | 0.65 |
| 23:DB:1722:A:H2' | 23:DB:1723:G:C8 | 2.31 | 0.65 |
| 23:DB:18:U:H2' | 23:DB:19:A:H8 | 1.62 | 0.65 |
| 23:DB:2229:U:H2' | 23:DB:2230:G:H8 | 1.62 | 0.65 |
| 23:DB:2901:C:H2' | 23:DB:2902:C:H6 | 1.59 | 0.65 |
| 30:DH:125:THR:HA | 30:DH:146:VAL:HB | 1.77 | 0.65 |
| 37:DP:45:VAL:N | 37:DP:60:VAL:HB | 2.11 | 0.65 |
| 38:DQ:97:ILE:HG13 | 38:DQ:105:PHE:HB2 | 1.77 | 0.65 |
| 43:DW:23:LYS:HZ3 | 43:DW:24:ARG:HG3 | 1.60 | 0.65 |
| 1:AA:1320:C:N4 | 18:AS:36:ARG:HG2 | 2.11 | 0.65 |
| 20:AB:195:VAL:HG12 | 20:AB:197:PHE:H | 1.62 | 0.65 |
| 23:BB:643:A:C2 | 48:B1:43:ARG:HD2 | 2.31 | 0.65 |
| 23:BB:1461:C:H2' | 23:BB:1462:C:C6 | 2.32 | 0.65 |
| 31:BJ:13:ARG:O | 31:BJ:52:ASP:HA | 1.97 | 0.65 |
| 31:BJ:25:LEU:HD13 | 31:BJ:26:GLY:N | 2.12 | 0.65 |
| 35:BN:78:LYS:HG3 | 35:BN:83:LEU:HG | 1.76 | 0.65 |
| 1:CA:1085:U:H3' | 1:CA:1086:U:C5 | 2.31 | 0.65 |
| 1:CA:373:A:H2' | 1:CA:374:A:H8 | 1.61 | 0.65 |
| 12:CM:2:ARG:HD3 | 12:CM:2:ARG:H | 1.59 | 0.65 |
| 18:CS:30:LEU:HD12 | 18:CS:48:ILE:HG12 | 1.78 | 0.65 |
| 49:D2:30:VAL:HA | 49:D2:33:ARG:NH2 | 2.11 | 0.65 |
| 23:DB:1241:A:H2' | 23:DB:1242:U:H5' | 1.79 | 0.65 |
| 23:DB:1381:G:H2' | 23:DB:1382:G:H5' | 1.79 | 0.65 |
| 23:DB:2457:U:H2' | 23:DB:2458:G:H5' | 1.77 | 0.65 |
| 25:DC:4:LYS:HD2 | 25:DC:5:CYS:N | 2.12 | 0.65 |
| 26:DD:107:VAL:HG13 | 26:DD:203:VAL:HG23 | 1.77 | 0.65 |
| 26:DD:182:ALA:O | 26:DD:184:ARG:HG2 | 1.96 | 0.65 |
| 32:DK:112:PHE:O | 32:DK:115:ILE:HG22 | 1.97 | 0.65 |
| 1:AA:1270:G:H2' | 1:AA:1271:A:H8 | 1.61 | 0.65 |
| 1:AA:1307:U:H2' | 1:AA:1308:U:C6 | 2.32 | 0.65 |
| 1:AA:1347:G:N2 | 1:AA:1373:G:H2' | 2.11 | 0.65 |
| 1:AA:677:U:H2' | 1:AA:678:U:H6 | 1.61 | 0.65 |
| 3:AD:123:MET:SD | 3:AD:145:ARG:HD2 | 2.37 | 0.65 |
| 3:AD:84:ASN:ND2 | 4:AE:101:GLY:HA3 | 2.12 | 0.65 |
| 10:AK:28:ASN:HD21 | 10:AK:46:ALA:HB3 | 1.61 | 0.65 |
| 16:AQ:13:SER:HB3 | 16:AQ:21:VAL:HB | 1.77 | 0.65 |
| 51:B4:9:LYS:H | 51:B4:9:LYS:HD3 | 1.60 | 0.65 |
| 23:BB:118:A:OP2 | 23:BB:119:A:H2' | 1.97 | 0.65 |
| 23:BB:1549:A:H2' | 23:BB:1550:C:C6 | 2.32 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:162:U:H4' | 23:BB:163:C:OP1 | 1.96 | 0.65 |
| 23:BB:1949:G:H2' | 23:BB:1950:G:C8 | 2.32 | 0.65 |
| 23:BB:2502:G:H5' | 23:BB:2503:A:C5' | 2.26 | 0.65 |
| 32:BK:20:MET:O | 32:BK:41:ILE:HG13 | 1.97 | 0.65 |
| 33:BL:56:PRO:HD2 | 33:BL:59:ARG:HG3 | 1.79 | 0.65 |
| 39:BR:78:ARG:HB3 | 39:BR:83:TYR:HB3 | 1.78 | 0.65 |
| 23:BB:329:G:H1 | 42:BU:16:LYS:HE3 | 1.60 | 0.65 |
| 45:BY:12:ALA:HA | 45:BY:15:ARG:HD3 | 1.79 | 0.65 |
| 1:CA:473:U:H2' | 1:CA:474:G:C8 | 2.31 | 0.65 |
| 1:CA:834:U:H2' | 1:CA:835:U:C6 | 2.31 | 0.65 |
| 20:CB:114:LYS:HE2 | 20:CB:151:LYS:HZ1 | 1.62 | 0.65 |
| 20:CB:14:HIS:HB2 | 20:CB:208:ALA:HB2 | 1.79 | 0.65 |
| 1:CA:1103:C:H5'' | 20:CB:96:LEU:HD12 | 1.79 | 0.65 |
| 14:CO:7:THR:O | 14:CO:11:VAL:HG23 | 1.96 | 0.65 |
| 16:CQ:59:GLU:O | 16:CQ:75:VAL:HG22 | 1.96 | 0.65 |
| 23:DB:2557:G:H2' | 23:DB:2558:C:C6 | 2.31 | 0.65 |
| 23:DB:784:G:O2' | 23:DB:785:G:H5'' | 1.97 | 0.65 |
| 28:DF:134:GLN:NE2 | 28:DF:136:ILE:HD13 | 2.11 | 0.65 |
| 39:DR:49:ILE:HD13 | 39:DR:53:PHE:N | 2.11 | 0.65 |
| 14:AO:7:THR:O | 14:AO:11:VAL:HG23 | 1.96 | 0.65 |
| 23:BB:962:G:H21 | 23:BB:2250:G:N2 | 1.92 | 0.65 |
| 28:BF:139:GLU:HG2 | 28:BF:140:ILE:N | 2.11 | 0.65 |
| 28:BF:87:LYS:HG3 | 28:BF:88:VAL:H | 1.61 | 0.65 |
| 30:BH:104:THR:HG23 | 30:BH:105:ALA:H | 1.59 | 0.65 |
| 30:BH:81:ALA:HA | 30:BH:147:VAL:H | 1.60 | 0.65 |
| 32:BK:60:ALA:HA | 32:BK:87:LEU:HD23 | 1.79 | 0.65 |
| 23:BB:329:G:H1 | 42:BU:16:LYS:HG2 | 1.60 | 0.65 |
| 43:BW:39:GLN:NE2 | 43:BW:43:LYS:HB2 | 2.12 | 0.65 |
| 44:BX:31:GLN:HG2 | 44:BX:37:LEU:HB2 | 1.79 | 0.65 |
| 3:CD:122:ILE:O | 3:CD:128:VAL:HG23 | 1.96 | 0.65 |
| 13:CN:58:ARG:HB3 | 13:CN:58:ARG:HH11 | 1.62 | 0.65 |
| 18:CS:42:ASN:N | 18:CS:42:ASN:HD22 | 1.95 | 0.65 |
| 23:DB:1387:A:C4' | 23:DB:1469:A:H1' | 2.26 | 0.65 |
| 23:DB:2086:U:H2' | 23:DB:2087:G:C8 | 2.32 | 0.65 |
| 23:DB:2895:G:H2' | 23:DB:2896:C:C6 | 2.32 | 0.65 |
| 29:DG:84:LYS:HG3 | 29:DG:131:VAL:CA | 2.27 | 0.65 |
| 35:DN:70:THR:HB | 35:DN:75:ILE:HD11 | 1.78 | 0.65 |
| 36:DO:83:LEU:HD21 | 36:DO:114:GLY:HA3 | 1.78 | 0.65 |
| 37:DP:93:LYS:HB3 | 37:DP:96:LEU:HD12 | 1.79 | 0.65 |
| 42:DU:25:LYS:HE3 | 42:DU:36:GLU:HA | 1.79 | 0.65 |
| 1:AA:706:A:H4' | 10:AK:30:ILE:HD11 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:78:A:H3' | 1:AA:79:G:C8 | 2.31 | 0.65 |
| 1:AA:810:C:O2' | 1:AA:811:C:H5' | 1.96 | 0.65 |
| 23:BB:1241:A:H2' | 23:BB:1242:U:H5' | 1.77 | 0.65 |
| 23:BB:145:C:H2' | 23:BB:146:A:C8 | 2.32 | 0.65 |
| 23:BB:2834:G:H1' | 23:BB:2883:A:H61 | 1.61 | 0.65 |
| 34:BM:66:ARG:NE | 34:BM:101:VAL:HG11 | 2.11 | 0.65 |
| 37:BP:61:ARG:HD3 | 37:BP:70:GLU:HG3 | 1.78 | 0.65 |
| 40:BS:4:ILE:HG22 | 40:BS:106:VAL:HG13 | 1.79 | 0.65 |
| 18:CS:41:PRO:O | 18:CS:44:ILE:HG22 | 1.97 | 0.65 |
| 23:DB:2624:G:H1' | 47:D0:18:HIS:NE2 | 2.12 | 0.65 |
| 23:DB:1028:A:H2' | 23:DB:1029:A:C8 | 2.31 | 0.65 |
| 25:DC:142:ASN:HA | 25:DC:153:LEU:O | 1.97 | 0.65 |
| 25:DC:173:LEU:HD13 | 25:DC:173:LEU:H | 1.60 | 0.65 |
| 26:DD:91:THR:HG23 | 26:DD:92:VAL:H | 1.60 | 0.65 |
| 34:DM:21:ALA:CB | 34:DM:100:LYS:HG2 | 2.26 | 0.65 |
| 1:AA:1213:A:H2' | 1:AA:1215:G:N7 | 2.12 | 0.65 |
| 1:AA:208:U:H2' | 1:AA:210:C:C4 | 2.31 | 0.65 |
| 1:AA:673:A:H2' | 1:AA:674:G:C8 | 2.32 | 0.65 |
| 5:AF:3:HIS:CE1 | 5:AF:95:ALA:H | 2.15 | 0.65 |
| 10:AK:28:ASN:ND2 | 10:AK:46:ALA:HB3 | 2.12 | 0.65 |
| 10:AK:75:GLU:H | 10:AK:75:GLU:CD | 2.00 | 0.65 |
| 12:AM:3:ILE:O | 12:AM:56:ARG:HG3 | 1.97 | 0.65 |
| 22:BA:46:A:H2' | 22:BA:47:C:O4' | 1.96 | 0.65 |
| 23:BB:419:U:H2' | 23:BB:420:C:C6 | 2.32 | 0.65 |
| 23:BB:496:G:H1' | 40:BS:61:ASN:HD21 | 1.62 | 0.65 |
| 25:BC:123:ILE:HD12 | 25:BC:191:LEU:HD13 | 1.79 | 0.65 |
| 26:BD:33:ARG:NE | 26:BD:74:GLU:HB3 | 2.12 | 0.65 |
| 31:BJ:32:LEU:O | 31:BJ:36:LEU:HD23 | 1.97 | 0.65 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:H8 | 1.60 | 0.65 |
| 1:CA:1432:G:H5'' | 37:DP:105:LYS:HG2 | 1.79 | 0.65 |
| 1:CA:51:A:H5'' | 1:CA:52:C:H5'' | 1.78 | 0.65 |
| 1:CA:678:U:H2' | 1:CA:679:C:C6 | 2.32 | 0.65 |
| 3:CD:36:ALA:HA | 3:CD:41:GLY:HA3 | 1.77 | 0.65 |
| 33:DL:112:LEU:HG | 33:DL:113:ALA:H | 1.62 | 0.65 |
| 40:DS:73:LYS:HE3 | 40:DS:74:ILE:H | 1.61 | 0.65 |
| 43:DW:18:LYS:H | 43:DW:35:ILE:HG23 | 1.62 | 0.65 |
| 1:AA:695:A:H61 | 1:AA:797:C:H1' | 1.59 | 0.65 |
| 20:AB:14:HIS:HB2 | 20:AB:208:ALA:HB2 | 1.79 | 0.65 |
| 3:AD:25:ARG:CZ | 3:AD:26:ALA:HB2 | 2.26 | 0.65 |
| 23:BB:1046:A:C3' | 23:BB:1047:G:H5'' | 2.27 | 0.65 |
| 28:BF:62:GLN:OE1 | 28:BF:94:ARG:HG2 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BJ:56:VAL:HG12 | 31:BJ:57:LEU:H | 1.62 | 0.65 |
| 34:BM:96:ILE:HD11 | 34:BM:126:ILE:HG12 | 1.79 | 0.65 |
| 23:BB:532:A:H3' | 38:BQ:27:ARG:NH1 | 2.12 | 0.65 |
| 39:BR:14:VAL:HG22 | 39:BR:15:SER:N | 2.10 | 0.65 |
| 39:BR:49:ILE:HD13 | 39:BR:53:PHE:N | 2.12 | 0.65 |
| 45:BY:7:THR:HB | 45:BY:55:LYS:H | 1.61 | 0.65 |
| 5:CF:38:ARG:HH21 | 5:CF:63:ASN:HD21 | 1.43 | 0.65 |
| 7:CH:63:LYS:HD2 | 7:CH:70:VAL:HG21 | 1.78 | 0.65 |
| 8:CI:25:GLY:HA3 | 8:CI:57:VAL:CA | 2.27 | 0.65 |
| 11:CL:106:VAL:HG23 | 11:CL:116:TYR:HB3 | 1.79 | 0.65 |
| 16:CQ:13:SER:HB3 | 16:CQ:21:VAL:HB | 1.78 | 0.65 |
| 23:DB:1346:G:O2' | 23:DB:1347:A:H5' | 1.97 | 0.65 |
| 23:DB:1439:A:C6 | 23:DB:1552:A:N7 | 2.65 | 0.65 |
| 23:DB:1674:G:H21 | 23:DB:1677:A:N6 | 1.94 | 0.65 |
| 23:DB:1911:U:H2' | 23:DB:1918:A:N1 | 2.11 | 0.65 |
| 23:DB:70:G:H3' | 23:DB:113:U:H4' | 1.79 | 0.65 |
| 27:DE:69:ARG:O | 27:DE:70:SER:HB3 | 1.97 | 0.65 |
| 36:DO:7:ARG:HA | 36:DO:10:ARG:CZ | 2.27 | 0.65 |
| 1:AA:1072:G:H21 | 20:AB:105:THR:HG21 | 1.62 | 0.64 |
| 1:AA:1423:G:H2' | 1:AA:1424:U:C6 | 2.32 | 0.64 |
| 1:AA:802:A:H2' | 1:AA:803:G:O4' | 1.97 | 0.64 |
| 1:AA:82:G:H2' | 1:AA:83:C:O4' | 1.98 | 0.64 |
| 13:AN:68:ARG:NH1 | 13:AN:71:GLY:H | 1.95 | 0.64 |
| 15:AP:57:ILE:O | 15:AP:61:VAL:HG23 | 1.96 | 0.64 |
| 23:BB:2188:U:H2' | 23:BB:2189:U:C6 | 2.31 | 0.64 |
| 23:BB:720:U:H2' | 23:BB:721:A:C8 | 2.32 | 0.64 |
| 26:BD:141:ARG:HG3 | 26:BD:141:ARG:O | 1.95 | 0.64 |
| 29:BG:87:GLN:HE21 | 29:BG:164:ALA:HA | 1.61 | 0.64 |
| 30:BH:78:VAL:HB | 30:BH:143:ILE:HG12 | 1.78 | 0.64 |
| 45:BY:16:LEU:H | 45:BY:16:LEU:HD22 | 1.61 | 0.64 |
| 1:CA:662:U:H2' | 1:CA:663:A:C8 | 2.31 | 0.64 |
| 4:CE:85:LYS:HG3 | 4:CE:93:VAL:O | 1.96 | 0.64 |
| 6:CG:45:ALA:HB1 | 6:CG:120:ALA:HB2 | 1.79 | 0.64 |
| 23:DB:2693:G:H2' | 23:DB:2694:G:H8 | 1.61 | 0.64 |
| 23:DB:807:U:H2' | 23:DB:808:G:C8 | 2.31 | 0.64 |
| 32:DK:68:GLY:HA3 | 32:DK:78:ARG:HB3 | 1.77 | 0.64 |
| 35:DN:32:GLU:O | 35:DN:114:GLU:HA | 1.97 | 0.64 |
| 37:DP:52:ARG:HH11 | 37:DP:52:ARG:HG2 | 1.62 | 0.64 |
| 38:DQ:60:TRP:O | 38:DQ:64:ILE:HG12 | 1.96 | 0.64 |
| 24:DV:80:HIS:CD2 | 24:DV:83:LYS:H | 2.15 | 0.64 |
| 1:AA:218:U:H2' | 1:AA:219:U:C6 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:229:U:H2' | 1:AA:230:G:C8 | 2.31 | 0.64 |
| 20:AB:186:VAL:HB | 20:AB:190:SER:CB | 2.28 | 0.64 |
| 9:AJ:52:LEU:H | 9:AJ:52:LEU:HD12 | 1.63 | 0.64 |
| 23:BB:2471:A:O2' | 23:BB:2472:G:H8 | 1.79 | 0.64 |
| 23:BB:273:G:O2' | 23:BB:274:C:H5' | 1.97 | 0.64 |
| 23:BB:65:U:H2' | 23:BB:66:C:H6 | 1.61 | 0.64 |
| 23:BB:775:G:H4' | 23:BB:776:G:H5' | 1.77 | 0.64 |
| 42:BU:38:ILE:HG23 | 42:BU:39:ASN:N | 2.06 | 0.64 |
| 42:BU:70:ALA:HB1 | 42:BU:79:ALA:CB | 2.28 | 0.64 |
| 1:CA:1258:G:H2' | 1:CA:1259:C:C6 | 2.33 | 0.64 |
| 2:CC:48:LYS:HE2 | 2:CC:48:LYS:N | 2.07 | 0.64 |
| 8:CI:20:ILE:HD12 | 8:CI:20:ILE:H | 1.62 | 0.64 |
| 23:DB:106:C:H2' | 23:DB:107:G:H8 | 1.61 | 0.64 |
| 23:DB:1324:G:H1' | 23:DB:1616:A:N6 | 2.12 | 0.64 |
| 23:DB:155:A:H2' | 23:DB:156:A:H8 | 1.62 | 0.64 |
| 23:DB:1771:C:H2' | 23:DB:1772:A:C8 | 2.32 | 0.64 |
| 23:DB:1947:C:H2' | 23:DB:1948:G:H8 | 1.62 | 0.64 |
| 34:DM:60:GLN:H | 34:DM:60:GLN:HE21 | 1.44 | 0.64 |
| 39:DR:78:ARG:HH21 | 39:DR:78:ARG:HG3 | 1.61 | 0.64 |
| 1:AA:376:G:H5'' | 15:AP:5:ARG:HB2 | 1.77 | 0.64 |
| 1:AA:78:A:H3' | 1:AA:79:G:H8 | 1.62 | 0.64 |
| 5:AF:40:GLU:HB2 | 5:AF:61:LEU:HB2 | 1.79 | 0.64 |
| 8:AI:51:LEU:HD13 | 8:AI:56:MET:HG2 | 1.79 | 0.64 |
| 23:BB:171:U:H2' | 23:BB:172:A:H8 | 1.61 | 0.64 |
| 23:BB:17:G:H2' | 23:BB:18:U:C6 | 2.32 | 0.64 |
| 23:BB:2861:U:H2' | 23:BB:2862:G:H8 | 1.61 | 0.64 |
| 26:BD:107:VAL:H | 26:BD:205:PRO:HA | 1.62 | 0.64 |
| 40:BS:32:ALA:O | 40:BS:35:ILE:HB | 1.97 | 0.64 |
| 44:BX:1:MET:HB3 | 44:BX:4:LYS:HD3 | 1.78 | 0.64 |
| 46:BZ:40:VAL:CG2 | 46:BZ:45:ARG:H | 2.09 | 0.64 |
| 1:CA:1132:C:H2' | 1:CA:1133:G:C8 | 2.32 | 0.64 |
| 1:CA:1270:G:H2' | 1:CA:1271:A:H8 | 1.62 | 0.64 |
| 1:CA:658:C:H2' | 1:CA:659:U:H6 | 1.62 | 0.64 |
| 1:CA:707:U:H2' | 1:CA:708:C:C6 | 2.33 | 0.64 |
| 5:CF:40:GLU:HB2 | 5:CF:61:LEU:HB2 | 1.80 | 0.64 |
| 10:CK:108:ASN:ND2 | 21:CU:6:ARG:HB2 | 2.12 | 0.64 |
| 21:CU:16:ARG:CA | 21:CU:16:ARG:HE | 2.01 | 0.64 |
| 23:DB:173:A:H2' | 23:DB:174:U:C6 | 2.33 | 0.64 |
| 23:DB:1856:U:H2' | 23:DB:1857:G:O4' | 1.97 | 0.64 |
| 23:DB:2331:G:H21 | 23:DB:2336:A:H8 | 1.44 | 0.64 |
| 23:DB:962:G:H21 | 23:DB:2250:G:N2 | 1.92 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DD:118:PHE:O | 26:DD:119:ALA:HB3 | 1.97 | 0.64 |
| 33:DL:141:LYS:HD3 | 33:DL:142:ILE:H | 1.61 | 0.64 |
| 23:DB:532:A:H3' | 38:DQ:27:ARG:NH1 | 2.11 | 0.64 |
| 38:DQ:91:ARG:HG2 | 38:DQ:93:ILE:HG22 | 1.79 | 0.64 |
| 38:DQ:63:ARG:HH12 | 38:DQ:96:ASP:HA | 1.63 | 0.64 |
| 39:DR:39:LEU:HA | 39:DR:53:PHE:HA | 1.78 | 0.64 |
| 40:DS:36:LEU:H | 40:DS:36:LEU:HD22 | 1.62 | 0.64 |
| 1:AA:1342:C:H2' | 1:AA:1343:G:C8 | 2.32 | 0.64 |
| 2:AC:13:ILE:O | 2:AC:14:VAL:HG22 | 1.97 | 0.64 |
| 2:AC:59:PRO:HG2 | 2:AC:62:SER:OG | 1.97 | 0.64 |
| 49:B2:33:ARG:HH21 | 49:B2:33:ARG:HB2 | 1.62 | 0.64 |
| 23:BB:1412:U:H2' | 23:BB:1413:A:C8 | 2.31 | 0.64 |
| 23:BB:1464:G:H2' | 23:BB:1465:G:C8 | 2.33 | 0.64 |
| 23:BB:2893:A:H5'' | 23:BB:2894:G:H5' | 1.79 | 0.64 |
| 26:BD:113:SER:HB3 | 26:BD:168:GLU:N | 2.12 | 0.64 |
| 29:BG:84:LYS:HG3 | 29:BG:131:VAL:CA | 2.26 | 0.64 |
| 35:BN:32:GLU:O | 35:BN:114:GLU:HA | 1.97 | 0.64 |
| 38:BQ:63:ARG:HH22 | 38:BQ:96:ASP:CA | 2.04 | 0.64 |
| 38:BQ:91:ARG:HH12 | 39:BR:10:LYS:HB3 | 1.62 | 0.64 |
| 1:CA:71:A:O2' | 1:CA:72:A:H5'' | 1.98 | 0.64 |
| 1:CA:825:A:H2' | 1:CA:826:C:C6 | 2.33 | 0.64 |
| 1:CA:927:G:H4' | 1:CA:1503:A:N7 | 2.12 | 0.64 |
| 8:CI:79:ARG:NH2 | 8:CI:102:PHE:HA | 2.11 | 0.64 |
| 10:CK:75:GLU:H | 10:CK:75:GLU:CD | 1.98 | 0.64 |
| 11:CL:113:ARG:HG2 | 11:CL:118:VAL:HB | 1.80 | 0.64 |
| 23:DB:1021:A:H61 | 23:DB:1142:A:N6 | 1.95 | 0.64 |
| 23:DB:132:G:H2' | 23:DB:133:U:C6 | 2.32 | 0.64 |
| 23:DB:2473:U:H2' | 23:DB:2473:U:O2 | 1.96 | 0.64 |
| 23:DB:2502:G:H5' | 23:DB:2503:A:C5' | 2.23 | 0.64 |
| 23:DB:72:U:O2' | 23:DB:73:A:H5' | 1.97 | 0.64 |
| 32:DK:64:ARG:O | 32:DK:82:ASN:HA | 1.98 | 0.64 |
| 1:AA:1432:G:H1' | 1:AA:1468:A:N6 | 2.13 | 0.64 |
| 5:AF:18:VAL:HG21 | 5:AF:58:HIS:ND1 | 2.13 | 0.64 |
| 23:BB:1060:U:O4 | 52:BI:131:THR:HG22 | 1.97 | 0.64 |
| 23:BB:1485:U:H2' | 23:BB:1486:U:C6 | 2.32 | 0.64 |
| 23:BB:2229:U:H2' | 23:BB:2230:G:H8 | 1.62 | 0.64 |
| 52:BI:25:PRO:O | 52:BI:29:GLN:HG2 | 1.98 | 0.64 |
| 42:BU:25:LYS:HE3 | 42:BU:36:GLU:HA | 1.79 | 0.64 |
| 1:CA:735:C:O2' | 1:CA:736:C:H5' | 1.97 | 0.64 |
| 1:CA:763:G:H2' | 1:CA:764:C:H6 | 1.62 | 0.64 |
| 23:DB:1690:A:H2' | 23:DB:1691:C:O4' | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1812:U:H2' | 23:DB:1813:G:H8 | 1.61 | 0.64 |
| 23:DB:2182:U:H2' | 23:DB:2183:A:C8 | 2.32 | 0.64 |
| 23:DB:2425:A:H5' | 23:DB:2427:C:O4' | 1.96 | 0.64 |
| 23:DB:365:U:H2' | 23:DB:366:C:C6 | 2.31 | 0.64 |
| 28:DF:139:GLU:HG2 | 28:DF:140:ILE:N | 2.10 | 0.64 |
| 29:DG:152:ARG:HG3 | 29:DG:153:PRO:HD2 | 1.80 | 0.64 |
| 42:DU:11:ILE:HG22 | 42:DU:70:ALA:HB3 | 1.80 | 0.64 |
| 1:AA:845:A:H5'' | 1:AA:846:G:N7 | 2.12 | 0.64 |
| 50:B3:41:ARG:HA | 50:B3:44:ARG:HH21 | 1.60 | 0.64 |
| 23:BB:1220:G:H2' | 23:BB:1221:C:C6 | 2.33 | 0.64 |
| 23:BB:246:C:H2' | 23:BB:247:G:H5' | 1.78 | 0.64 |
| 23:BB:72:U:O2' | 23:BB:73:A:H5' | 1.97 | 0.64 |
| 23:BB:587:C:O2' | 33:BL:19:LEU:HD13 | 1.98 | 0.64 |
| 37:BP:61:ARG:HH21 | 37:BP:61:ARG:HB3 | 1.61 | 0.64 |
| 1:CA:131:A:H2' | 1:CA:132:C:H6 | 1.62 | 0.64 |
| 3:CD:106:PHE:CD1 | 3:CD:144:ILE:HD11 | 2.32 | 0.64 |
| 43:DW:49:ASN:HB2 | 43:DW:61:LYS:H | 1.60 | 0.64 |
| 45:DY:16:LEU:H | 45:DY:16:LEU:HD22 | 1.61 | 0.64 |
| 1:AA:859:G:H2' | 1:AA:860:A:H8 | 1.63 | 0.64 |
| 23:BB:154:U:H2' | 23:BB:155:A:C8 | 2.33 | 0.64 |
| 23:BB:2019:A:H2 | 23:BB:2035:G:H22 | 1.42 | 0.64 |
| 26:BD:8:LYS:HB2 | 26:BD:201:LEU:HD21 | 1.78 | 0.64 |
| 30:BH:80:ILE:HD12 | 30:BH:144:VAL:HG22 | 1.79 | 0.64 |
| 40:BS:90:LYS:HD2 | 40:BS:92:ARG:HH12 | 1.62 | 0.64 |
| 1:CA:1008:U:H5'' | 13:CN:23:ARG:NH2 | 2.13 | 0.64 |
| 20:CB:115:ASP:O | 20:CB:119:GLN:HG2 | 1.97 | 0.64 |
| 3:CD:29:THR:HB | 3:CD:30:LYS:NZ | 2.12 | 0.64 |
| 4:CE:125:LYS:HD2 | 4:CE:126:ALA:N | 2.12 | 0.64 |
| 49:D2:10:LEU:HD11 | 49:D2:14:ARG:NH1 | 2.13 | 0.64 |
| 51:D4:9:LYS:H | 51:D4:9:LYS:HD3 | 1.62 | 0.64 |
| 23:DB:2213:U:O2 | 23:DB:2213:U:H2' | 1.95 | 0.64 |
| 23:DB:2804:U:H2' | 23:DB:2805:C:H6 | 1.62 | 0.64 |
| 27:DE:176:ASP:HB3 | 27:DE:179:SER:HB2 | 1.80 | 0.64 |
| 31:DJ:136:GLN:N | 31:DJ:137:PRO:HD3 | 2.13 | 0.64 |
| 32:DK:118:LEU:C | 32:DK:120:PRO:HD2 | 2.18 | 0.64 |
| 37:DP:61:ARG:HH21 | 37:DP:61:ARG:HB3 | 1.61 | 0.64 |
| 38:DQ:104:ALA:HA | 39:DR:46:GLU:OE1 | 1.97 | 0.64 |
| 1:AA:1437:A:H2' | 1:AA:1438:G:H8 | 1.63 | 0.64 |
| 1:AA:229:U:H2' | 1:AA:230:G:H8 | 1.62 | 0.64 |
| 1:AA:415:A:H3' | 1:AA:416:G:H8 | 1.63 | 0.64 |
| 3:AD:88:ASN:O | 3:AD:92:LEU:HD23 | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:AG:56:SER:HB3 | 6:AG:59:GLU:HG3 | 1.80 | 0.64 |
| 22:BA:56:G:H4' | 22:BA:57:A:H5' | 1.78 | 0.64 |
| 23:BB:1654:A:H2' | 23:BB:1655:A:C8 | 2.33 | 0.64 |
| 23:BB:173:A:H2' | 23:BB:174:U:C6 | 2.32 | 0.64 |
| 23:BB:1802:A:H2' | 23:BB:1803:A:C8 | 2.33 | 0.64 |
| 23:BB:2352:A:H2' | 23:BB:2353:G:O4' | 1.98 | 0.64 |
| 23:BB:414:C:H2' | 23:BB:415:A:C8 | 2.32 | 0.64 |
| 27:BE:117:ARG:O | 27:BE:186:VAL:HG12 | 1.98 | 0.64 |
| 32:BK:105:ARG:HD3 | 32:BK:106:GLU:OE1 | 1.98 | 0.64 |
| 35:BN:77:ALA:O | 35:BN:81:ASN:HB2 | 1.98 | 0.64 |
| 1:CA:845:A:H5'' | 1:CA:846:G:N7 | 2.13 | 0.64 |
| 20:CB:186:VAL:HB | 20:CB:190:SER:CB | 2.28 | 0.64 |
| 4:CE:105:ILE:HD11 | 4:CE:123:LEU:HB3 | 1.80 | 0.64 |
| 7:CH:6:ILE:HD11 | 7:CH:31:LEU:HD23 | 1.79 | 0.64 |
| 7:CH:51:GLU:HG2 | 7:CH:52:GLY:H | 1.61 | 0.64 |
| 10:CK:28:ASN:ND2 | 10:CK:46:ALA:HB3 | 2.12 | 0.64 |
| 49:D2:1:MET:HG2 | 49:D2:2:LYS:H | 1.63 | 0.64 |
| 23:DB:1407:G:H2' | 23:DB:1408:G:H8 | 1.63 | 0.64 |
| 23:DB:145:C:H2' | 23:DB:146:A:C8 | 2.32 | 0.64 |
| 26:DD:34:VAL:HB | 26:DD:48:ILE:HD11 | 1.80 | 0.64 |
| 27:DE:189:THR:O | 27:DE:193:VAL:HG23 | 1.96 | 0.64 |
| 27:DE:33:VAL:O | 27:DE:36:ALA:HB3 | 1.97 | 0.64 |
| 23:DB:1163:G:H4' | 39:DR:92:TRP:NE1 | 2.13 | 0.64 |
| 41:DT:38:ALA:HB3 | 41:DT:81:LYS:NZ | 2.12 | 0.64 |
| 23:DB:2269:G:C4' | 43:DW:19:ARG:HH12 | 2.11 | 0.64 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:C6 | 2.33 | 0.64 |
| 1:AA:270:A:H2' | 1:AA:271:C:C6 | 2.32 | 0.64 |
| 20:AB:128:LEU:HD12 | 20:AB:132:GLU:HB3 | 1.79 | 0.64 |
| 8:AI:23:GLY:H | 8:AI:60:LEU:HA | 1.63 | 0.64 |
| 13:AN:58:ARG:HH11 | 13:AN:58:ARG:HB3 | 1.63 | 0.64 |
| 23:BB:155:A:H2' | 23:BB:156:A:H8 | 1.63 | 0.64 |
| 23:BB:2720:U:H5'' | 37:BP:52:ARG:HH21 | 1.62 | 0.64 |
| 23:BB:2804:U:H2' | 23:BB:2805:C:H6 | 1.63 | 0.64 |
| 26:BD:115:GLY:HA2 | 26:BD:167:ASN:HB2 | 1.79 | 0.64 |
| 26:BD:91:THR:HG23 | 26:BD:92:VAL:H | 1.62 | 0.64 |
| 37:BP:5:LYS:HE2 | 37:BP:5:LYS:HA | 1.80 | 0.64 |
| 40:BS:36:LEU:H | 40:BS:36:LEU:HD22 | 1.61 | 0.64 |
| 1:CA:1320:C:N4 | 18:CS:36:ARG:HG2 | 2.13 | 0.64 |
| 1:CA:1323:G:H4' | 1:CA:1362:A:C4 | 2.33 | 0.64 |
| 1:CA:412:A:H4' | 1:CA:413:G:OP1 | 1.98 | 0.64 |
| 1:CA:69:G:N2 | 1:CA:71:A:H62 | 1.96 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:CD:25:ARG:CZ | 3:CD:26:ALA:HB2 | 2.26 | 0.64 |
| 12:CM:3:ILE:O | 12:CM:56:ARG:HG3 | 1.98 | 0.64 |
| 49:D2:33:ARG:HH21 | 49:D2:33:ARG:CB | 2.11 | 0.64 |
| 23:DB:1100:C:H2' | 23:DB:1101:U:H6 | 1.62 | 0.64 |
| 23:DB:1292:G:H2' | 23:DB:1293:C:C6 | 2.32 | 0.64 |
| 23:DB:2443:C:H2' | 23:DB:2444:G:H8 | 1.63 | 0.64 |
| 26:DD:113:SER:CB | 26:DD:168:GLU:H | 2.10 | 0.64 |
| 29:DG:132:LEU:HD23 | 29:DG:132:LEU:H | 1.63 | 0.64 |
| 20:AB:115:ASP:O | 20:AB:119:GLN:HG2 | 1.97 | 0.64 |
| 7:AH:94:VAL:HG23 | 7:AH:101:ALA:HB2 | 1.80 | 0.64 |
| 9:AJ:52:LEU:HA | 9:AJ:62:ARG:HA | 1.79 | 0.64 |
| 23:BB:2749:A:C3' | 23:BB:2750:A:H5'' | 2.28 | 0.64 |
| 25:BC:142:ASN:HA | 25:BC:153:LEU:O | 1.98 | 0.64 |
| 26:BD:114:LYS:HZ2 | 26:BD:116:LYS:NZ | 1.84 | 0.64 |
| 26:BD:118:PHE:O | 26:BD:119:ALA:HB3 | 1.97 | 0.64 |
| 26:BD:51:THR:CG2 | 26:BD:76:GLY:HA3 | 2.28 | 0.64 |
| 30:BH:131:SER:HB3 | 30:BH:141:LYS:HA | 1.79 | 0.64 |
| 30:BH:133:GLN:HB2 | 30:BH:139:PHE:CB | 2.27 | 0.64 |
| 37:BP:4:ILE:C | 37:BP:6:GLN:H | 2.00 | 0.64 |
| 46:BZ:71:LEU:HD13 | 46:BZ:76:GLU:HB3 | 1.80 | 0.64 |
| 1:CA:129:A:H1' | 1:CA:130:A:C8 | 2.33 | 0.64 |
| 1:CA:131:A:H2' | 1:CA:132:C:C6 | 2.33 | 0.64 |
| 1:CA:1404:C:H2' | 1:CA:1405:G:C8 | 2.33 | 0.64 |
| 1:CA:524:G:H2' | 1:CA:525:C:C6 | 2.33 | 0.64 |
| 20:CB:62:ARG:H | 20:CB:62:ARG:HD2 | 1.63 | 0.64 |
| 3:CD:153:ARG:HG3 | 3:CD:154:VAL:H | 1.63 | 0.64 |
| 5:CF:47:LEU:HD21 | 5:CF:57:ALA:HB3 | 1.80 | 0.64 |
| 8:CI:42:THR:HA | 8:CI:45:MET:SD | 2.37 | 0.64 |
| 9:CJ:52:LEU:HA | 9:CJ:62:ARG:HA | 1.80 | 0.64 |
| 26:DD:51:THR:CG2 | 26:DD:76:GLY:HA3 | 2.28 | 0.64 |
| 29:DG:87:GLN:HE21 | 29:DG:164:ALA:HA | 1.63 | 0.64 |
| 33:DL:60:ARG:HB2 | 33:DL:60:ARG:HH21 | 1.63 | 0.64 |
| 1:AA:1210:C:H1' | 1:AA:1214:C:H2' | 1.80 | 0.63 |
| 1:AA:499:A:H4' | 1:AA:500:G:H5' | 1.80 | 0.63 |
| 1:AA:763:G:H2' | 1:AA:764:C:C6 | 2.32 | 0.63 |
| 1:AA:921:U:H2' | 1:AA:922:G:C8 | 2.33 | 0.63 |
| 21:AU:33:ARG:HG2 | 21:AU:34:ARG:H | 1.64 | 0.63 |
| 23:BB:1324:G:H1' | 23:BB:1616:A:N6 | 2.13 | 0.63 |
| 23:BB:287:G:H2' | 23:BB:288:U:H6 | 1.63 | 0.63 |
| 23:BB:401:A:H2' | 23:BB:402:A:C8 | 2.33 | 0.63 |
| 23:BB:547:A:C2' | 23:BB:548:G:H5' | 2.26 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BC:145:MET:HB2 | 25:BC:152:GLN:HE22 | 1.64 | 0.63 |
| 28:BF:16:MET:O | 28:BF:20:ASN:HA | 1.97 | 0.63 |
| 33:BL:60:ARG:HH21 | 33:BL:60:ARG:HB2 | 1.63 | 0.63 |
| 34:BM:21:ALA:CB | 34:BM:100:LYS:HG2 | 2.28 | 0.63 |
| 41:BT:67:VAL:C | 41:BT:68:LYS:HD3 | 2.19 | 0.63 |
| 1:CA:1004:A:H3' | 1:CA:1024:G:N2 | 2.12 | 0.63 |
| 1:CA:1347:G:N2 | 1:CA:1373:G:H2' | 2.13 | 0.63 |
| 1:CA:1148:U:H5' | 8:CI:6:TYR:OH | 1.98 | 0.63 |
| 1:CA:958:A:H61 | 18:CS:53:GLY:HA3 | 1.64 | 0.63 |
| 22:DA:7:G:H1' | 36:DO:38:GLN:HE22 | 1.63 | 0.63 |
| 23:DB:1047:G:H1' | 23:DB:1110:G:N2 | 2.12 | 0.63 |
| 23:DB:1486:U:H2' | 23:DB:1487:U:H6 | 1.62 | 0.63 |
| 23:DB:2019:A:H2 | 23:DB:2035:G:H22 | 1.44 | 0.63 |
| 23:DB:2183:A:H2' | 23:DB:2184:A:C8 | 2.33 | 0.63 |
| 23:DB:720:U:H2' | 23:DB:721:A:C8 | 2.32 | 0.63 |
| 26:DD:13:ARG:HH12 | 37:DP:74:GLN:NE2 | 1.96 | 0.63 |
| 28:DF:101:ARG:HA | 28:DF:105:ILE:HD13 | 1.78 | 0.63 |
| 35:DN:101:GLY:HA2 | 35:DN:110:MET:H | 1.59 | 0.63 |
| 42:DU:85:ARG:CD | 42:DU:86:PHE:H | 2.02 | 0.63 |
| 1:AA:41:G:H2' | 1:AA:42:G:C8 | 2.33 | 0.63 |
| 1:AA:865:A:C2 | 1:AA:918:A:H4' | 2.33 | 0.63 |
| 48:B1:26:LYS:HB2 | 48:B1:52:LYS:HZ2 | 1.63 | 0.63 |
| 23:BB:1439:A:C6 | 23:BB:1552:A:N7 | 2.66 | 0.63 |
| 23:BB:549:G:H3' | 23:BB:549:G:OP2 | 1.98 | 0.63 |
| 32:BK:64:ARG:O | 32:BK:82:ASN:HA | 1.97 | 0.63 |
| 44:BX:39:GLN:O | 44:BX:42:LEU:HB2 | 1.98 | 0.63 |
| 3:CD:25:ARG:NH1 | 3:CD:26:ALA:HB2 | 2.12 | 0.63 |
| 6:CG:49:LEU:HD21 | 6:CG:60:ALA:HB3 | 1.79 | 0.63 |
| 23:DB:1060:U:O4 | 23:DB:1088:A:N6 | 2.31 | 0.63 |
| 23:DB:699:A:H4' | 23:DB:1634:A:N7 | 2.12 | 0.63 |
| 23:DB:189:G:H2' | 23:DB:205:G:N2 | 2.13 | 0.63 |
| 23:DB:1935:G:H1' | 23:DB:1964:G:N2 | 2.13 | 0.63 |
| 23:DB:300:A:H2' | 23:DB:334:C:H1' | 1.80 | 0.63 |
| 52:DI:41:PHE:O | 52:DI:45:THR:HG23 | 1.98 | 0.63 |
| 31:DJ:13:ARG:O | 31:DJ:52:ASP:HA | 1.98 | 0.63 |
| 22:DA:28:C:OP1 | 36:DO:31:THR:HG21 | 1.98 | 0.63 |
| 1:AA:865:A:H5' | 1:AA:1078:U:O4 | 1.99 | 0.63 |
| 1:AA:51:A:H5'' | 1:AA:52:C:H5'' | 1.80 | 0.63 |
| 1:AA:918:A:H2' | 1:AA:919:A:C8 | 2.32 | 0.63 |
| 4:AE:37:VAL:HG11 | 4:AE:113:VAL:HG12 | 1.81 | 0.63 |
| 8:AI:27:ILE:HB | 8:AI:34:LEU:HB2 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1341:G:H3' | 23:BB:1397:U:O2 | 1.99 | 0.63 |
| 23:BB:2443:C:H2' | 23:BB:2444:G:C8 | 2.34 | 0.63 |
| 23:BB:968:C:H2' | 23:BB:969:G:H8 | 1.63 | 0.63 |
| 23:BB:98:G:H1 | 42:BU:6:ARG:HH12 | 1.47 | 0.63 |
| 25:BC:77:VAL:HG22 | 25:BC:113:ASP:H | 1.63 | 0.63 |
| 23:BB:2393:U:H5'' | 33:BL:62:PRO:HG3 | 1.80 | 0.63 |
| 37:BP:24:THR:O | 37:BP:25:VAL:HG22 | 1.98 | 0.63 |
| 41:BT:1:MET:HB2 | 41:BT:2:ILE:HD13 | 1.80 | 0.63 |
| 22:BA:98:G:N1 | 24:BV:14:LYS:HB2 | 2.12 | 0.63 |
| 43:BW:77:LYS:O | 43:BW:78:PHE:HB2 | 1.97 | 0.63 |
| 1:CA:1330:U:H4' | 12:CM:69:ARG:HH12 | 1.63 | 0.63 |
| 1:CA:370:C:O2' | 1:CA:371:A:H5' | 1.99 | 0.63 |
| 1:CA:492:C:H2' | 1:CA:493:A:N3 | 2.12 | 0.63 |
| 1:CA:859:G:H2' | 1:CA:860:A:H8 | 1.61 | 0.63 |
| 20:CB:101:THR:HG22 | 20:CB:174:GLU:OE1 | 1.98 | 0.63 |
| 2:CC:62:SER:HA | 2:CC:97:PRO:O | 1.98 | 0.63 |
| 1:CA:437:U:H4' | 3:CD:153:ARG:HH12 | 1.63 | 0.63 |
| 11:CL:40:THR:HG22 | 11:CL:41:PRO:HD2 | 1.79 | 0.63 |
| 22:DA:15:A:H3' | 22:DA:15:A:OP2 | 1.97 | 0.63 |
| 22:DA:46:A:H2' | 22:DA:47:C:O4' | 1.98 | 0.63 |
| 23:DB:1050:A:H2' | 23:DB:1051:G:O4' | 1.98 | 0.63 |
| 23:DB:2861:U:H2' | 23:DB:2862:G:H8 | 1.62 | 0.63 |
| 23:DB:2898:U:H2' | 23:DB:2899:A:H8 | 1.63 | 0.63 |
| 26:DD:178:VAL:HG12 | 26:DD:179:ARG:H | 1.64 | 0.63 |
| 27:DE:97:ASN:HD21 | 27:DE:100:MET:HG3 | 1.62 | 0.63 |
| 31:DJ:89:PHE:HE1 | 31:DJ:93:ILE:HD13 | 1.64 | 0.63 |
| 32:DK:43:ILE:HG21 | 32:DK:46:ALA:HB2 | 1.80 | 0.63 |
| 33:DL:57:LEU:O | 33:DL:61:LEU:HD13 | 1.98 | 0.63 |
| 36:DO:40:ILE:HA | 36:DO:47:VAL:HA | 1.80 | 0.63 |
| 45:DY:6:ILE:HA | 45:DY:56:VAL:HG13 | 1.79 | 0.63 |
| 1:AA:978:A:H5' | 1:AA:1362:A:N6 | 2.14 | 0.63 |
| 3:AD:25:ARG:NH1 | 3:AD:26:ALA:HB2 | 2.14 | 0.63 |
| 13:AN:26:LEU:HA | 13:AN:29:ILE:HD12 | 1.81 | 0.63 |
| 13:AN:9:GLU:HB2 | 13:AN:62:ARG:NE | 2.13 | 0.63 |
| 23:BB:2144:G:O2' | 23:BB:2146:C:H5' | 1.99 | 0.63 |
| 25:BC:158:GLY:N | 25:BC:194:VAL:HG13 | 2.13 | 0.63 |
| 29:BG:89:VAL:HG12 | 29:BG:90:GLY:H | 1.63 | 0.63 |
| 1:CA:1342:C:H2' | 1:CA:1343:G:H8 | 1.63 | 0.63 |
| 23:DB:1857:G:HO2' | 23:DB:1858:A:H8 | 1.46 | 0.63 |
| 25:DC:77:VAL:HG22 | 25:DC:113:ASP:H | 1.64 | 0.63 |
| 26:DD:68:PHE:HB3 | 26:DD:73:VAL:HA | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:DU:27:VAL:HG23 | 42:DU:33:VAL:HG12 | 1.80 | 0.63 |
| 23:DB:2353:G:H1' | 43:DW:30:VAL:CG1 | 2.28 | 0.63 |
| 43:DW:44:PHE:O | 43:DW:78:PHE:HA | 1.98 | 0.63 |
| 8:AI:20:ILE:HD12 | 8:AI:20:ILE:H | 1.62 | 0.63 |
| 51:B4:2:LYS:HG2 | 51:B4:3:VAL:H | 1.64 | 0.63 |
| 23:BB:1346:G:O2' | 23:BB:1347:A:H5' | 1.98 | 0.63 |
| 23:BB:2331:G:N2 | 23:BB:2336:A:H8 | 1.96 | 0.63 |
| 23:BB:2895:G:H2' | 23:BB:2896:C:C6 | 2.34 | 0.63 |
| 32:BK:7:MET:SD | 32:BK:20:MET:HB2 | 2.39 | 0.63 |
| 43:BW:44:PHE:O | 43:BW:78:PHE:HA | 1.99 | 0.63 |
| 11:CL:122:LYS:HD2 | 11:CL:123:ALA:H | 1.64 | 0.63 |
| 18:CS:5:LYS:O | 18:CS:6:LYS:HD2 | 1.97 | 0.63 |
| 23:DB:1220:G:H2' | 23:DB:1221:C:C6 | 2.34 | 0.63 |
| 23:DB:1508:A:H5' | 23:DB:1509:A:N6 | 2.14 | 0.63 |
| 23:DB:1735:A:H2' | 23:DB:1736:U:C6 | 2.34 | 0.63 |
| 23:DB:548:G:H2' | 23:DB:548:G:N3 | 2.12 | 0.63 |
| 28:DF:60:SER:HB2 | 28:DF:62:GLN:OE1 | 1.99 | 0.63 |
| 41:DT:67:VAL:C | 41:DT:68:LYS:HD3 | 2.19 | 0.63 |
| 44:DX:26:PHE:HD1 | 44:DX:27:ASN:HD22 | 1.44 | 0.63 |
| 1:AA:1173:U:H2' | 1:AA:1174:G:C8 | 2.33 | 0.63 |
| 1:AA:1258:G:H2' | 1:AA:1259:C:H6 | 1.64 | 0.63 |
| 3:AD:138:PRO:HA | 3:AD:181:PHE:CD2 | 2.31 | 0.63 |
| 4:AE:125:LYS:HD2 | 4:AE:126:ALA:N | 2.13 | 0.63 |
| 11:AL:49:ARG:HG2 | 11:AL:89:LEU:HD21 | 1.80 | 0.63 |
| 23:BB:155:A:H2' | 23:BB:156:A:C8 | 2.34 | 0.63 |
| 23:BB:2752:C:H3' | 23:BB:2753:A:H8 | 1.63 | 0.63 |
| 23:BB:2800:A:H2' | 23:BB:2801:G:O4' | 1.99 | 0.63 |
| 25:BC:20:ASN:HB3 | 25:BC:23:LEU:HD22 | 1.79 | 0.63 |
| 23:BB:2313:C:H4' | 28:BF:87:LYS:HB3 | 1.80 | 0.63 |
| 23:BB:2658:C:H5' | 29:BG:159:LYS:NZ | 2.14 | 0.63 |
| 38:BQ:63:ARG:HH12 | 38:BQ:96:ASP:HA | 1.63 | 0.63 |
| 41:BT:7:LEU:HA | 41:BT:9:LYS:HZ1 | 1.64 | 0.63 |
| 1:CA:1307:U:H2' | 1:CA:1308:U:C6 | 2.33 | 0.63 |
| 1:CA:1380:U:O4 | 6:CG:2:ARG:HB2 | 1.99 | 0.63 |
| 3:CD:160:LEU:HA | 3:CD:163:GLN:HG3 | 1.80 | 0.63 |
| 13:CN:42:ASN:O | 13:CN:46:LYS:HG2 | 1.99 | 0.63 |
| 21:CU:48:LYS:HA | 21:CU:51:ALA:HB3 | 1.80 | 0.63 |
| 23:DB:1205:A:H4' | 23:DB:1206:G:OP2 | 1.98 | 0.63 |
| 23:DB:1654:A:H2' | 23:DB:1655:A:C8 | 2.33 | 0.63 |
| 23:DB:1812:U:H1' | 25:DC:43:ASN:ND2 | 2.06 | 0.63 |
| 23:DB:195:A:H1' | 23:DB:250:G:N2 | 2.12 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:DG:89:VAL:HB | 29:DG:159:LYS:HA | 1.81 | 0.63 |
| 31:DJ:37:ARG:HE | 31:DJ:110:PRO:HG3 | 1.63 | 0.63 |
| 1:AA:1234:C:O2' | 1:AA:1235:U:H5' | 1.99 | 0.63 |
| 1:AA:1236:A:H4' | 1:AA:1304:G:H4' | 1.81 | 0.63 |
| 4:AE:106:ALA:HB1 | 4:AE:110:MET:HB3 | 1.81 | 0.63 |
| 5:AF:42:TRP:HB2 | 5:AF:59:TYR:HB2 | 1.78 | 0.63 |
| 23:BB:1373:A:H2' | 23:BB:1374:G:O4' | 1.98 | 0.63 |
| 23:BB:1551:A:H3' | 23:BB:1552:A:H5'' | 1.81 | 0.63 |
| 23:BB:1735:A:H2' | 23:BB:1736:U:C6 | 2.33 | 0.63 |
| 23:BB:350:G:H2' | 23:BB:351:C:O4' | 1.99 | 0.63 |
| 23:BB:37:C:H4' | 23:BB:451:U:OP1 | 1.98 | 0.63 |
| 26:BD:97:SER:HB3 | 26:BD:99:GLU:HG2 | 1.80 | 0.63 |
| 38:BQ:91:ARG:HG2 | 38:BQ:93:ILE:HG22 | 1.79 | 0.63 |
| 8:CI:23:GLY:H | 8:CI:60:LEU:HA | 1.62 | 0.63 |
| 9:CJ:56:HIS:O | 9:CJ:57:VAL:HG12 | 1.99 | 0.63 |
| 17:CR:55:ALA:HA | 17:CR:58:ILE:HD13 | 1.80 | 0.63 |
| 38:DQ:86:SER:O | 39:DR:51:VAL:HA | 1.99 | 0.63 |
| 24:DV:28:ALA:HA | 24:DV:88:HIS:CE1 | 2.33 | 0.63 |
| 46:DZ:71:LEU:HD13 | 46:DZ:76:GLU:HB3 | 1.81 | 0.63 |
| 1:AA:412:A:H4' | 1:AA:413:G:OP1 | 1.99 | 0.63 |
| 1:AA:825:A:H2' | 1:AA:826:C:H6 | 1.62 | 0.63 |
| 1:AA:950:U:H2' | 1:AA:951:G:C8 | 2.33 | 0.63 |
| 12:AM:63:VAL:HG13 | 12:AM:67:ASP:HB2 | 1.81 | 0.63 |
| 13:AN:63:CYS:HB3 | 13:AN:67:GLY:H | 1.64 | 0.63 |
| 19:AT:4:LYS:HZ1 | 19:AT:6:ALA:HB2 | 1.63 | 0.63 |
| 21:AU:48:LYS:HA | 21:AU:51:ALA:HB3 | 1.79 | 0.63 |
| 22:BA:28:C:OP1 | 36:BO:31:THR:HG21 | 1.99 | 0.63 |
| 23:BB:1060:U:O4 | 23:BB:1088:A:N6 | 2.31 | 0.63 |
| 23:BB:140:C:H4' | 23:BB:141:G:N2 | 2.12 | 0.63 |
| 23:BB:1722:A:H2' | 23:BB:1723:G:C8 | 2.34 | 0.63 |
| 23:BB:1856:U:H2' | 23:BB:1857:G:O4' | 1.99 | 0.63 |
| 23:BB:2748:A:H5'' | 29:BG:3:VAL:HG21 | 1.81 | 0.63 |
| 23:BB:654:A:H2' | 23:BB:655:A:H5'' | 1.81 | 0.63 |
| 33:BL:141:LYS:HD3 | 33:BL:142:ILE:H | 1.63 | 0.63 |
| 35:BN:70:THR:HB | 35:BN:75:ILE:HD11 | 1.78 | 0.63 |
| 1:CA:950:U:H2' | 1:CA:951:G:C8 | 2.34 | 0.63 |
| 10:CK:28:ASN:HD21 | 10:CK:46:ALA:HB3 | 1.62 | 0.63 |
| 49:D2:27:GLY:O | 49:D2:30:VAL:HB | 1.99 | 0.63 |
| 22:DA:6:G:H2' | 22:DA:7:G:H8 | 1.64 | 0.63 |
| 23:DB:2080:A:H4' | 46:DZ:19:SER:OG | 1.98 | 0.63 |
| 23:DB:2428:G:H21 | 33:DL:60:ARG:HE | 1.47 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:286:U:H2' | 23:DB:287:G:H8 | 1.63 | 0.63 |
| 25:DC:20:ASN:HB3 | 25:DC:23:LEU:HD22 | 1.81 | 0.63 |
| 41:DT:32:LEU:N | 41:DT:83:ALA:HB3 | 2.13 | 0.63 |
| 46:DZ:40:VAL:CG2 | 46:DZ:45:ARG:H | 2.11 | 0.63 |
| 4:AE:45:VAL:HG12 | 4:AE:116:VAL:HG23 | 1.79 | 0.63 |
| 23:BB:1723:G:N7 | 23:BB:1737:G:N2 | 2.47 | 0.63 |
| 23:BB:274:C:H2' | 23:BB:275:C:O4' | 1.99 | 0.63 |
| 23:BB:2834:G:H2' | 23:BB:2879:A:N6 | 2.13 | 0.63 |
| 26:BD:40:LEU:HA | 26:BD:45:TYR:N | 2.14 | 0.63 |
| 42:BU:27:VAL:HG23 | 42:BU:33:VAL:HG12 | 1.79 | 0.63 |
| 45:BY:8:GLN:CG | 45:BY:31:ILE:HA | 2.21 | 0.63 |
| 1:CA:204:G:H2' | 1:CA:205:A:C8 | 2.34 | 0.63 |
| 1:CA:376:G:H2' | 1:CA:377:G:H8 | 1.64 | 0.63 |
| 1:CA:462:G:H2' | 1:CA:462:G:N3 | 2.13 | 0.63 |
| 1:CA:677:U:H2' | 1:CA:678:U:H6 | 1.63 | 0.63 |
| 1:CA:620:C:C2 | 3:CD:131:ILE:HD13 | 2.33 | 0.63 |
| 3:CD:29:THR:HG22 | 3:CD:30:LYS:H | 1.64 | 0.63 |
| 4:CE:158:LYS:HZ3 | 7:CH:63:LYS:HD3 | 1.62 | 0.63 |
| 7:CH:94:VAL:HG23 | 7:CH:101:ALA:HB2 | 1.80 | 0.63 |
| 47:D0:8:THR:HG23 | 47:D0:11:LYS:H | 1.64 | 0.63 |
| 23:DB:1080:A:H2' | 23:DB:1081:U:C6 | 2.32 | 0.63 |
| 23:DB:1593:A:H2' | 23:DB:1594:U:C6 | 2.34 | 0.63 |
| 23:DB:1796:U:H2' | 23:DB:1797:G:H8 | 1.63 | 0.63 |
| 23:DB:401:A:H2' | 23:DB:402:A:C8 | 2.33 | 0.63 |
| 23:DB:521:U:H2' | 23:DB:522:A:C8 | 2.34 | 0.63 |
| 23:DB:594:U:H2' | 23:DB:595:C:H6 | 1.64 | 0.63 |
| 23:DB:963:U:H5'' | 56:DB:3697:HOH:O | 1.99 | 0.63 |
| 52:DI:72:THR:HG22 | 52:DI:115:ASP:OD2 | 1.98 | 0.63 |
| 52:DI:78:LEU:HA | 52:DI:81:LYS:HE2 | 1.81 | 0.63 |
| 35:DN:77:ALA:O | 35:DN:81:ASN:HB2 | 1.99 | 0.63 |
| 36:DO:17:LYS:O | 36:DO:21:LEU:HB2 | 1.99 | 0.63 |
| 45:DY:12:ALA:HA | 45:DY:15:ARG:HD3 | 1.81 | 0.63 |
| 1:AA:1134:G:C2 | 1:AA:1135:U:H1' | 2.33 | 0.62 |
| 1:AA:154:U:H2' | 1:AA:155:A:C8 | 2.33 | 0.62 |
| 1:AA:208:U:H2' | 1:AA:210:C:N3 | 2.14 | 0.62 |
| 1:AA:437:U:H4' | 3:AD:153:ARG:HH12 | 1.62 | 0.62 |
| 8:AI:42:THR:HA | 8:AI:45:MET:SD | 2.38 | 0.62 |
| 23:BB:1166:G:H2' | 23:BB:1167:C:H6 | 1.64 | 0.62 |
| 23:BB:1309:G:OP1 | 49:B2:9:VAL:HG12 | 1.99 | 0.62 |
| 23:BB:1508:A:H5' | 23:BB:1509:A:N6 | 2.13 | 0.62 |
| 23:BB:1678:A:H2' | 23:BB:1679:A:H8 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2277:G:H5'' | 34:BM:86:LYS:HB2 | 1.81 | 0.62 |
| 23:BB:2841:C:H2' | 23:BB:2842:G:C8 | 2.33 | 0.62 |
| 25:BC:202:ARG:HH11 | 25:BC:213:ARG:NE | 1.96 | 0.62 |
| 34:BM:34:LYS:HB3 | 34:BM:129:THR:HG22 | 1.80 | 0.62 |
| 38:BQ:14:LYS:O | 38:BQ:18:LYS:HB2 | 1.98 | 0.62 |
| 24:BV:80:HIS:CD2 | 24:BV:83:LYS:HB2 | 2.33 | 0.62 |
| 8:CI:25:GLY:HA3 | 8:CI:57:VAL:N | 2.13 | 0.62 |
| 9:CJ:28:THR:O | 9:CJ:32:THR:HG22 | 1.98 | 0.62 |
| 9:CJ:52:LEU:H | 9:CJ:52:LEU:HD12 | 1.64 | 0.62 |
| 23:DB:414:C:H2' | 23:DB:415:A:H8 | 1.63 | 0.62 |
| 23:DB:581:C:H2' | 23:DB:582:A:C8 | 2.33 | 0.62 |
| 29:DG:26:LYS:HB3 | 29:DG:26:LYS:HZ2 | 1.64 | 0.62 |
| 23:DB:1080:A:H4' | 52:DI:126:ARG:HD3 | 1.81 | 0.62 |
| 32:DK:7:MET:SD | 32:DK:20:MET:HB2 | 2.39 | 0.62 |
| 1:AA:462:G:N3 | 1:AA:462:G:H2' | 2.12 | 0.62 |
| 1:AA:750:C:O2 | 14:AO:22:GLY:HA3 | 2.00 | 0.62 |
| 23:BB:1244:A:H5'' | 33:BL:8:PRO:CD | 2.27 | 0.62 |
| 23:BB:1341:G:N2 | 23:BB:1398:C:H4' | 2.13 | 0.62 |
| 23:BB:1690:A:H2' | 23:BB:1691:C:O4' | 1.98 | 0.62 |
| 23:BB:2898:U:H2' | 23:BB:2899:A:H8 | 1.64 | 0.62 |
| 26:BD:117:GLY:HA2 | 26:BD:164:GLN:CD | 2.19 | 0.62 |
| 26:BD:179:ARG:HB3 | 26:BD:179:ARG:HH11 | 1.64 | 0.62 |
| 28:BF:102:LEU:HD22 | 28:BF:103:ILE:H | 1.65 | 0.62 |
| 29:BG:152:ARG:HG3 | 29:BG:153:PRO:HD2 | 1.81 | 0.62 |
| 30:BH:58:LEU:O | 30:BH:62:LEU:HG | 1.99 | 0.62 |
| 40:BS:17:VAL:C | 40:BS:19:LEU:H | 2.01 | 0.62 |
| 24:BV:28:ALA:HA | 24:BV:88:HIS:CE1 | 2.34 | 0.62 |
| 1:CA:600:A:H2' | 1:CA:601:G:H8 | 1.63 | 0.62 |
| 1:CA:978:A:HO2' | 1:CA:1322:C:H5 | 1.46 | 0.62 |
| 22:DA:29:A:H3' | 22:DA:30:C:H6 | 1.64 | 0.62 |
| 23:DB:1287:A:N7 | 35:DN:105:GLY:HA3 | 2.13 | 0.62 |
| 23:DB:1853:A:N1 | 23:DB:2087:G:H1' | 2.14 | 0.62 |
| 23:DB:2141:G:H2' | 23:DB:2142:A:C8 | 2.34 | 0.62 |
| 23:DB:639:U:H2' | 23:DB:640:C:H6 | 1.64 | 0.62 |
| 52:DI:121:ILE:N | 52:DI:121:ILE:HD13 | 2.13 | 0.62 |
| 33:DL:85:VAL:HG21 | 33:DL:94:THR:HB | 1.81 | 0.62 |
| 1:AA:1278:G:H4' | 1:AA:1279:G:C5' | 2.29 | 0.62 |
| 1:AA:792:A:H1' | 1:AA:794:A:N7 | 2.14 | 0.62 |
| 3:AD:56:GLU:HG2 | 3:AD:198:LEU:HD12 | 1.81 | 0.62 |
| 7:AH:25:THR:HA | 7:AH:58:LEU:O | 1.99 | 0.62 |
| 7:AH:6:ILE:HB | 7:AH:76:ARG:NH1 | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AJ:28:THR:O | 9:AJ:32:THR:HG22 | 1.99 | 0.62 |
| 13:AN:42:ASN:O | 13:AN:46:LYS:HG2 | 1.99 | 0.62 |
| 18:AS:31:ARG:HA | 18:AS:49:ALA:HB3 | 1.81 | 0.62 |
| 23:BB:135:U:O2' | 23:BB:136:G:H5' | 1.99 | 0.62 |
| 23:BB:1847:A:H4' | 23:BB:1848:A:C8 | 2.34 | 0.62 |
| 23:BB:2563:U:H2' | 23:BB:2565:A:OP2 | 2.00 | 0.62 |
| 23:BB:988:A:H3' | 45:BY:13:ILE:HD11 | 1.80 | 0.62 |
| 25:BC:36:ASN:HD21 | 25:BC:85:ASN:ND2 | 1.97 | 0.62 |
| 28:BF:168:LEU:HD13 | 28:BF:169:LEU:N | 2.14 | 0.62 |
| 30:BH:5:LEU:O | 30:BH:6:LEU:HD12 | 1.99 | 0.62 |
| 52:BI:105:LEU:HD11 | 52:BI:139:VAL:HG11 | 1.80 | 0.62 |
| 6:CG:14:ASP:CB | 6:CG:19:SER:H | 2.12 | 0.62 |
| 6:CG:86:VAL:HG13 | 6:CG:151:ALA:O | 1.98 | 0.62 |
| 9:CJ:24:GLU:HG3 | 9:CJ:90:LEU:HD11 | 1.81 | 0.62 |
| 50:D3:54:LEU:O | 50:D3:58:ILE:HG13 | 1.98 | 0.62 |
| 23:DB:264:C:C2' | 23:DB:265:A:H5'' | 2.28 | 0.62 |
| 23:DB:2841:C:H2' | 23:DB:2842:G:C8 | 2.34 | 0.62 |
| 23:DB:2898:U:H2' | 23:DB:2899:A:C8 | 2.35 | 0.62 |
| 23:DB:718:A:H3' | 23:DB:719:C:H6 | 1.64 | 0.62 |
| 23:DB:987:C:H2' | 23:DB:988:A:O4' | 1.99 | 0.62 |
| 25:DC:136:VAL:HG12 | 25:DC:137:GLY:H | 1.64 | 0.62 |
| 23:DB:784:G:C6 | 25:DC:227:VAL:HG11 | 2.34 | 0.62 |
| 26:DD:136:ASN:HD21 | 26:DD:139:SER:C | 2.03 | 0.62 |
| 26:DD:8:LYS:HB2 | 26:DD:201:LEU:HD21 | 1.80 | 0.62 |
| 28:DF:168:LEU:HD13 | 28:DF:169:LEU:N | 2.14 | 0.62 |
| 30:DH:53:GLU:HB2 | 30:DH:57:LYS:HB3 | 1.82 | 0.62 |
| 52:DI:27:LEU:HD12 | 52:DI:32:VAL:HG11 | 1.79 | 0.62 |
| 33:DL:79:LEU:HD23 | 33:DL:82:LEU:HD11 | 1.81 | 0.62 |
| 41:DT:7:LEU:HA | 41:DT:9:LYS:HZ1 | 1.62 | 0.62 |
| 42:DU:87:GLU:OE2 | 42:DU:88:ASP:HB3 | 1.98 | 0.62 |
| 2:AC:62:SER:HA | 2:AC:97:PRO:O | 1.99 | 0.62 |
| 5:AF:47:LEU:HD21 | 5:AF:57:ALA:HB3 | 1.81 | 0.62 |
| 6:AG:45:ALA:HB1 | 6:AG:120:ALA:HB2 | 1.79 | 0.62 |
| 9:AJ:55:PRO:HA | 13:AN:80:ARG:NH2 | 2.15 | 0.62 |
| 14:AO:52:ARG:HD2 | 23:BB:715:A:N6 | 2.13 | 0.62 |
| 23:BB:1407:G:H2' | 23:BB:1408:G:H8 | 1.63 | 0.62 |
| 23:BB:1535:A:H5'' | 23:BB:1536:C:H5 | 1.64 | 0.62 |
| 23:BB:195:A:H1' | 23:BB:250:G:N2 | 2.14 | 0.62 |
| 26:BD:136:ASN:HD21 | 26:BD:139:SER:C | 2.03 | 0.62 |
| 26:BD:178:VAL:HG12 | 26:BD:179:ARG:H | 1.64 | 0.62 |
| 36:BO:17:LYS:O | 36:BO:21:LEU:HB2 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:BU:11:ILE:HG22 | 42:BU:70:ALA:HB3 | 1.80 | 0.62 |
| 1:CA:1144:G:H21 | 1:CA:1146:A:H62 | 1.46 | 0.62 |
| 1:CA:750:C:O2 | 14:CO:22:GLY:HA3 | 1.98 | 0.62 |
| 18:CS:10:ILE:HD12 | 18:CS:15:LEU:HG | 1.81 | 0.62 |
| 23:DB:1341:G:N2 | 23:DB:1398:C:H4' | 2.13 | 0.62 |
| 23:DB:1353:A:H2' | 23:DB:1354:A:C8 | 2.34 | 0.62 |
| 23:DB:2654:A:N1 | 23:DB:2665:A:H5'' | 2.14 | 0.62 |
| 26:DD:109:VAL:HG11 | 26:DD:193:VAL:HB | 1.81 | 0.62 |
| 26:DD:115:GLY:HA2 | 26:DD:167:ASN:HB2 | 1.81 | 0.62 |
| 29:DG:89:VAL:HG12 | 29:DG:90:GLY:H | 1.64 | 0.62 |
| 31:DJ:40:HIS:ND1 | 31:DJ:41:LYS:HG3 | 2.14 | 0.62 |
| 32:DK:38:ILE:O | 32:DK:39:ILE:HD13 | 2.00 | 0.62 |
| 42:DU:71:ILE:HD11 | 42:DU:82:VAL:HG22 | 1.82 | 0.62 |
| 1:AA:1004:A:H3' | 1:AA:1024:G:N2 | 2.14 | 0.62 |
| 1:AA:1085:U:H3' | 1:AA:1086:U:C5 | 2.34 | 0.62 |
| 1:AA:97:G:H2' | 1:AA:98:A:O4' | 1.99 | 0.62 |
| 11:AL:40:THR:HG22 | 11:AL:41:PRO:HD2 | 1.81 | 0.62 |
| 22:BA:74:U:H2' | 22:BA:75:G:C8 | 2.33 | 0.62 |
| 23:BB:1260:A:H2' | 23:BB:1261:C:C6 | 2.34 | 0.62 |
| 23:BB:2066:C:O2' | 23:BB:2067:G:H5' | 1.98 | 0.62 |
| 23:BB:2810:A:H2' | 23:BB:2811:G:O4' | 1.99 | 0.62 |
| 23:BB:445:C:O2' | 23:BB:446:G:H5' | 1.99 | 0.62 |
| 23:BB:495:G:H1' | 40:BS:57:ASN:ND2 | 2.15 | 0.62 |
| 23:BB:946:C:H2' | 23:BB:947:A:H8 | 1.65 | 0.62 |
| 32:BK:38:ILE:O | 32:BK:39:ILE:HD13 | 1.99 | 0.62 |
| 22:BA:7:G:H1' | 36:BO:38:GLN:HE22 | 1.63 | 0.62 |
| 1:CA:1053:G:H4' | 1:CA:1054:C:H5' | 1.81 | 0.62 |
| 1:CA:946:A:H2' | 1:CA:947:G:H8 | 1.63 | 0.62 |
| 2:CC:59:PRO:HG2 | 2:CC:62:SER:OG | 2.00 | 0.62 |
| 23:DB:1198:U:H2' | 23:DB:1199:U:C6 | 2.35 | 0.62 |
| 23:DB:545:U:H4' | 23:DB:550:C:O2 | 2.00 | 0.62 |
| 26:DD:105:LYS:HE3 | 26:DD:176:ASP:OD1 | 1.99 | 0.62 |
| 28:DF:62:GLN:OE1 | 28:DF:94:ARG:HG2 | 2.00 | 0.62 |
| 30:DH:41:LYS:O | 30:DH:44:ILE:HG12 | 1.99 | 0.62 |
| 32:DK:70:ARG:HB3 | 32:DK:76:VAL:HG22 | 1.82 | 0.62 |
| 38:DQ:57:ARG:CB | 38:DQ:57:ARG:HH11 | 2.12 | 0.62 |
| 38:DQ:74:SER:OG | 38:DQ:77:LYS:HD3 | 2.00 | 0.62 |
| 6:AG:14:ASP:N | 6:AG:23:ALA:HB2 | 2.13 | 0.62 |
| 8:AI:126:PHE:CE1 | 8:AI:129:ARG:HD3 | 2.35 | 0.62 |
| 11:AL:113:ARG:HG2 | 11:AL:118:VAL:HB | 1.82 | 0.62 |
| 19:AT:24:ARG:HD2 | 19:AT:28:ARG:NH2 | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1593:A:H2' | 23:BB:1594:U:C6 | 2.35 | 0.62 |
| 23:BB:1704:C:O2' | 23:BB:1705:A:H5' | 1.99 | 0.62 |
| 23:BB:172:A:H2' | 23:BB:173:A:H8 | 1.63 | 0.62 |
| 23:BB:639:U:H2' | 23:BB:640:C:H6 | 1.64 | 0.62 |
| 23:BB:675:A:H4' | 27:BE:62:GLN:HE22 | 1.63 | 0.62 |
| 28:BF:104:THR:C | 28:BF:108:PRO:HG2 | 2.20 | 0.62 |
| 31:BJ:23:LYS:HE2 | 31:BJ:142:ILE:HA | 1.82 | 0.62 |
| 32:BK:43:ILE:HG21 | 32:BK:46:ALA:HB2 | 1.80 | 0.62 |
| 36:BO:53:THR:HB | 36:BO:65:THR:HG22 | 1.81 | 0.62 |
| 1:CA:162:A:H2' | 1:CA:163:C:O4' | 2.00 | 0.62 |
| 1:CA:482:A:H2' | 1:CA:483:C:O4' | 2.00 | 0.62 |
| 1:CA:763:G:H2' | 1:CA:764:C:C6 | 2.34 | 0.62 |
| 20:CB:205:ALA:O | 20:CB:209:VAL:HG22 | 1.98 | 0.62 |
| 4:CE:37:VAL:HG11 | 4:CE:113:VAL:HG12 | 1.82 | 0.62 |
| 8:CI:18:VAL:HG11 | 8:CI:82:ILE:HG12 | 1.81 | 0.62 |
| 13:CN:26:LEU:HA | 13:CN:29:ILE:HD12 | 1.82 | 0.62 |
| 23:DB:2064:C:H2' | 23:DB:2065:C:C6 | 2.33 | 0.62 |
| 23:DB:2102:G:H2' | 23:DB:2103:C:O4' | 1.99 | 0.62 |
| 25:DC:94:LEU:HA | 25:DC:100:ARG:HB3 | 1.80 | 0.62 |
| 28:DF:72:SER:HA | 28:DF:80:GLN:N | 2.15 | 0.62 |
| 34:DM:71:LYS:HB3 | 34:DM:93:VAL:HG12 | 1.81 | 0.62 |
| 37:DP:24:THR:O | 37:DP:25:VAL:HG22 | 1.99 | 0.62 |
| 38:DQ:14:LYS:O | 38:DQ:18:LYS:HB2 | 1.99 | 0.62 |
| 44:DX:1:MET:HB3 | 44:DX:4:LYS:HD3 | 1.80 | 0.62 |
| 1:AA:1323:G:H4' | 1:AA:1362:A:C4 | 2.35 | 0.62 |
| 1:AA:46:G:O2' | 1:AA:365:U:H1' | 1.99 | 0.62 |
| 3:AD:96:ARG:HB3 | 3:AD:98:ASP:OD2 | 2.00 | 0.62 |
| 23:BB:1133:A:H4' | 23:BB:1134:A:O5' | 2.00 | 0.62 |
| 23:BB:1406:U:H2' | 23:BB:1407:G:C8 | 2.35 | 0.62 |
| 23:BB:1657:U:O2' | 23:BB:1658:C:H5' | 2.00 | 0.62 |
| 23:BB:1674:G:H21 | 23:BB:1677:A:N6 | 1.96 | 0.62 |
| 23:BB:189:G:H2' | 23:BB:205:G:N2 | 2.14 | 0.62 |
| 23:BB:2312:U:O2 | 28:BF:38:GLY:HA3 | 1.99 | 0.62 |
| 23:BB:784:G:N1 | 25:BC:227:VAL:HG11 | 2.15 | 0.62 |
| 28:BF:36:ASN:HA | 28:BF:87:LYS:HA | 1.82 | 0.62 |
| 29:BG:132:LEU:HD23 | 29:BG:132:LEU:H | 1.64 | 0.62 |
| 38:BQ:65:ASN:CB | 38:BQ:75:TYR:HB2 | 2.29 | 0.62 |
| 46:BZ:6:GLN:NE2 | 46:BZ:50:ARG:H | 1.94 | 0.62 |
| 1:CA:154:U:H2' | 1:CA:155:A:C8 | 2.35 | 0.62 |
| 3:CD:84:ASN:ND2 | 4:CE:101:GLY:HA3 | 2.14 | 0.62 |
| 1:CA:1092:A:H5" | 6:CG:3:ARG:HH11 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:CM:63:VAL:HG13 | 12:CM:67:ASP:HB2 | 1.82 | 0.62 |
| 13:CN:63:CYS:HB3 | 13:CN:67:GLY:H | 1.63 | 0.62 |
| 23:DB:2834:G:H1' | 23:DB:2883:A:H61 | 1.63 | 0.62 |
| 23:DB:522:A:H2' | 23:DB:523:C:C6 | 2.35 | 0.62 |
| 32:DK:104:THR:H | 32:DK:107:LEU:HD12 | 1.64 | 0.62 |
| 34:DM:64:TRP:HB2 | 34:DM:104:GLU:HB2 | 1.81 | 0.62 |
| 1:AA:1132:C:H2' | 1:AA:1133:G:C8 | 2.34 | 0.62 |
| 1:AA:131:A:H2' | 1:AA:132:C:C6 | 2.34 | 0.62 |
| 1:AA:1414:U:H2' | 1:AA:1415:G:H8 | 1.65 | 0.62 |
| 1:AA:678:U:H2' | 1:AA:679:C:C6 | 2.35 | 0.62 |
| 6:AG:78:ARG:HH11 | 6:AG:81:GLY:H | 1.47 | 0.62 |
| 23:BB:1760:C:H2' | 23:BB:1761:C:O4' | 1.99 | 0.62 |
| 23:BB:1778:U:H2' | 23:BB:1784:A:H62 | 1.64 | 0.62 |
| 23:BB:2737:G:H2' | 23:BB:2738:A:C8 | 2.34 | 0.62 |
| 23:BB:2772:C:H2' | 23:BB:2773:C:H6 | 1.64 | 0.62 |
| 23:BB:2820:A:H4' | 35:BN:3:HIS:ND1 | 2.15 | 0.62 |
| 23:BB:2073:C:H5'' | 25:BC:227:VAL:HG12 | 1.80 | 0.62 |
| 28:BF:41:GLU:O | 28:BF:43:ILE:HG22 | 2.00 | 0.62 |
| 28:BF:72:SER:HA | 28:BF:80:GLN:N | 2.15 | 0.62 |
| 30:BH:32:PRO:O | 30:BH:33:GLN:HB2 | 1.99 | 0.62 |
| 31:BJ:136:GLN:N | 31:BJ:137:PRO:HD3 | 2.15 | 0.62 |
| 42:BU:11:ILE:O | 42:BU:12:VAL:HB | 2.00 | 0.62 |
| 46:BZ:45:ARG:HE | 46:BZ:47:VAL:CG1 | 2.13 | 0.62 |
| 1:CA:865:A:C2 | 1:CA:918:A:H4' | 2.34 | 0.62 |
| 20:CB:71:THR:CG2 | 20:CB:94:ARG:H | 2.12 | 0.62 |
| 11:CL:14:LYS:HG2 | 11:CL:16:ALA:H | 1.63 | 0.62 |
| 19:CT:4:LYS:HZ1 | 19:CT:6:ALA:HB2 | 1.63 | 0.62 |
| 23:DB:1549:A:H2' | 23:DB:1550:C:C6 | 2.34 | 0.62 |
| 23:DB:1760:C:H2' | 23:DB:1761:C:O4' | 1.98 | 0.62 |
| 23:DB:1778:U:H2' | 23:DB:1784:A:N6 | 2.15 | 0.62 |
| 23:DB:2156:G:H2' | 23:DB:2157:G:H4' | 1.81 | 0.62 |
| 23:DB:2443:C:H2' | 23:DB:2444:G:C8 | 2.35 | 0.62 |
| 23:DB:557:C:H2' | 23:DB:558:U:C6 | 2.35 | 0.62 |
| 23:DB:947:A:H2' | 23:DB:948:C:C6 | 2.35 | 0.62 |
| 23:DB:946:C:H2' | 23:DB:947:A:H8 | 1.64 | 0.62 |
| 36:DO:111:ARG:HD2 | 36:DO:117:PHE:O | 2.00 | 0.62 |
| 36:DO:67:ASN:HB3 | 36:DO:70:ALA:HB2 | 1.82 | 0.62 |
| 38:DQ:91:ARG:HH12 | 39:DR:10:LYS:CB | 2.12 | 0.62 |
| 42:DU:9:GLU:HG3 | 42:DU:21:ARG:HD2 | 1.81 | 0.62 |
| 45:DY:7:THR:HB | 45:DY:55:LYS:H | 1.64 | 0.62 |
| 1:AA:1151:A:HO2' | 1:AA:1152:A:H8 | 1.45 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1238:A:H5' | 1:AA:1336:C:H41 | 1.64 | 0.62 |
| 1:AA:266:G:O2' | 1:AA:267:C:H3' | 1.99 | 0.62 |
| 1:AA:658:C:H2' | 1:AA:659:U:H6 | 1.63 | 0.62 |
| 1:AA:806:C:H2' | 1:AA:807:A:C8 | 2.35 | 0.62 |
| 1:AA:834:U:H2' | 1:AA:835:U:C6 | 2.35 | 0.62 |
| 20:AB:221:ARG:HG3 | 20:AB:222:GLU:N | 2.15 | 0.62 |
| 20:AB:62:ARG:H | 20:AB:62:ARG:HD2 | 1.65 | 0.62 |
| 18:AS:42:ASN:N | 18:AS:42:ASN:HD22 | 1.95 | 0.62 |
| 21:AU:40:PRO:HA | 21:AU:44:ARG:HB2 | 1.80 | 0.62 |
| 23:BB:1149:G:H2' | 23:BB:1150:C:C6 | 2.35 | 0.62 |
| 23:BB:1287:A:H3' | 23:BB:1288:G:H21 | 1.64 | 0.62 |
| 23:BB:18:U:H2' | 23:BB:19:A:H8 | 1.64 | 0.62 |
| 23:BB:2269:G:C4' | 43:BW:19:ARG:HH12 | 2.12 | 0.62 |
| 23:BB:2898:U:H2' | 23:BB:2899:A:C8 | 2.35 | 0.62 |
| 52:BI:85:ILE:HD13 | 52:BI:137:LEU:HD21 | 1.82 | 0.62 |
| 33:BL:19:LEU:O | 33:BL:21:ARG:HG2 | 2.00 | 0.62 |
| 1:CA:487:A:H2' | 1:CA:488:C:O4' | 2.00 | 0.62 |
| 5:CF:3:HIS:CE1 | 5:CF:95:ALA:H | 2.18 | 0.62 |
| 23:DB:704:G:H2' | 23:DB:726:G:N2 | 2.14 | 0.62 |
| 25:DC:70:LYS:HE2 | 25:DC:99:GLU:HB3 | 1.82 | 0.62 |
| 25:DC:36:ASN:HD21 | 25:DC:85:ASN:HD21 | 1.46 | 0.62 |
| 30:DH:83:LYS:O | 30:DH:90:LEU:HA | 2.00 | 0.62 |
| 31:DJ:40:HIS:CE1 | 31:DJ:41:LYS:HG3 | 2.35 | 0.62 |
| 32:DK:71:ARG:HG3 | 32:DK:105:ARG:HH21 | 1.65 | 0.62 |
| 24:DV:80:HIS:CD2 | 24:DV:83:LYS:HB2 | 2.35 | 0.62 |
| 43:DW:39:GLN:NE2 | 43:DW:43:LYS:HB2 | 2.14 | 0.62 |
| 1:AA:1053:G:H4' | 1:AA:1054:C:H5' | 1.82 | 0.62 |
| 1:AA:1296:C:H4' | 1:AA:1302:C:N3 | 2.15 | 0.62 |
| 1:AA:1463:U:H2' | 1:AA:1464:U:C6 | 2.34 | 0.62 |
| 1:AA:335:C:H2' | 1:AA:336:A:C8 | 2.34 | 0.62 |
| 1:AA:482:A:H2' | 1:AA:483:C:O4' | 2.00 | 0.62 |
| 20:AB:72:LYS:HE3 | 20:AB:203:ASP:O | 2.00 | 0.62 |
| 16:AQ:58:VAL:HG12 | 16:AQ:77:VAL:HA | 1.80 | 0.62 |
| 22:BA:75:G:H1' | 24:BV:29:ILE:HG12 | 1.81 | 0.62 |
| 23:BB:1109:C:H2' | 23:BB:1110:G:C4 | 2.35 | 0.62 |
| 23:BB:2693:G:H2' | 23:BB:2694:G:H8 | 1.63 | 0.62 |
| 28:BF:31:GLU:O | 28:BF:32:LYS:HD3 | 2.00 | 0.62 |
| 36:BO:40:ILE:HA | 36:BO:47:VAL:HA | 1.80 | 0.62 |
| 41:BT:32:LEU:N | 41:BT:83:ALA:HB3 | 2.13 | 0.62 |
| 1:CA:1141:C:H2' | 1:CA:1142:G:H8 | 1.65 | 0.62 |
| 1:CA:1149:C:H2' | 1:CA:1150:A:C8 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1432:G:H1' | 1:CA:1468:A:N6 | 2.14 | 0.62 |
| 1:CA:255:G:H2' | 1:CA:256:U:C6 | 2.34 | 0.62 |
| 1:CA:539:A:H2' | 1:CA:540:G:C8 | 2.35 | 0.62 |
| 1:CA:678:U:H2' | 1:CA:679:C:H6 | 1.64 | 0.62 |
| 1:CA:909:A:H2' | 1:CA:910:C:O4' | 1.99 | 0.62 |
| 6:CG:14:ASP:N | 6:CG:23:ALA:HB2 | 2.14 | 0.62 |
| 51:D4:2:LYS:HG2 | 51:D4:3:VAL:H | 1.64 | 0.62 |
| 22:DA:32:U:H4' | 22:DA:52:A:N6 | 2.15 | 0.62 |
| 23:DB:1024:G:C3' | 23:DB:1025:G:H5'' | 2.28 | 0.62 |
| 23:DB:1149:G:H2' | 23:DB:1150:C:C6 | 2.34 | 0.62 |
| 23:DB:1485:U:H2' | 23:DB:1486:U:C6 | 2.35 | 0.62 |
| 23:DB:1518:C:H2' | 23:DB:1519:G:C8 | 2.35 | 0.62 |
| 23:DB:1557:C:H3' | 23:DB:1558:C:H5'' | 1.82 | 0.62 |
| 23:DB:1802:A:H2' | 23:DB:1803:A:C8 | 2.35 | 0.62 |
| 23:DB:2815:C:H2' | 23:DB:2816:G:H8 | 1.65 | 0.62 |
| 23:DB:2895:G:H2' | 23:DB:2896:C:H6 | 1.64 | 0.62 |
| 23:DB:321:U:OP2 | 27:DE:130:LYS:HD3 | 2.00 | 0.62 |
| 23:DB:359:G:H2' | 23:DB:360:U:H5' | 1.80 | 0.62 |
| 23:DB:62:U:O2' | 23:DB:63:A:H5' | 1.98 | 0.62 |
| 23:DB:64:A:H2' | 23:DB:65:U:C6 | 2.35 | 0.62 |
| 23:DB:721:A:H2' | 23:DB:722:A:H8 | 1.65 | 0.62 |
| 27:DE:188:MET:HG2 | 27:DE:193:VAL:HG22 | 1.82 | 0.62 |
| 28:DF:41:GLU:O | 28:DF:43:ILE:HG22 | 1.99 | 0.62 |
| 1:AA:735:C:O2' | 1:AA:736:C:H5' | 1.99 | 0.61 |
| 3:AD:12:ARG:HA | 3:AD:33:ILE:HD12 | 1.82 | 0.61 |
| 18:AS:5:LYS:O | 18:AS:6:LYS:HD2 | 2.00 | 0.61 |
| 23:BB:2264:C:H41 | 43:BW:11:ASN:HD21 | 1.48 | 0.61 |
| 23:BB:2743:U:H2' | 23:BB:2744:G:O4' | 1.99 | 0.61 |
| 23:BB:592:A:H2' | 23:BB:593:U:C6 | 2.35 | 0.61 |
| 23:BB:717:C:H3' | 23:BB:718:A:H5'' | 1.82 | 0.61 |
| 23:BB:753:A:H2' | 23:BB:754:U:C6 | 2.35 | 0.61 |
| 25:BC:127:ASN:O | 25:BC:190:THR:HA | 1.99 | 0.61 |
| 26:BD:13:ARG:HD3 | 26:BD:15:PHE:HE1 | 1.65 | 0.61 |
| 27:BE:117:ARG:HH12 | 33:BL:2:ARG:HB2 | 1.64 | 0.61 |
| 52:BI:18:ASN:N | 52:BI:19:PRO:HD2 | 2.14 | 0.61 |
| 3:CD:123:MET:HB3 | 3:CD:128:VAL:HA | 1.82 | 0.61 |
| 4:CE:93:VAL:HG13 | 4:CE:126:ALA:HB2 | 1.82 | 0.61 |
| 6:CG:2:ARG:HH11 | 6:CG:2:ARG:CB | 2.13 | 0.61 |
| 9:CJ:53:ILE:HG22 | 9:CJ:61:ALA:HB1 | 1.82 | 0.61 |
| 23:DB:1013:C:H2' | 23:DB:1014:A:H8 | 1.64 | 0.61 |
| 23:DB:155:A:H2' | 23:DB:156:A:C8 | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:37:C:O2' | 27:DE:45:ALA:HA | 2.00 | 0.61 |
| 23:DB:419:U:H2' | 23:DB:420:C:C6 | 2.35 | 0.61 |
| 23:DB:441:U:H2' | 23:DB:442:G:H8 | 1.65 | 0.61 |
| 23:DB:63:A:OP2 | 23:DB:63:A:H8 | 1.83 | 0.61 |
| 42:DU:70:ALA:HB1 | 42:DU:79:ALA:CB | 2.30 | 0.61 |
| 1:AA:1179:A:H2' | 1:AA:1180:A:O4' | 2.01 | 0.61 |
| 1:AA:600:A:H2' | 1:AA:601:G:H8 | 1.64 | 0.61 |
| 20:AB:202:ASN:HD22 | 20:AB:204:ASP:N | 1.90 | 0.61 |
| 3:AD:29:THR:HG22 | 3:AD:30:LYS:HD3 | 1.80 | 0.61 |
| 56:AA:2260:HOH:O | 8:AI:110:VAL:HG13 | 1.99 | 0.61 |
| 8:AI:7:GLY:HA2 | 8:AI:85:ALA:HB2 | 1.82 | 0.61 |
| 12:AM:89:ARG:HD3 | 12:AM:95:PRO:O | 1.99 | 0.61 |
| 23:BB:1591:A:H2' | 23:BB:1592:C:O4' | 2.00 | 0.61 |
| 23:BB:987:C:H2' | 23:BB:988:A:O4' | 2.00 | 0.61 |
| 23:BB:633:A:OP1 | 33:BL:68:SER:HB2 | 2.00 | 0.61 |
| 41:BT:11:LEU:N | 41:BT:11:LEU:HD22 | 2.15 | 0.61 |
| 46:BZ:6:GLN:HE22 | 46:BZ:50:ARG:N | 1.95 | 0.61 |
| 1:CA:46:G:O2' | 1:CA:365:U:H1' | 2.00 | 0.61 |
| 5:CF:36:ILE:HG13 | 5:CF:64:VAL:HG13 | 1.81 | 0.61 |
| 16:CQ:58:VAL:HG12 | 16:CQ:77:VAL:HA | 1.82 | 0.61 |
| 19:CT:79:THR:HA | 19:CT:82:ILE:HG12 | 1.82 | 0.61 |
| 21:CU:33:ARG:HG2 | 21:CU:34:ARG:H | 1.65 | 0.61 |
| 23:DB:1373:A:H2' | 23:DB:1374:G:O4' | 1.99 | 0.61 |
| 23:DB:2810:A:H2' | 23:DB:2811:G:O4' | 1.99 | 0.61 |
| 23:DB:441:U:H2' | 23:DB:442:G:C8 | 2.36 | 0.61 |
| 23:DB:443:A:C5 | 27:DE:40:ARG:HD3 | 2.34 | 0.61 |
| 23:DB:27:G:H1' | 23:DB:513:A:H61 | 1.63 | 0.61 |
| 26:DD:113:SER:HB3 | 26:DD:168:GLU:N | 2.13 | 0.61 |
| 26:DD:40:LEU:HA | 26:DD:45:TYR:N | 2.14 | 0.61 |
| 28:DF:37:MET:HB2 | 28:DF:56:LEU:HD21 | 1.82 | 0.61 |
| 30:DH:3:VAL:HG12 | 30:DH:38:PRO:HA | 1.81 | 0.61 |
| 36:DO:53:THR:HB | 36:DO:65:THR:HG22 | 1.81 | 0.61 |
| 44:DX:49:ASP:O | 44:DX:53:VAL:HG23 | 1.99 | 0.61 |
| 1:AA:1239:A:H4' | 1:AA:1240:U:H5' | 1.82 | 0.61 |
| 1:AA:131:A:H2' | 1:AA:132:C:H6 | 1.64 | 0.61 |
| 1:AA:1342:C:H2' | 1:AA:1343:G:H8 | 1.63 | 0.61 |
| 20:AB:187:ASP:HB3 | 20:AB:201:GLY:O | 2.01 | 0.61 |
| 8:AI:25:GLY:HA3 | 8:AI:57:VAL:CA | 2.30 | 0.61 |
| 18:AS:50:VAL:O | 18:AS:57:VAL:HG22 | 1.99 | 0.61 |
| 49:B2:27:GLY:O | 49:B2:30:VAL:HB | 2.00 | 0.61 |
| 23:BB:1535:A:H5'' | 23:BB:1536:C:C5 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2366:A:H2' | 23:BB:2367:G:O4' | 2.01 | 0.61 |
| 23:BB:300:A:H2' | 23:BB:334:C:H1' | 1.81 | 0.61 |
| 23:BB:355:U:H2' | 23:BB:356:G:H8 | 1.65 | 0.61 |
| 23:BB:670:A:H4' | 33:BL:42:SER:HB2 | 1.82 | 0.61 |
| 25:BC:136:VAL:HG12 | 25:BC:137:GLY:H | 1.64 | 0.61 |
| 35:BN:24:MET:HG3 | 35:BN:44:LEU:HD22 | 1.82 | 0.61 |
| 38:BQ:93:ILE:HG23 | 38:BQ:94:LEU:HD22 | 1.81 | 0.61 |
| 42:BU:81:ARG:HB2 | 42:BU:96:LYS:CG | 2.29 | 0.61 |
| 1:CA:1244:G:H2' | 1:CA:1245:C:C6 | 2.35 | 0.61 |
| 1:CA:1409:C:H4' | 23:DB:1915:U:O4 | 2.00 | 0.61 |
| 1:CA:410:G:P | 3:CD:25:ARG:HD2 | 2.40 | 0.61 |
| 21:CU:40:PRO:HA | 21:CU:44:ARG:HB2 | 1.82 | 0.61 |
| 23:DB:1591:A:H2' | 23:DB:1592:C:O4' | 2.00 | 0.61 |
| 23:DB:233:A:H61 | 23:DB:428:A:N6 | 1.98 | 0.61 |
| 23:DB:417:C:H2' | 23:DB:418:C:C6 | 2.36 | 0.61 |
| 23:DB:851:C:O2 | 45:DY:42:ALA:HB1 | 2.00 | 0.61 |
| 28:DF:71:LYS:HE2 | 28:DF:73:VAL:HB | 1.81 | 0.61 |
| 42:DU:26:ASN:N | 42:DU:26:ASN:HD22 | 1.96 | 0.61 |
| 1:AA:1029:U:H1' | 1:AA:1032:G:O6 | 2.00 | 0.61 |
| 1:AA:253:A:H2' | 1:AA:254:G:C8 | 2.35 | 0.61 |
| 1:AA:512:U:H2' | 1:AA:513:C:C6 | 2.36 | 0.61 |
| 1:AA:825:A:H2' | 1:AA:826:C:C6 | 2.34 | 0.61 |
| 20:AB:163:ILE:HG23 | 20:AB:164:ASP:N | 2.15 | 0.61 |
| 4:AE:105:ILE:HD11 | 4:AE:123:LEU:HB3 | 1.83 | 0.61 |
| 4:AE:61:LYS:O | 4:AE:65:LYS:HG2 | 2.01 | 0.61 |
| 6:AG:2:ARG:HB3 | 6:AG:3:ARG:NH1 | 2.15 | 0.61 |
| 50:B3:54:LEU:HG | 50:B3:58:ILE:HD11 | 1.82 | 0.61 |
| 23:BB:1024:G:C3' | 23:BB:1025:G:H5'' | 2.30 | 0.61 |
| 23:BB:1518:C:H2' | 23:BB:1519:G:C8 | 2.35 | 0.61 |
| 23:BB:1592:C:H2' | 23:BB:1593:A:H8 | 1.65 | 0.61 |
| 23:BB:1684:G:H2' | 23:BB:1685:C:C6 | 2.35 | 0.61 |
| 23:BB:233:A:H61 | 23:BB:428:A:N6 | 1.98 | 0.61 |
| 23:BB:49:A:H5'' | 23:BB:51:G:O4' | 2.01 | 0.61 |
| 23:BB:27:G:H1' | 23:BB:513:A:H61 | 1.65 | 0.61 |
| 25:BC:103:ILE:HG22 | 25:BC:105:ALA:H | 1.64 | 0.61 |
| 25:BC:94:LEU:HA | 25:BC:100:ARG:HB3 | 1.81 | 0.61 |
| 31:BJ:101:ILE:O | 31:BJ:105:VAL:HG22 | 2.01 | 0.61 |
| 31:BJ:111:LYS:HB3 | 31:BJ:113:PRO:HD2 | 1.81 | 0.61 |
| 31:BJ:40:HIS:ND1 | 31:BJ:41:LYS:HG3 | 2.15 | 0.61 |
| 35:BN:85:PRO:HA | 35:BN:88:ALA:HB2 | 1.82 | 0.61 |
| 38:BQ:79:ILE:O | 38:BQ:82:LEU:HB2 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BT:45:ALA:HA | 41:BT:48:GLN:HB2 | 1.82 | 0.61 |
| 1:CA:1029:U:H1' | 1:CA:1032:G:O6 | 2.00 | 0.61 |
| 1:CA:1382:C:H4' | 6:CG:78:ARG:NH2 | 2.15 | 0.61 |
| 1:CA:1463:U:H2' | 1:CA:1464:U:C6 | 2.36 | 0.61 |
| 8:CI:17:ARG:O | 8:CI:64:ILE:HA | 2.00 | 0.61 |
| 19:CT:66:ILE:HG22 | 19:CT:67:HIS:N | 2.15 | 0.61 |
| 23:DB:1847:A:H4' | 23:DB:1848:A:C8 | 2.35 | 0.61 |
| 23:DB:1917:U:H2' | 23:DB:1918:A:H5' | 1.82 | 0.61 |
| 23:DB:2041:U:H2' | 23:DB:2042:A:C8 | 2.35 | 0.61 |
| 23:DB:402:A:H2' | 23:DB:403:U:O4' | 1.99 | 0.61 |
| 23:DB:639:U:H2' | 23:DB:640:C:C6 | 2.35 | 0.61 |
| 25:DC:202:ARG:HH11 | 25:DC:213:ARG:NE | 1.97 | 0.61 |
| 52:DI:128:ILE:HA | 52:DI:131:THR:HG23 | 1.81 | 0.61 |
| 23:DB:1100:C:OP2 | 52:DI:2:LYS:HB3 | 2.00 | 0.61 |
| 35:DN:9:GLN:HA | 35:DN:17:ARG:NE | 2.15 | 0.61 |
| 39:DR:4:VAL:HG21 | 39:DR:39:LEU:HG | 1.81 | 0.61 |
| 1:AA:1343:G:H2' | 1:AA:1344:C:C6 | 2.36 | 0.61 |
| 20:AB:101:THR:HG22 | 20:AB:174:GLU:OE1 | 1.99 | 0.61 |
| 16:AQ:75:VAL:HG23 | 16:AQ:76:ARG:HG2 | 1.82 | 0.61 |
| 1:AA:958:A:H61 | 18:AS:53:GLY:HA3 | 1.65 | 0.61 |
| 22:BA:24:G:O2' | 22:BA:25:U:H5'' | 2.01 | 0.61 |
| 23:BB:1485:U:H2' | 23:BB:1486:U:H6 | 1.66 | 0.61 |
| 23:BB:63:A:H8 | 23:BB:63:A:OP2 | 1.83 | 0.61 |
| 1:CA:335:C:H2' | 1:CA:336:A:H8 | 1.64 | 0.61 |
| 1:CA:41:G:H2' | 1:CA:42:G:C8 | 2.35 | 0.61 |
| 1:CA:978:A:H5' | 1:CA:1362:A:N6 | 2.14 | 0.61 |
| 1:CA:987:G:O2' | 1:CA:988:G:H5' | 2.00 | 0.61 |
| 4:CE:81:GLN:H | 4:CE:146:MET:CE | 2.14 | 0.61 |
| 5:CF:42:TRP:HB2 | 5:CF:59:TYR:HB2 | 1.82 | 0.61 |
| 8:CI:29:ILE:HD13 | 8:CI:78:ILE:HD13 | 1.81 | 0.61 |
| 13:CN:9:GLU:HB2 | 13:CN:62:ARG:NE | 2.15 | 0.61 |
| 18:CS:62:THR:HG22 | 18:CS:63:ASP:H | 1.66 | 0.61 |
| 23:DB:1550:C:H2' | 23:DB:1551:A:C8 | 2.36 | 0.61 |
| 23:DB:1579:A:H2' | 23:DB:1580:A:C8 | 2.35 | 0.61 |
| 23:DB:2366:A:H2' | 23:DB:2367:G:O4' | 2.01 | 0.61 |
| 23:DB:246:C:H2' | 23:DB:247:G:H5' | 1.81 | 0.61 |
| 23:DB:2472:G:H2' | 23:DB:2475:C:H42 | 1.66 | 0.61 |
| 23:DB:401:A:H2' | 23:DB:402:A:H8 | 1.66 | 0.61 |
| 31:DJ:101:ILE:O | 31:DJ:105:VAL:HG22 | 2.00 | 0.61 |
| 31:DJ:20:ALA:HA | 31:DJ:23:LYS:HG2 | 1.81 | 0.61 |
| 33:DL:19:LEU:O | 33:DL:21:ARG:HG2 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:2415:G:H4' | 33:DL:66:PHE:HB2 | 1.81 | 0.61 |
| 34:DM:36:VAL:HB | 34:DM:127:LYS:O | 2.01 | 0.61 |
| 39:DR:5:PHE:O | 39:DR:11:GLN:HA | 2.00 | 0.61 |
| 1:AA:473:U:H2' | 1:AA:474:G:H8 | 1.65 | 0.61 |
| 3:AD:153:ARG:HG3 | 3:AD:154:VAL:H | 1.65 | 0.61 |
| 23:BB:2639:A:H2' | 23:BB:2640:G:O4' | 1.99 | 0.61 |
| 25:BC:70:LYS:HE2 | 25:BC:99:GLU:HB3 | 1.83 | 0.61 |
| 29:BG:137:LYS:HA | 29:BG:140:ILE:HD11 | 1.81 | 0.61 |
| 1:CA:1213:A:H2' | 1:CA:1215:G:N7 | 2.16 | 0.61 |
| 1:CA:668:G:O2' | 14:CO:45:HIS:HB3 | 2.00 | 0.61 |
| 1:CA:792:A:H1' | 1:CA:794:A:N7 | 2.15 | 0.61 |
| 18:CS:30:LEU:H | 18:CS:48:ILE:HA | 1.66 | 0.61 |
| 23:DB:1152:C:O2' | 23:DB:1153:C:H5' | 2.01 | 0.61 |
| 23:DB:1335:C:H2' | 23:DB:1336:A:H8 | 1.65 | 0.61 |
| 23:DB:1461:C:H2' | 23:DB:1462:C:C6 | 2.34 | 0.61 |
| 25:DC:104:LEU:O | 25:DC:105:ALA:HB3 | 2.01 | 0.61 |
| 25:DC:145:MET:HB2 | 25:DC:152:GLN:NE2 | 2.14 | 0.61 |
| 25:DC:158:GLY:N | 25:DC:194:VAL:HG13 | 2.15 | 0.61 |
| 26:DD:97:SER:HB3 | 26:DD:99:GLU:HG2 | 1.81 | 0.61 |
| 29:DG:152:ARG:NH1 | 29:DG:162:ARG:HA | 2.15 | 0.61 |
| 52:DI:20:SER:O | 52:DI:25:PRO:HD2 | 2.00 | 0.61 |
| 31:DJ:72:LYS:O | 31:DJ:73:VAL:HG13 | 2.00 | 0.61 |
| 37:DP:6:GLN:HA | 37:DP:9:GLN:HG2 | 1.82 | 0.61 |
| 41:DT:45:ALA:HA | 41:DT:48:GLN:HB2 | 1.81 | 0.61 |
| 43:DW:24:ARG:HD2 | 43:DW:25:PHE:N | 2.16 | 0.61 |
| 1:AA:204:G:H2' | 1:AA:205:A:C8 | 2.36 | 0.61 |
| 1:AA:524:G:H2' | 1:AA:525:C:C6 | 2.36 | 0.61 |
| 3:AD:106:PHE:CD1 | 3:AD:144:ILE:HD11 | 2.36 | 0.61 |
| 5:AF:79:ARG:NH2 | 5:AF:87:SER:HB3 | 2.14 | 0.61 |
| 49:B2:1:MET:HG2 | 49:B2:2:LYS:H | 1.65 | 0.61 |
| 23:BB:1013:C:H2' | 23:BB:1014:A:H8 | 1.66 | 0.61 |
| 23:BB:1381:G:H2' | 23:BB:1382:G:H5' | 1.81 | 0.61 |
| 23:BB:581:C:H2' | 23:BB:582:A:C8 | 2.35 | 0.61 |
| 23:BB:62:U:O2' | 23:BB:63:A:H5' | 2.00 | 0.61 |
| 52:BI:20:SER:O | 52:BI:25:PRO:HD2 | 2.01 | 0.61 |
| 52:BI:7:TYR:HB2 | 52:BI:58:ILE:O | 2.00 | 0.61 |
| 33:BL:70:LYS:O | 33:BL:73:ILE:HG12 | 2.01 | 0.61 |
| 41:BT:11:LEU:HA | 41:BT:34:VAL:HG12 | 1.81 | 0.61 |
| 44:BX:26:PHE:HD1 | 44:BX:27:ASN:HD22 | 1.48 | 0.61 |
| 1:CA:1210:C:H1' | 1:CA:1214:C:H2' | 1.83 | 0.61 |
| 1:CA:335:C:H2' | 1:CA:336:A:C8 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:CB:20:ARG:HA | 20:CB:38:HIS:HE1 | 1.65 | 0.61 |
| 12:CM:79:LEU:HD21 | 12:CM:86:ARG:HH21 | 1.65 | 0.61 |
| 48:D1:29:LYS:HE2 | 48:D1:31:GLU:OE1 | 2.00 | 0.61 |
| 50:D3:51:LYS:HA | 50:D3:54:LEU:HB2 | 1.81 | 0.61 |
| 23:DB:138:U:O3' | 23:DB:139:U:H3' | 1.99 | 0.61 |
| 23:DB:1550:C:H2' | 23:DB:1551:A:H8 | 1.66 | 0.61 |
| 23:DB:1871:A:H2' | 23:DB:1872:A:C8 | 2.35 | 0.61 |
| 23:DB:2097:A:H2' | 23:DB:2098:U:H6 | 1.65 | 0.61 |
| 23:DB:2457:U:C2' | 23:DB:2458:G:H5' | 2.31 | 0.61 |
| 23:DB:593:U:H2' | 23:DB:594:U:C6 | 2.35 | 0.61 |
| 27:DE:117:ARG:O | 27:DE:186:VAL:HG12 | 2.00 | 0.61 |
| 30:DH:5:LEU:O | 30:DH:6:LEU:HD12 | 2.01 | 0.61 |
| 52:DI:25:PRO:O | 52:DI:29:GLN:HG3 | 2.00 | 0.61 |
| 52:DI:42:ASN:HA | 52:DI:45:THR:OG1 | 1.99 | 0.61 |
| 44:DX:39:GLN:O | 44:DX:42:LEU:HB2 | 2.00 | 0.61 |
| 1:AA:1486:G:H2' | 1:AA:1487:G:C1' | 2.30 | 0.61 |
| 3:AD:169:TRP:CE2 | 3:AD:185:PRO:HB3 | 2.35 | 0.61 |
| 4:AE:28:ARG:NH1 | 4:AE:30:PHE:HB3 | 2.15 | 0.61 |
| 23:BB:1130:U:C2 | 23:BB:2025:C:H5'' | 2.36 | 0.61 |
| 23:BB:2722:G:H2' | 23:BB:2723:C:C6 | 2.36 | 0.61 |
| 23:BB:402:A:H2' | 23:BB:403:U:O4' | 2.01 | 0.61 |
| 23:BB:967:U:H2' | 23:BB:968:C:C6 | 2.36 | 0.61 |
| 23:BB:1843:C:H5'' | 25:BC:250:GLN:HE21 | 1.66 | 0.61 |
| 25:BC:75:ALA:HB2 | 25:BC:95:TYR:HA | 1.83 | 0.61 |
| 31:BJ:8:PRO:HG3 | 31:BJ:48:VAL:HG22 | 1.83 | 0.61 |
| 32:BK:104:THR:H | 32:BK:107:LEU:HD12 | 1.65 | 0.61 |
| 34:BM:71:LYS:HB3 | 34:BM:93:VAL:HG12 | 1.81 | 0.61 |
| 23:BB:1287:A:N7 | 35:BN:105:GLY:HA3 | 2.15 | 0.61 |
| 37:BP:4:ILE:HG22 | 37:BP:5:LYS:N | 2.14 | 0.61 |
| 1:CA:1278:G:H4' | 1:CA:1279:G:C5' | 2.29 | 0.61 |
| 1:CA:512:U:H2' | 1:CA:513:C:C6 | 2.36 | 0.61 |
| 5:CF:100:SER:HA | 17:CR:23:LYS:CE | 2.30 | 0.61 |
| 12:CM:89:ARG:NH2 | 12:CM:94:LEU:HD12 | 2.15 | 0.61 |
| 23:DB:1061:U:O4' | 23:DB:1070:A:H1' | 2.00 | 0.61 |
| 23:DB:154:U:H2' | 23:DB:155:A:C8 | 2.35 | 0.61 |
| 23:DB:1812:U:H2' | 23:DB:1813:G:C8 | 2.36 | 0.61 |
| 23:DB:2626:C:O2' | 23:DB:2627:G:H5' | 2.00 | 0.61 |
| 23:DB:2639:A:H2' | 23:DB:2640:G:O4' | 2.00 | 0.61 |
| 26:DD:136:ASN:HD21 | 26:DD:140:HIS:N | 1.99 | 0.61 |
| 34:DM:19:GLY:H | 34:DM:38:ARG:NH1 | 1.98 | 0.61 |
| 36:DO:94:ARG:O | 36:DO:97:PHE:HB2 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DQ:86:SER:HB3 | 39:DR:51:VAL:CA | 2.30 | 0.61 |
| 40:DS:36:LEU:HB3 | 40:DS:48:LYS:HB2 | 1.81 | 0.61 |
| 42:DU:11:ILE:O | 42:DU:12:VAL:HB | 2.01 | 0.61 |
| 1:AA:1144:G:H21 | 1:AA:1146:A:H62 | 1.48 | 0.61 |
| 1:AA:1271:A:H5' | 1:AA:1314:C:H5'' | 1.83 | 0.61 |
| 1:AA:1411:C:O2' | 1:AA:1412:C:H5' | 2.00 | 0.61 |
| 1:AA:253:A:H2' | 1:AA:254:G:H8 | 1.66 | 0.61 |
| 1:AA:946:A:H2' | 1:AA:947:G:H8 | 1.65 | 0.61 |
| 9:AJ:24:GLU:HG3 | 9:AJ:90:LEU:HD11 | 1.83 | 0.61 |
| 47:B0:8:THR:HG23 | 47:B0:11:LYS:H | 1.66 | 0.61 |
| 22:BA:94:A:H2' | 22:BA:95:U:O4' | 2.00 | 0.61 |
| 23:BB:1597:A:H5'' | 23:BB:1598:A:H5' | 1.83 | 0.61 |
| 23:BB:807:U:H2' | 23:BB:808:G:C8 | 2.35 | 0.61 |
| 23:BB:975:A:H1' | 23:BB:990:A:C2 | 2.36 | 0.61 |
| 28:BF:90:LEU:C | 28:BF:91:ARG:HD3 | 2.21 | 0.61 |
| 35:BN:49:GLU:OE2 | 35:BN:95:THR:HG22 | 2.00 | 0.61 |
| 37:BP:52:ARG:HH11 | 37:BP:52:ARG:HG2 | 1.65 | 0.61 |
| 20:CB:221:ARG:HG3 | 20:CB:222:GLU:N | 2.15 | 0.61 |
| 14:CO:72:LYS:O | 14:CO:73:ASP:HB2 | 2.01 | 0.61 |
| 23:DB:2091:C:H1' | 46:DZ:34:HIS:CD2 | 2.35 | 0.61 |
| 23:DB:2353:G:N3 | 43:DW:30:VAL:HG13 | 2.16 | 0.61 |
| 23:DB:2529:G:H4' | 29:DG:174:LYS:CD | 2.31 | 0.61 |
| 35:DN:34:ILE:O | 35:DN:112:TYR:HA | 2.01 | 0.61 |
| 43:DW:47:GLY:HA3 | 43:DW:80:SER:HA | 1.81 | 0.61 |
| 1:AA:1038:C:H2' | 1:AA:1039:G:C8 | 2.36 | 0.61 |
| 1:AA:651:C:H2' | 1:AA:652:U:C6 | 2.36 | 0.61 |
| 1:AA:87:C:H2' | 1:AA:88:U:H4' | 1.83 | 0.61 |
| 3:AD:123:MET:HB3 | 3:AD:128:VAL:HA | 1.82 | 0.61 |
| 4:AE:143:LEU:O | 4:AE:146:MET:HG2 | 2.00 | 0.61 |
| 9:AJ:56:HIS:O | 9:AJ:57:VAL:HG12 | 2.01 | 0.61 |
| 12:AM:21:ILE:HB | 12:AM:24:VAL:CG2 | 2.29 | 0.61 |
| 47:B0:38:LEU:HD23 | 47:B0:39:ARG:H | 1.65 | 0.61 |
| 50:B3:51:LYS:HA | 50:B3:54:LEU:HB2 | 1.82 | 0.61 |
| 23:BB:1419:A:H2' | 23:BB:1421:G:N7 | 2.16 | 0.61 |
| 23:BB:1592:C:H2' | 23:BB:1593:A:C8 | 2.35 | 0.61 |
| 23:BB:1914:C:H2' | 23:BB:1915:U:O4' | 2.01 | 0.61 |
| 23:BB:2852:G:H2' | 23:BB:2853:C:C6 | 2.36 | 0.61 |
| 23:BB:64:A:H2' | 23:BB:65:U:C6 | 2.36 | 0.61 |
| 31:BJ:40:HIS:CE1 | 31:BJ:41:LYS:HG3 | 2.36 | 0.61 |
| 40:BS:36:LEU:HB3 | 40:BS:48:LYS:HB2 | 1.83 | 0.61 |
| 42:BU:82:VAL:HG13 | 42:BU:93:ARG:HB3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:13:ILE:O | 2:CC:14:VAL:HG22 | 2.00 | 0.61 |
| 7:CH:11:THR:HG22 | 7:CH:14:ARG:HH22 | 1.65 | 0.61 |
| 23:DB:1133:A:H4' | 23:DB:1134:A:O5' | 2.01 | 0.61 |
| 23:DB:1164:C:H2' | 23:DB:1165:A:C8 | 2.36 | 0.61 |
| 23:DB:2088:A:H2' | 23:DB:2089:C:C6 | 2.36 | 0.61 |
| 52:DI:27:LEU:CD2 | 52:DI:27:LEU:H | 2.14 | 0.61 |
| 31:DJ:111:LYS:HB3 | 31:DJ:113:PRO:HD2 | 1.82 | 0.61 |
| 43:DW:37:VAL:HG11 | 43:DW:38:ARG:HH11 | 1.66 | 0.61 |
| 1:AA:195:A:H2' | 1:AA:196:A:C8 | 2.36 | 0.60 |
| 1:AA:255:G:H2' | 1:AA:256:U:C6 | 2.36 | 0.60 |
| 1:AA:751:U:H4' | 14:AO:23:SER:HA | 1.82 | 0.60 |
| 3:AD:160:LEU:HA | 3:AD:163:GLN:HG3 | 1.83 | 0.60 |
| 8:AI:18:VAL:HG11 | 8:AI:82:ILE:HG12 | 1.83 | 0.60 |
| 14:AO:72:LYS:O | 14:AO:73:ASP:HB2 | 2.01 | 0.60 |
| 18:AS:18:VAL:CG2 | 18:AS:43:MET:HG2 | 2.29 | 0.60 |
| 19:AT:79:THR:HA | 19:AT:82:ILE:HG12 | 1.83 | 0.60 |
| 23:BB:2369:A:O2' | 23:BB:2370:G:H5' | 2.00 | 0.60 |
| 23:BB:417:C:H2' | 23:BB:418:C:C6 | 2.35 | 0.60 |
| 23:BB:639:U:H2' | 23:BB:640:C:C6 | 2.35 | 0.60 |
| 25:BC:76:VAL:HG12 | 25:BC:114:GLN:HG2 | 1.83 | 0.60 |
| 27:BE:104:ALA:O | 27:BE:108:ILE:HG22 | 2.01 | 0.60 |
| 27:BE:176:ASP:HB3 | 27:BE:179:SER:HB2 | 1.82 | 0.60 |
| 27:BE:29:HIS:NE2 | 33:BL:8:PRO:HG3 | 2.16 | 0.60 |
| 27:BE:98:LYS:HZ2 | 27:BE:99:LYS:HG2 | 1.65 | 0.60 |
| 28:BF:125:GLY:HA2 | 28:BF:162:ASP:HA | 1.82 | 0.60 |
| 52:BI:11:GLN:HA | 52:BI:55:PRO:HA | 1.82 | 0.60 |
| 35:BN:9:GLN:HA | 35:BN:17:ARG:NE | 2.16 | 0.60 |
| 37:BP:93:LYS:HB3 | 37:BP:96:LEU:HD12 | 1.82 | 0.60 |
| 23:BB:992:C:H4' | 39:BR:74:ILE:HD13 | 1.82 | 0.60 |
| 43:BW:37:VAL:HG11 | 43:BW:38:ARG:HH11 | 1.66 | 0.60 |
| 44:BX:48:ARG:O | 44:BX:51:ALA:HB3 | 2.00 | 0.60 |
| 44:BX:49:ASP:O | 44:BX:53:VAL:HG23 | 2.01 | 0.60 |
| 1:CA:1071:C:H2' | 1:CA:1072:G:H8 | 1.65 | 0.60 |
| 1:CA:1296:C:H4' | 1:CA:1302:C:C4 | 2.36 | 0.60 |
| 13:CN:41:TRP:HB3 | 13:CN:44:VAL:HB | 1.83 | 0.60 |
| 18:CS:50:VAL:O | 18:CS:57:VAL:HG22 | 2.00 | 0.60 |
| 23:DB:17:G:H2' | 23:DB:18:U:C6 | 2.36 | 0.60 |
| 23:DB:360:U:H2' | 23:DB:361:G:O4' | 2.01 | 0.60 |
| 26:DD:169:ARG:O | 26:DD:170:VAL:HG22 | 2.00 | 0.60 |
| 28:DF:104:THR:C | 28:DF:108:PRO:HG2 | 2.21 | 0.60 |
| 30:DH:69:ALA:HB1 | 30:DH:73:ASN:ND2 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:DI:123:ALA:HA | 52:DI:126:ARG:HH12 | 1.66 | 0.60 |
| 31:DJ:24:THR:HA | 31:DJ:63:ALA:HB3 | 1.83 | 0.60 |
| 44:DX:57:LEU:H | 44:DX:60:LYS:HG3 | 1.66 | 0.60 |
| 1:AA:620:C:C2 | 3:AD:131:ILE:HD13 | 2.36 | 0.60 |
| 1:AA:707:U:H2' | 1:AA:708:C:C6 | 2.36 | 0.60 |
| 13:AN:14:ALA:O | 13:AN:18:LYS:HG2 | 2.01 | 0.60 |
| 18:AS:62:THR:HG22 | 18:AS:63:ASP:H | 1.66 | 0.60 |
| 23:BB:125:A:H5' | 49:B2:19:ARG:HG3 | 1.82 | 0.60 |
| 23:BB:1771:C:H2' | 23:BB:1772:A:C8 | 2.36 | 0.60 |
| 23:BB:2101:A:C3' | 23:BB:2102:G:H5'' | 2.31 | 0.60 |
| 23:BB:2297:A:H61 | 23:BB:2319:G:H1' | 1.66 | 0.60 |
| 23:BB:2457:U:C2' | 23:BB:2458:G:H5' | 2.31 | 0.60 |
| 23:BB:45:G:H5' | 23:BB:46:G:OP1 | 2.02 | 0.60 |
| 23:BB:3:U:H2' | 23:BB:4:U:C6 | 2.36 | 0.60 |
| 25:BC:77:VAL:CG2 | 25:BC:112:GLY:H | 2.06 | 0.60 |
| 26:BD:178:VAL:HB | 26:BD:188:LEU:HB2 | 1.82 | 0.60 |
| 27:BE:98:LYS:HZ1 | 27:BE:99:LYS:HE2 | 1.66 | 0.60 |
| 33:BL:79:LEU:HB3 | 33:BL:115:GLU:O | 2.01 | 0.60 |
| 33:BL:93:ASN:O | 33:BL:95:LEU:N | 2.35 | 0.60 |
| 36:BO:94:ARG:O | 36:BO:97:PHE:HB2 | 2.00 | 0.60 |
| 46:BZ:70:GLU:C | 46:BZ:72:ARG:H | 2.03 | 0.60 |
| 1:CA:1238:A:N3 | 1:CA:1238:A:H2' | 2.16 | 0.60 |
| 1:CA:1388:C:H2' | 1:CA:1389:C:C6 | 2.35 | 0.60 |
| 1:CA:195:A:H2' | 1:CA:196:A:C8 | 2.36 | 0.60 |
| 1:CA:218:U:H2' | 1:CA:219:U:C6 | 2.36 | 0.60 |
| 1:CA:253:A:H2' | 1:CA:254:G:C8 | 2.36 | 0.60 |
| 8:CI:7:GLY:HA2 | 8:CI:85:ALA:HB2 | 1.82 | 0.60 |
| 10:CK:70:ALA:O | 10:CK:74:LYS:HB2 | 2.01 | 0.60 |
| 10:CK:81:LEU:HD11 | 10:CK:99:LEU:HD23 | 1.81 | 0.60 |
| 23:DB:1199:U:H2' | 23:DB:1200:C:H6 | 1.66 | 0.60 |
| 23:DB:2497:A:H5'' | 56:DB:3696:HOH:O | 2.01 | 0.60 |
| 23:DB:2737:G:H2' | 23:DB:2738:A:C8 | 2.36 | 0.60 |
| 23:DB:660:C:H2' | 23:DB:661:A:H8 | 1.66 | 0.60 |
| 26:DD:179:ARG:HB2 | 26:DD:188:LEU:HD12 | 1.83 | 0.60 |
| 28:DF:155:ILE:O | 28:DF:156:THR:HB | 2.01 | 0.60 |
| 30:DH:32:PRO:O | 30:DH:33:GLN:HB2 | 2.01 | 0.60 |
| 33:DL:70:LYS:O | 33:DL:73:ILE:HG12 | 2.02 | 0.60 |
| 1:AA:10:A:H2' | 1:AA:11:G:C8 | 2.37 | 0.60 |
| 1:AA:1249:C:H4' | 8:AI:37:TYR:OH | 2.00 | 0.60 |
| 1:AA:1405:G:O4' | 1:AA:1519:A:H4' | 2.01 | 0.60 |
| 1:AA:487:A:H2' | 1:AA:488:C:O4' | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:909:A:H2' | 1:AA:910:C:O4' | 2.01 | 0.60 |
| 18:AS:16:LYS:O | 18:AS:20:LYS:HB2 | 2.01 | 0.60 |
| 49:B2:3:ARG:HE | 49:B2:4:THR:HG22 | 1.66 | 0.60 |
| 22:BA:6:G:H2' | 22:BA:7:G:C8 | 2.36 | 0.60 |
| 23:BB:1443:U:H2' | 23:BB:1444:G:C8 | 2.37 | 0.60 |
| 23:BB:264:C:C2' | 23:BB:265:A:H5'' | 2.31 | 0.60 |
| 23:BB:716:A:H2' | 23:BB:717:C:H5'' | 1.83 | 0.60 |
| 27:BE:111:GLU:HB3 | 33:BL:2:ARG:HH12 | 1.66 | 0.60 |
| 35:BN:96:ARG:NH1 | 35:BN:116:VAL:HG23 | 2.08 | 0.60 |
| 40:BS:29:VAL:HG23 | 40:BS:70:LYS:HA | 1.83 | 0.60 |
| 40:BS:72:THR:OG1 | 40:BS:108:SER:HB3 | 2.01 | 0.60 |
| 45:BY:37:ARG:HG2 | 45:BY:43:ILE:HD11 | 1.84 | 0.60 |
| 1:CA:17:U:O2' | 1:CA:1079:G:H1' | 2.01 | 0.60 |
| 20:CB:20:ARG:HA | 20:CB:38:HIS:CE1 | 2.36 | 0.60 |
| 5:CF:18:VAL:HG21 | 5:CF:58:HIS:ND1 | 2.16 | 0.60 |
| 7:CH:46:GLU:HB2 | 7:CH:61:THR:HB | 1.82 | 0.60 |
| 1:CA:1343:G:H4' | 8:CI:123:ARG:O | 2.01 | 0.60 |
| 10:CK:81:LEU:HD21 | 10:CK:104:PHE:HB3 | 1.83 | 0.60 |
| 12:CM:95:PRO:N | 12:CM:108:ARG:HG2 | 2.16 | 0.60 |
| 19:CT:19:HIS:O | 19:CT:23:ARG:HG2 | 2.01 | 0.60 |
| 50:D3:44:ARG:N | 50:D3:45:PRO:HD2 | 2.17 | 0.60 |
| 22:DA:28:C:H2' | 22:DA:29:A:O4' | 2.01 | 0.60 |
| 23:DB:1015:U:H2' | 23:DB:1016:G:C8 | 2.36 | 0.60 |
| 23:DB:1419:A:H2' | 23:DB:1421:G:N7 | 2.16 | 0.60 |
| 23:DB:1535:A:H3' | 23:DB:1536:C:H6 | 1.66 | 0.60 |
| 23:DB:1704:C:O2' | 23:DB:1705:A:H5' | 2.02 | 0.60 |
| 23:DB:395:U:H2' | 23:DB:396:G:N7 | 2.16 | 0.60 |
| 23:DB:594:U:H2' | 23:DB:595:C:C6 | 2.36 | 0.60 |
| 25:DC:75:ALA:O | 25:DC:114:GLN:HA | 2.01 | 0.60 |
| 28:DF:125:GLY:HA2 | 28:DF:162:ASP:HA | 1.81 | 0.60 |
| 30:DH:117:LEU:HB2 | 30:DH:130:VAL:HG13 | 1.84 | 0.60 |
| 35:DN:33:ILE:HD12 | 35:DN:33:ILE:O | 2.01 | 0.60 |
| 41:DT:31:VAL:HA | 41:DT:84:TYR:H | 1.66 | 0.60 |
| 42:DU:95:PHE:CE1 | 42:DU:102:ILE:HB | 2.36 | 0.60 |
| 1:AA:239:U:C5' | 1:AA:239:U:H6 | 2.14 | 0.60 |
| 1:AA:376:G:H2' | 1:AA:377:G:H8 | 1.65 | 0.60 |
| 8:AI:17:ARG:O | 8:AI:64:ILE:HA | 2.01 | 0.60 |
| 23:BB:136:G:H2' | 23:BB:137:U:H6 | 1.64 | 0.60 |
| 23:BB:2025:C:H2' | 23:BB:2026:U:C6 | 2.36 | 0.60 |
| 23:BB:2626:C:O2' | 23:BB:2627:G:H5' | 2.01 | 0.60 |
| 23:BB:594:U:H2' | 23:BB:595:C:H6 | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:79:C:O2' | 23:BB:346:A:H1' | 2.01 | 0.60 |
| 23:BB:820:A:H1' | 23:BB:943:A:O2' | 2.01 | 0.60 |
| 32:BK:13:ASN:ND2 | 32:BK:98:ARG:H | 1.99 | 0.60 |
| 35:BN:34:ILE:O | 35:BN:112:TYR:HA | 2.01 | 0.60 |
| 38:BQ:86:SER:HB3 | 39:BR:51:VAL:HA | 1.82 | 0.60 |
| 43:BW:49:ASN:HB2 | 43:BW:61:LYS:H | 1.65 | 0.60 |
| 6:CG:145:GLU:HA | 6:CG:148:LYS:HB2 | 1.84 | 0.60 |
| 8:CI:25:GLY:HA3 | 8:CI:57:VAL:H | 1.65 | 0.60 |
| 11:CL:26:CYS:SG | 11:CL:29:LYS:HE2 | 2.41 | 0.60 |
| 23:DB:1443:U:H2' | 23:DB:1444:G:C8 | 2.37 | 0.60 |
| 23:DB:2078:C:H2' | 23:DB:2079:U:C6 | 2.36 | 0.60 |
| 23:DB:1060:U:C5 | 52:DI:131:THR:HG22 | 2.36 | 0.60 |
| 31:DJ:57:LEU:HD21 | 31:DJ:128:ASN:HA | 1.84 | 0.60 |
| 31:DJ:8:PRO:HG3 | 31:DJ:48:VAL:HG22 | 1.84 | 0.60 |
| 43:DW:35:ILE:HG13 | 43:DW:57:THR:OG1 | 2.01 | 0.60 |
| 1:AA:162:A:H2' | 1:AA:163:C:O4' | 2.01 | 0.60 |
| 1:AA:719:C:O2' | 17:AR:37:LYS:HB2 | 2.02 | 0.60 |
| 23:BB:1082:U:N3 | 23:BB:1086:A:C6 | 2.70 | 0.60 |
| 23:BB:1240:U:O2' | 23:BB:1241:A:H5'' | 2.02 | 0.60 |
| 23:BB:184:C:H2' | 23:BB:185:G:H8 | 1.66 | 0.60 |
| 23:BB:2041:U:H2' | 23:BB:2042:A:C8 | 2.35 | 0.60 |
| 23:BB:2100:G:H2' | 23:BB:2101:A:O4' | 2.00 | 0.60 |
| 23:BB:248:G:H5' | 23:BB:250:G:N7 | 2.16 | 0.60 |
| 23:BB:2758:A:H2' | 23:BB:2759:G:O4' | 2.02 | 0.60 |
| 26:BD:136:ASN:HD21 | 26:BD:140:HIS:N | 1.99 | 0.60 |
| 26:BD:92:VAL:O | 26:BD:94:GLN:N | 2.34 | 0.60 |
| 52:BI:89:SER:HA | 52:BI:97:VAL:HG21 | 1.83 | 0.60 |
| 42:BU:9:GLU:HG3 | 42:BU:21:ARG:HD2 | 1.82 | 0.60 |
| 1:CA:1427:C:H2' | 1:CA:1428:A:C8 | 2.37 | 0.60 |
| 20:CB:72:LYS:HE3 | 20:CB:203:ASP:O | 2.02 | 0.60 |
| 6:CG:62:GLU:O | 6:CG:66:GLU:HG3 | 2.01 | 0.60 |
| 13:CN:30:ILE:HG21 | 13:CN:44:VAL:HG21 | 1.83 | 0.60 |
| 18:CS:16:LYS:O | 18:CS:20:LYS:HB2 | 2.01 | 0.60 |
| 49:D2:33:ARG:HB2 | 49:D2:33:ARG:HH21 | 1.65 | 0.60 |
| 22:DA:94:A:H2' | 22:DA:95:U:O4' | 2.01 | 0.60 |
| 23:DB:1291:C:O2' | 23:DB:1292:G:H5' | 2.02 | 0.60 |
| 23:DB:172:A:H2' | 23:DB:173:A:H8 | 1.64 | 0.60 |
| 23:DB:717:C:H3' | 23:DB:718:A:H5'' | 1.82 | 0.60 |
| 28:DF:90:LEU:C | 28:DF:91:ARG:HD3 | 2.21 | 0.60 |
| 35:DN:103:ARG:HG2 | 35:DN:104:ALA:H | 1.66 | 0.60 |
| 35:DN:85:PRO:HA | 35:DN:88:ALA:HB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:DW:18:LYS:HG3 | 43:DW:19:ARG:NE | 2.16 | 0.60 |
| 43:DW:37:VAL:HG13 | 43:DW:55:ASP:O | 2.02 | 0.60 |
| 23:DB:96:C:H4' | 44:DX:41:HIS:CE1 | 2.36 | 0.60 |
| 1:AA:1492:A:H2' | 23:BB:1913:A:C2 | 2.36 | 0.60 |
| 1:AA:35:G:H2' | 1:AA:36:C:C6 | 2.36 | 0.60 |
| 20:AB:205:ALA:O | 20:AB:209:VAL:HG22 | 2.01 | 0.60 |
| 20:AB:16:GLY:HA3 | 20:AB:39:ILE:HA | 1.82 | 0.60 |
| 8:AI:79:ARG:NH2 | 8:AI:102:PHE:HA | 2.15 | 0.60 |
| 12:AM:77:LYS:HG2 | 12:AM:81:ASP:OD2 | 2.01 | 0.60 |
| 23:BB:1292:G:H2' | 23:BB:1293:C:C6 | 2.36 | 0.60 |
| 23:BB:1857:G:H1' | 23:BB:1885:A:N6 | 2.16 | 0.60 |
| 25:BC:161:VAL:HG12 | 25:BC:162:GLN:N | 2.16 | 0.60 |
| 26:BD:29:VAL:O | 26:BD:185:ASN:HB3 | 2.01 | 0.60 |
| 26:BD:55:LYS:NZ | 26:BD:59:ARG:HD2 | 2.16 | 0.60 |
| 28:BF:60:SER:HB2 | 28:BF:62:GLN:OE1 | 2.01 | 0.60 |
| 28:BF:62:GLN:CB | 28:BF:91:ARG:HE | 2.15 | 0.60 |
| 24:BV:24:ASN:O | 24:BV:44:HIS:HB2 | 2.01 | 0.60 |
| 1:CA:270:A:H2' | 1:CA:271:C:C6 | 2.35 | 0.60 |
| 1:CA:473:U:H2' | 1:CA:474:G:H8 | 1.66 | 0.60 |
| 4:CE:106:ALA:HB1 | 4:CE:110:MET:HB3 | 1.84 | 0.60 |
| 6:CG:26:VAL:HB | 6:CG:39:GLU:HG2 | 1.83 | 0.60 |
| 23:DB:1199:U:H2' | 23:DB:1200:C:C6 | 2.36 | 0.60 |
| 23:DB:1843:C:H5'' | 25:DC:250:GLN:HE21 | 1.67 | 0.60 |
| 23:DB:2143:C:H3' | 23:DB:2144:G:C8 | 2.36 | 0.60 |
| 23:DB:2229:U:H2' | 23:DB:2230:G:C8 | 2.37 | 0.60 |
| 23:DB:2387:U:H1' | 43:DW:38:ARG:CZ | 2.32 | 0.60 |
| 23:DB:2804:U:H2' | 23:DB:2805:C:C6 | 2.36 | 0.60 |
| 23:DB:2899:A:H2' | 23:DB:2900:A:C8 | 2.36 | 0.60 |
| 23:DB:716:A:H2' | 23:DB:717:C:H5'' | 1.83 | 0.60 |
| 26:DD:178:VAL:HB | 26:DD:188:LEU:HB2 | 1.83 | 0.60 |
| 30:DH:21:VAL:HG22 | 30:DH:22:LYS:H | 1.67 | 0.60 |
| 40:DS:42:LYS:O | 40:DS:45:VAL:HG22 | 2.01 | 0.60 |
| 43:DW:49:ASN:HD22 | 43:DW:59:PHE:HB3 | 1.66 | 0.60 |
| 23:BB:1490:A:H2' | 25:BC:97:ASP:OD1 | 2.02 | 0.60 |
| 23:BB:1842:G:H2' | 23:BB:1843:C:C6 | 2.37 | 0.60 |
| 23:BB:1871:A:H2' | 23:BB:1872:A:C8 | 2.37 | 0.60 |
| 23:BB:2064:C:H2' | 23:BB:2065:C:H6 | 1.66 | 0.60 |
| 23:BB:2649:C:H2' | 23:BB:2650:U:C6 | 2.37 | 0.60 |
| 28:BF:111:ARG:HH22 | 28:BF:113:PHE:HB2 | 1.65 | 0.60 |
| 30:BH:50:ARG:H | 30:BH:50:ARG:NE | 2.00 | 0.60 |
| 33:BL:80:SER:HA | 33:BL:115:GLU:HB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2277:G:C5' | 34:BM:86:LYS:HB2 | 2.32 | 0.60 |
| 23:BB:751:A:H5' | 40:BS:90:LYS:HA | 1.84 | 0.60 |
| 43:BW:24:ARG:HD3 | 43:BW:65:LYS:CG | 2.31 | 0.60 |
| 1:CA:208:U:H2' | 1:CA:210:C:N3 | 2.16 | 0.60 |
| 1:CA:91:U:H2' | 1:CA:92:U:C6 | 2.36 | 0.60 |
| 4:CE:143:LEU:O | 4:CE:146:MET:HG2 | 2.02 | 0.60 |
| 23:DB:1406:U:H2' | 23:DB:1407:G:C8 | 2.36 | 0.60 |
| 23:DB:1484:U:H2' | 23:DB:1485:U:C6 | 2.36 | 0.60 |
| 23:DB:1513:U:O2' | 23:DB:1514:G:H5' | 2.00 | 0.60 |
| 23:DB:191:A:H2' | 23:DB:192:C:H6 | 1.65 | 0.60 |
| 23:DB:2645:G:H3' | 23:DB:2646:C:C5' | 2.32 | 0.60 |
| 25:DC:123:ILE:HD12 | 25:DC:191:LEU:HD13 | 1.84 | 0.60 |
| 29:DG:72:ASN:O | 29:DG:76:ILE:HG12 | 2.02 | 0.60 |
| 34:DM:34:LYS:HB3 | 34:DM:129:THR:HG22 | 1.82 | 0.60 |
| 1:AA:1149:C:H2' | 1:AA:1150:A:H8 | 1.65 | 0.60 |
| 1:AA:919:A:O2' | 1:AA:920:U:H5' | 2.01 | 0.60 |
| 1:AA:532:A:N6 | 2:AC:191:THR:HB | 2.16 | 0.60 |
| 5:AF:29:ILE:HG23 | 5:AF:66:ALA:HB2 | 1.82 | 0.60 |
| 13:AN:30:ILE:HG21 | 13:AN:44:VAL:HG21 | 1.83 | 0.60 |
| 23:BB:1535:A:H3' | 23:BB:1536:C:H6 | 1.65 | 0.60 |
| 23:BB:2359:C:H2' | 23:BB:2360:G:C8 | 2.37 | 0.60 |
| 23:BB:2654:A:N1 | 23:BB:2665:A:H5'' | 2.16 | 0.60 |
| 23:BB:594:U:H2' | 23:BB:595:C:C6 | 2.36 | 0.60 |
| 30:BH:27:ARG:NH1 | 46:BZ:64:ILE:HD11 | 2.16 | 0.60 |
| 41:BT:76:ARG:HH21 | 41:BT:77:ARG:HB2 | 1.67 | 0.60 |
| 41:BT:31:VAL:HA | 41:BT:84:TYR:H | 1.66 | 0.60 |
| 43:BW:64:GLY:HA2 | 43:BW:84:GLU:HG2 | 1.84 | 0.60 |
| 41:BT:14:PRO:HD2 | 44:BX:33:ALA:HB3 | 1.83 | 0.60 |
| 1:CA:1001:C:H2' | 1:CA:1002:G:C8 | 2.36 | 0.60 |
| 1:CA:1437:A:H2' | 1:CA:1438:G:H8 | 1.67 | 0.60 |
| 1:CA:276:G:H5' | 16:CQ:16:MET:SD | 2.42 | 0.60 |
| 1:CA:923:A:H2' | 1:CA:924:C:C6 | 2.37 | 0.60 |
| 4:CE:100:GLU:HA | 4:CE:121:ASN:ND2 | 2.16 | 0.60 |
| 6:CG:24:LYS:HA | 6:CG:27:ASN:HD22 | 1.66 | 0.60 |
| 7:CH:25:THR:HA | 7:CH:58:LEU:O | 2.01 | 0.60 |
| 8:CI:9:GLY:HA3 | 8:CI:81:GLY:H | 1.67 | 0.60 |
| 23:DB:1857:G:H1' | 23:DB:1885:A:N6 | 2.15 | 0.60 |
| 23:DB:2103:C:H3' | 23:DB:2104:C:C2 | 2.37 | 0.60 |
| 23:DB:2720:U:H5'' | 37:DP:52:ARG:NH2 | 2.16 | 0.60 |
| 23:DB:592:A:H2' | 23:DB:593:U:C6 | 2.37 | 0.60 |
| 26:DD:117:GLY:HA2 | 26:DD:164:GLN:CD | 2.21 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DD:55:LYS:NZ | 26:DD:59:ARG:HD2 | 2.17 | 0.60 |
| 40:DS:90:LYS:HD2 | 40:DS:92:ARG:HH12 | 1.65 | 0.60 |
| 1:AA:1001:C:H2' | 1:AA:1002:G:C8 | 2.37 | 0.60 |
| 1:AA:1053:G:HO2' | 1:AA:1199:U:H5 | 1.48 | 0.60 |
| 1:AA:1218:C:H2' | 1:AA:1219:A:C8 | 2.37 | 0.60 |
| 1:AA:1330:U:H4' | 12:AM:69:ARG:HH12 | 1.67 | 0.60 |
| 8:AI:29:ILE:HD13 | 8:AI:78:ILE:HD13 | 1.82 | 0.60 |
| 10:AK:70:ALA:O | 10:AK:74:LYS:HB2 | 2.01 | 0.60 |
| 12:AM:58:GLU:O | 12:AM:61:LYS:HG2 | 2.02 | 0.60 |
| 5:AF:86:ARG:HH12 | 17:AR:63:TYR:HB3 | 1.66 | 0.60 |
| 18:AS:10:ILE:HD12 | 18:AS:15:LEU:HG | 1.82 | 0.60 |
| 23:BB:1054:A:H2' | 23:BB:1055:G:C8 | 2.37 | 0.60 |
| 23:BB:1220:G:H2' | 23:BB:1221:C:H6 | 1.67 | 0.60 |
| 23:BB:1796:U:H2' | 23:BB:1797:G:H8 | 1.65 | 0.60 |
| 23:BB:191:A:H2' | 23:BB:192:C:H6 | 1.66 | 0.60 |
| 23:BB:521:U:H2' | 23:BB:522:A:C8 | 2.37 | 0.60 |
| 26:BD:176:ASP:HB2 | 26:BD:190:LYS:HG2 | 1.84 | 0.60 |
| 29:BG:155:PRO:HA | 29:BG:170:THR:HA | 1.84 | 0.60 |
| 32:BK:118:LEU:C | 32:BK:120:PRO:HD2 | 2.22 | 0.60 |
| 35:BN:62:ASN:N | 35:BN:62:ASN:HD22 | 2.00 | 0.60 |
| 24:BV:30:ILE:HG13 | 24:BV:40:ILE:HD12 | 1.84 | 0.60 |
| 1:CA:1236:A:H4' | 1:CA:1304:G:H4' | 1.81 | 0.60 |
| 1:CA:1302:C:H5' | 12:CM:16:ILE:HG13 | 1.84 | 0.60 |
| 1:CA:1386:G:H2' | 1:CA:1387:G:H8 | 1.67 | 0.60 |
| 1:CA:190:A:O5' | 1:CA:190:A:H8 | 1.85 | 0.60 |
| 1:CA:35:G:H2' | 1:CA:36:C:C6 | 2.37 | 0.60 |
| 20:CB:187:ASP:HB3 | 20:CB:201:GLY:O | 2.02 | 0.60 |
| 20:CB:202:ASN:HD22 | 20:CB:204:ASP:N | 1.88 | 0.60 |
| 11:CL:7:VAL:HG22 | 16:CQ:33:TYR:HD1 | 1.66 | 0.60 |
| 12:CM:79:LEU:HD11 | 12:CM:86:ARG:HH21 | 1.66 | 0.60 |
| 23:DB:1535:A:H5'' | 23:DB:1536:C:H5 | 1.66 | 0.60 |
| 23:DB:2852:G:H2' | 23:DB:2853:C:C6 | 2.37 | 0.60 |
| 25:DC:76:VAL:HG12 | 25:DC:114:GLN:HG2 | 1.84 | 0.60 |
| 29:DG:68:ARG:HH12 | 29:DG:72:ASN:HD22 | 1.49 | 0.60 |
| 32:DK:54:LYS:N | 32:DK:54:LYS:HD2 | 2.17 | 0.60 |
| 23:DB:2376:A:N1 | 36:DO:92:PHE:HD2 | 2.00 | 0.60 |
| 40:DS:72:THR:OG1 | 40:DS:108:SER:HB3 | 2.01 | 0.60 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:C6 | 2.37 | 0.60 |
| 1:AA:1238:A:N3 | 1:AA:1238:A:H2' | 2.16 | 0.60 |
| 1:AA:411:A:H62 | 1:AA:413:G:H21 | 1.49 | 0.60 |
| 1:AA:492:C:H2' | 1:AA:493:A:N3 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AD:22:SER:H | 3:AD:109:THR:HG22 | 1.66 | 0.60 |
| 1:AA:1382:C:H4' | 6:AG:78:ARG:NH2 | 2.16 | 0.60 |
| 1:AA:538:G:H5'' | 11:AL:110:LYS:HG2 | 1.83 | 0.60 |
| 11:AL:35:ARG:HA | 11:AL:35:ARG:NH1 | 2.17 | 0.60 |
| 23:BB:1198:U:H2' | 23:BB:1199:U:C6 | 2.36 | 0.60 |
| 23:BB:1491:G:H5' | 25:BC:97:ASP:OD1 | 2.02 | 0.60 |
| 23:BB:1501:G:O2' | 23:BB:1502:A:H5' | 2.01 | 0.60 |
| 23:BB:1925:C:C2' | 23:BB:1926:U:H5'' | 2.31 | 0.60 |
| 23:BB:2073:C:O2' | 23:BB:2074:U:H5' | 2.02 | 0.60 |
| 23:BB:2488:G:O2' | 23:BB:2489:U:H5' | 2.02 | 0.60 |
| 23:BB:2498:C:O2' | 23:BB:2499:C:H5' | 2.02 | 0.60 |
| 23:BB:2635:A:H4' | 26:BD:79:LEU:HB2 | 1.84 | 0.60 |
| 23:BB:784:G:O2' | 23:BB:785:G:H5'' | 2.01 | 0.60 |
| 30:BH:69:ALA:C | 30:BH:140:ALA:HB2 | 2.22 | 0.60 |
| 31:BJ:45:THR:HG21 | 31:BJ:50:THR:HG21 | 1.83 | 0.60 |
| 34:BM:108:VAL:HG11 | 34:BM:112:LEU:HD12 | 1.84 | 0.60 |
| 1:CA:1417:G:N2 | 1:CA:1482:G:H2' | 2.17 | 0.60 |
| 3:CD:29:THR:HG22 | 3:CD:30:LYS:HD3 | 1.83 | 0.60 |
| 5:CF:79:ARG:NH2 | 5:CF:87:SER:HB3 | 2.17 | 0.60 |
| 7:CH:24:VAL:HG12 | 7:CH:60:LEU:O | 2.01 | 0.60 |
| 47:D0:38:LEU:HD23 | 47:D0:39:ARG:H | 1.67 | 0.60 |
| 23:DB:1082:U:N3 | 23:DB:1086:A:C6 | 2.69 | 0.60 |
| 23:DB:1647:U:H3' | 23:DB:1647:U:P | 2.42 | 0.60 |
| 23:DB:2458:G:H1' | 23:DB:2460:U:O4 | 2.02 | 0.60 |
| 25:DC:141:HIS:CG | 25:DC:142:ASN:H | 2.20 | 0.60 |
| 29:DG:2:ARG:H | 29:DG:5:LYS:HE2 | 1.67 | 0.60 |
| 31:DJ:100:VAL:O | 31:DJ:104:ALA:HB2 | 2.02 | 0.60 |
| 32:DK:105:ARG:HD3 | 32:DK:106:GLU:OE1 | 2.01 | 0.60 |
| 35:DN:62:ASN:N | 35:DN:62:ASN:HD22 | 1.99 | 0.60 |
| 41:DT:29:THR:CA | 41:DT:86:THR:HA | 2.30 | 0.60 |
| 45:DY:35:VAL:HG22 | 45:DY:36:GLU:N | 2.16 | 0.60 |
| 1:AA:1329:A:OP1 | 12:AM:28:ARG:HB2 | 2.02 | 0.59 |
| 1:AA:1508:A:H2' | 1:AA:1509:C:C6 | 2.37 | 0.59 |
| 1:AA:410:G:P | 3:AD:25:ARG:HD2 | 2.42 | 0.59 |
| 1:AA:685:G:O2' | 1:AA:686:U:H5' | 2.02 | 0.59 |
| 4:AE:158:LYS:HZ3 | 7:AH:63:LYS:HD3 | 1.67 | 0.59 |
| 8:AI:93:LEU:O | 8:AI:97:LEU:HG | 2.02 | 0.59 |
| 47:B0:39:ARG:O | 47:B0:40:HIS:HB2 | 2.02 | 0.59 |
| 48:B1:29:LYS:HE2 | 48:B1:31:GLU:OE1 | 2.02 | 0.59 |
| 23:BB:1268:A:H2' | 23:BB:1269:A:O4' | 2.02 | 0.59 |
| 23:BB:1425:G:H2' | 23:BB:1426:G:C8 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:150:U:H2' | 23:BB:151:C:C6 | 2.37 | 0.59 |
| 23:BB:181:A:H2' | 23:BB:182:A:H8 | 1.64 | 0.59 |
| 23:BB:2651:C:O2' | 23:BB:2652:C:H5' | 2.02 | 0.59 |
| 23:BB:2728:U:H2' | 23:BB:2729:G:H8 | 1.67 | 0.59 |
| 23:BB:279:A:H2' | 23:BB:280:U:H5' | 1.84 | 0.59 |
| 23:BB:282:A:H2' | 23:BB:283:G:H8 | 1.66 | 0.59 |
| 23:BB:401:A:H2' | 23:BB:402:A:H8 | 1.64 | 0.59 |
| 23:BB:545:U:C4 | 23:BB:547:A:H5'' | 2.37 | 0.59 |
| 23:BB:741:U:H2' | 23:BB:742:A:C8 | 2.37 | 0.59 |
| 31:BJ:100:VAL:O | 31:BJ:104:ALA:HB2 | 2.02 | 0.59 |
| 31:BJ:25:LEU:HB2 | 31:BJ:62:VAL:CG2 | 2.32 | 0.59 |
| 27:BE:108:ILE:HG13 | 33:BL:2:ARG:HH22 | 1.66 | 0.59 |
| 43:BW:49:ASN:HD22 | 43:BW:59:PHE:HB3 | 1.67 | 0.59 |
| 1:CA:1271:A:H5' | 1:CA:1314:C:H5'' | 1.83 | 0.59 |
| 1:CA:182:A:O2' | 1:CA:183:C:H3' | 2.02 | 0.59 |
| 20:CB:31:PHE:N | 20:CB:39:ILE:O | 2.34 | 0.59 |
| 3:CD:138:PRO:HA | 3:CD:181:PHE:CD2 | 2.31 | 0.59 |
| 23:DB:1178:C:H2' | 23:DB:1179:G:H8 | 1.66 | 0.59 |
| 23:DB:2025:C:H2' | 23:DB:2026:U:C6 | 2.37 | 0.59 |
| 23:DB:1130:U:C2 | 23:DB:2025:C:H5'' | 2.37 | 0.59 |
| 23:DB:2031:A:C6 | 23:DB:2498:C:H1' | 2.37 | 0.59 |
| 23:DB:233:A:H61 | 23:DB:428:A:H61 | 1.48 | 0.59 |
| 23:DB:2392:A:H2' | 23:DB:2392:A:N3 | 2.17 | 0.59 |
| 23:DB:2834:G:H2' | 23:DB:2879:A:N6 | 2.17 | 0.59 |
| 32:DK:60:ALA:HA | 32:DK:87:LEU:CD2 | 2.32 | 0.59 |
| 23:DB:196:A:H5'' | 33:DL:47:ARG:HH12 | 1.66 | 0.59 |
| 45:DY:6:ILE:O | 45:DY:34:THR:HG23 | 2.02 | 0.59 |
| 1:AA:1301:U:O2 | 1:AA:1301:U:H2' | 2.01 | 0.59 |
| 20:AB:99:MET:HA | 20:AB:106:VAL:HG11 | 1.84 | 0.59 |
| 20:AB:65:LYS:H | 20:AB:158:ASP:CG | 2.04 | 0.59 |
| 3:AD:29:THR:HG22 | 3:AD:30:LYS:H | 1.67 | 0.59 |
| 8:AI:25:GLY:HA3 | 8:AI:57:VAL:N | 2.16 | 0.59 |
| 9:AJ:53:ILE:HG22 | 9:AJ:61:ALA:HB1 | 1.83 | 0.59 |
| 12:AM:39:ALA:HB3 | 12:AM:42:VAL:HG13 | 1.84 | 0.59 |
| 13:AN:16:ALA:HB2 | 13:AN:55:SER:N | 2.17 | 0.59 |
| 23:BB:1205:A:H4' | 23:BB:1206:G:OP2 | 2.01 | 0.59 |
| 23:BB:1281:G:H2' | 23:BB:1282:U:C6 | 2.37 | 0.59 |
| 23:BB:131:A:H2' | 23:BB:132:G:C8 | 2.37 | 0.59 |
| 23:BB:1484:U:H2' | 23:BB:1485:U:C6 | 2.38 | 0.59 |
| 23:BB:1853:A:N1 | 23:BB:2087:G:H1' | 2.17 | 0.59 |
| 23:BB:2229:U:H2' | 23:BB:2230:G:C8 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2884:U:H2' | 23:BB:2885:G:C8 | 2.37 | 0.59 |
| 23:BB:2598:A:H5'' | 25:BC:233:GLY:CA | 2.32 | 0.59 |
| 28:BF:42:ALA:HA | 28:BF:48:LEU:CD2 | 2.31 | 0.59 |
| 28:BF:71:LYS:HE2 | 28:BF:73:VAL:HB | 1.83 | 0.59 |
| 29:BG:115:GLN:CD | 29:BG:115:GLN:H | 2.06 | 0.59 |
| 29:BG:15:ASP:CB | 29:BG:26:LYS:H | 2.12 | 0.59 |
| 31:BJ:72:LYS:O | 31:BJ:73:VAL:HG13 | 2.02 | 0.59 |
| 32:BK:11:ALA:HB3 | 32:BK:85:VAL:HG22 | 1.84 | 0.59 |
| 35:BN:103:ARG:HG2 | 35:BN:104:ALA:H | 1.65 | 0.59 |
| 24:BV:80:HIS:HD2 | 24:BV:83:LYS:H | 1.48 | 0.59 |
| 1:CA:10:A:H2' | 1:CA:11:G:C8 | 2.37 | 0.59 |
| 1:CA:1151:A:HO2' | 1:CA:1152:A:H8 | 1.49 | 0.59 |
| 1:CA:1301:U:H2' | 1:CA:1301:U:O2 | 2.02 | 0.59 |
| 20:CB:163:ILE:HG23 | 20:CB:164:ASP:N | 2.17 | 0.59 |
| 3:CD:169:TRP:CE2 | 3:CD:185:PRO:HB3 | 2.36 | 0.59 |
| 8:CI:126:PHE:CE1 | 8:CI:129:ARG:HD3 | 2.37 | 0.59 |
| 10:CK:51:PHE:HB2 | 10:CK:55:ARG:HB3 | 1.84 | 0.59 |
| 47:D0:39:ARG:O | 47:D0:40:HIS:HB2 | 2.01 | 0.59 |
| 23:DB:1316:U:O2' | 23:DB:1317:G:H5' | 2.02 | 0.59 |
| 23:DB:2651:C:O2' | 23:DB:2652:C:H5' | 2.03 | 0.59 |
| 23:DB:712:G:H2' | 23:DB:713:G:O4' | 2.03 | 0.59 |
| 23:DB:857:G:O2' | 23:DB:858:G:H5' | 2.02 | 0.59 |
| 25:DC:131:MET:HE2 | 25:DC:189:ALA:HB2 | 1.84 | 0.59 |
| 23:DB:1993:U:H4' | 26:DD:133:THR:HG22 | 1.83 | 0.59 |
| 27:DE:3:LEU:H | 27:DE:13:THR:H | 1.50 | 0.59 |
| 28:DF:102:LEU:HA | 28:DF:106:ALA:CB | 2.32 | 0.59 |
| 33:DL:93:ASN:O | 33:DL:95:LEU:N | 2.36 | 0.59 |
| 37:DP:13:LYS:CD | 37:DP:76:HIS:HA | 2.31 | 0.59 |
| 44:DX:48:ARG:O | 44:DX:51:ALA:HB3 | 2.02 | 0.59 |
| 1:AA:370:C:O2' | 1:AA:371:A:H5' | 2.02 | 0.59 |
| 4:AE:81:GLN:H | 4:AE:146:MET:CE | 2.15 | 0.59 |
| 4:AE:82:HIS:HB2 | 4:AE:83:PRO:HD2 | 1.84 | 0.59 |
| 10:AK:51:PHE:HB2 | 10:AK:55:ARG:HB3 | 1.85 | 0.59 |
| 10:AK:81:LEU:HD11 | 10:AK:99:LEU:HD23 | 1.82 | 0.59 |
| 23:BB:2015:A:N3 | 47:B0:2:VAL:HG22 | 2.18 | 0.59 |
| 23:BB:1487:U:H2' | 23:BB:1488:C:C6 | 2.37 | 0.59 |
| 23:BB:2216:G:H2' | 23:BB:2217:G:H8 | 1.68 | 0.59 |
| 23:BB:2377:A:H2' | 23:BB:2378:A:C8 | 2.37 | 0.59 |
| 23:BB:2530:A:H3' | 29:BG:156:TYR:OH | 2.01 | 0.59 |
| 23:BB:2848:G:H22 | 23:BB:2867:G:N2 | 2.00 | 0.59 |
| 23:BB:365:U:H2' | 23:BB:366:C:C6 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BC:243:PRO:O | 25:BC:250:GLN:HA | 2.02 | 0.59 |
| 23:BB:321:U:OP2 | 27:BE:130:LYS:HD3 | 2.02 | 0.59 |
| 29:BG:59:ASP:O | 29:BG:63:GLN:HB2 | 2.01 | 0.59 |
| 32:BK:71:ARG:HG3 | 32:BK:105:ARG:HH21 | 1.67 | 0.59 |
| 34:BM:36:VAL:HB | 34:BM:127:LYS:O | 2.01 | 0.59 |
| 39:BR:5:PHE:O | 39:BR:11:GLN:HA | 2.01 | 0.59 |
| 1:CA:1179:A:H2' | 1:CA:1180:A:O4' | 2.02 | 0.59 |
| 1:CA:1258:G:H2' | 1:CA:1259:C:H6 | 1.68 | 0.59 |
| 1:CA:1296:C:H4' | 1:CA:1302:C:N3 | 2.18 | 0.59 |
| 1:CA:824:G:O2' | 1:CA:825:A:H5' | 2.02 | 0.59 |
| 20:CB:42:LEU:O | 20:CB:46:VAL:HG12 | 2.02 | 0.59 |
| 8:CI:27:ILE:HB | 8:CI:34:LEU:HB2 | 1.84 | 0.59 |
| 23:DB:125:A:O2' | 49:D2:13:ASN:HB3 | 2.02 | 0.59 |
| 22:DA:106:G:H2' | 22:DA:107:G:O4' | 2.03 | 0.59 |
| 23:DB:1552:A:H2' | 23:DB:1553:A:H5' | 1.83 | 0.59 |
| 23:DB:1993:U:H4' | 26:DD:133:THR:HG21 | 1.84 | 0.59 |
| 23:DB:2037:A:H2' | 23:DB:2038:G:C8 | 2.37 | 0.59 |
| 25:DC:1:ALA:HB3 | 25:DC:19:VAL:HG23 | 1.84 | 0.59 |
| 27:DE:104:ALA:O | 27:DE:108:ILE:HG22 | 2.01 | 0.59 |
| 52:DI:112:LYS:O | 52:DI:116:MET:HG3 | 2.02 | 0.59 |
| 32:DK:37:ASP:O | 32:DK:61:VAL:HA | 2.03 | 0.59 |
| 35:DN:24:MET:HG3 | 35:DN:44:LEU:HD22 | 1.83 | 0.59 |
| 37:DP:56:SER:O | 37:DP:74:GLN:HA | 2.03 | 0.59 |
| 41:DT:65:GLY:HA3 | 41:DT:76:ARG:HH22 | 1.67 | 0.59 |
| 1:AA:845:A:H3' | 1:AA:846:G:C8 | 2.37 | 0.59 |
| 2:AC:8:GLY:HA2 | 2:AC:11:LEU:HG | 1.83 | 0.59 |
| 5:AF:3:HIS:NE2 | 5:AF:95:ALA:HB2 | 2.18 | 0.59 |
| 5:AF:98:GLU:HG2 | 5:AF:99:ALA:N | 2.17 | 0.59 |
| 6:AG:64:ALA:HA | 6:AG:127:ALA:HA | 1.84 | 0.59 |
| 13:AN:68:ARG:NH1 | 13:AN:70:HIS:HB2 | 2.16 | 0.59 |
| 19:AT:66:ILE:HG22 | 19:AT:67:HIS:N | 2.16 | 0.59 |
| 23:BB:1063:G:O2' | 52:BI:88:GLY:HA3 | 2.02 | 0.59 |
| 23:BB:1164:C:H2' | 23:BB:1165:A:C8 | 2.38 | 0.59 |
| 23:BB:1552:A:H2' | 23:BB:1553:A:H5' | 1.85 | 0.59 |
| 23:BB:233:A:H61 | 23:BB:428:A:H61 | 1.49 | 0.59 |
| 23:BB:2666:C:O4' | 23:BB:2666:C:O2 | 2.20 | 0.59 |
| 23:BB:30:G:H2' | 23:BB:31:C:H6 | 1.68 | 0.59 |
| 23:BB:969:G:OP1 | 45:BY:17:PRO:HG3 | 2.02 | 0.59 |
| 29:BG:34:ARG:HG2 | 29:BG:34:ARG:HH11 | 1.67 | 0.59 |
| 30:BH:53:GLU:HA | 30:BH:57:LYS:HG2 | 1.83 | 0.59 |
| 31:BJ:25:LEU:HD22 | 31:BJ:26:GLY:N | 2.16 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BQ:91:ARG:CZ | 39:BR:11:GLN:H | 2.14 | 0.59 |
| 1:CA:806:C:H2' | 1:CA:807:A:C8 | 2.36 | 0.59 |
| 1:CA:918:A:H2' | 1:CA:919:A:C8 | 2.38 | 0.59 |
| 20:CB:23:ASN:HD22 | 20:CB:24:PRO:HD2 | 1.67 | 0.59 |
| 12:CM:58:GLU:O | 12:CM:61:LYS:HG2 | 2.01 | 0.59 |
| 1:CA:751:U:H4' | 14:CO:23:SER:HA | 1.83 | 0.59 |
| 23:DB:1400:U:H2' | 23:DB:1401:G:H8 | 1.67 | 0.59 |
| 23:DB:150:U:H2' | 23:DB:151:C:C6 | 2.37 | 0.59 |
| 23:DB:1551:A:H3' | 23:DB:1552:A:H5'' | 1.83 | 0.59 |
| 23:DB:1771:C:H2' | 23:DB:1772:A:H8 | 1.65 | 0.59 |
| 23:DB:1790:C:O2' | 25:DC:207:ALA:HB2 | 2.02 | 0.59 |
| 28:DF:66:ILE:HA | 28:DF:86:CYS:HB3 | 1.84 | 0.59 |
| 29:DG:34:ARG:HH11 | 29:DG:34:ARG:HG2 | 1.67 | 0.59 |
| 33:DL:4:ASN:ND2 | 33:DL:4:ASN:N | 2.50 | 0.59 |
| 38:DQ:91:ARG:CZ | 39:DR:11:GLN:H | 2.15 | 0.59 |
| 1:AA:182:A:O2' | 1:AA:183:C:H3' | 2.03 | 0.59 |
| 1:AA:275:G:H5' | 16:AQ:15:LYS:HD3 | 1.84 | 0.59 |
| 20:AB:31:PHE:N | 20:AB:39:ILE:O | 2.34 | 0.59 |
| 2:AC:183:TYR:HA | 2:AC:199:VAL:O | 2.02 | 0.59 |
| 6:AG:24:LYS:HA | 6:AG:27:ASN:HD22 | 1.67 | 0.59 |
| 4:AE:152:VAL:HG21 | 7:AH:98:LEU:HB3 | 1.82 | 0.59 |
| 11:AL:14:LYS:HG2 | 11:AL:16:ALA:H | 1.66 | 0.59 |
| 12:AM:79:LEU:HD11 | 12:AM:86:ARG:NH2 | 2.18 | 0.59 |
| 14:AO:43:ALA:O | 14:AO:46:LYS:HE3 | 2.03 | 0.59 |
| 23:BB:1061:U:H4' | 23:BB:1070:A:O3' | 2.03 | 0.59 |
| 23:BB:1551:A:H2' | 23:BB:1552:A:O4' | 2.01 | 0.59 |
| 23:BB:528:A:N1 | 23:BB:2042:A:H2' | 2.18 | 0.59 |
| 23:BB:2458:G:H1' | 23:BB:2460:U:O4 | 2.02 | 0.59 |
| 23:BB:721:A:H2' | 23:BB:722:A:H8 | 1.68 | 0.59 |
| 23:BB:78:U:H2' | 23:BB:79:C:C6 | 2.37 | 0.59 |
| 25:BC:141:HIS:CG | 25:BC:142:ASN:H | 2.20 | 0.59 |
| 25:BC:71:ASP:OD2 | 25:BC:118:GLY:HA2 | 2.02 | 0.59 |
| 29:BG:72:ASN:O | 29:BG:76:ILE:HG12 | 2.03 | 0.59 |
| 31:BJ:24:THR:HA | 31:BJ:63:ALA:HB3 | 1.84 | 0.59 |
| 32:BK:37:ASP:O | 32:BK:61:VAL:HA | 2.02 | 0.59 |
| 33:BL:30:THR:O | 33:BL:33:ARG:HG2 | 2.01 | 0.59 |
| 36:BO:55:GLU:HB2 | 36:BO:58:ILE:HD12 | 1.84 | 0.59 |
| 42:BU:26:ASN:HD22 | 42:BU:26:ASN:N | 1.98 | 0.59 |
| 43:BW:23:LYS:HD2 | 43:BW:24:ARG:N | 2.16 | 0.59 |
| 1:CA:336:A:O2' | 1:CA:337:G:H5' | 2.03 | 0.59 |
| 1:CA:699:C:C2' | 1:CA:700:G:H5'' | 2.30 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CI:93:LEU:O | 8:CI:97:LEU:HG | 2.02 | 0.59 |
| 12:CM:43:LYS:HD2 | 12:CM:43:LYS:H | 1.68 | 0.59 |
| 16:CQ:45:VAL:HG12 | 16:CQ:46:HIS:N | 2.18 | 0.59 |
| 50:D3:22:LYS:HA | 50:D3:47:ALA:O | 2.01 | 0.59 |
| 23:DB:1326:U:H2' | 23:DB:1327:A:H8 | 1.65 | 0.59 |
| 23:DB:1657:U:O2' | 23:DB:1658:C:H5' | 2.01 | 0.59 |
| 23:DB:2498:C:O2' | 23:DB:2499:C:H5' | 2.02 | 0.59 |
| 28:DF:102:LEU:HD22 | 28:DF:103:ILE:H | 1.68 | 0.59 |
| 28:DF:62:GLN:CB | 28:DF:91:ARG:HE | 2.14 | 0.59 |
| 34:DM:60:GLN:HG2 | 34:DM:108:VAL:HG23 | 1.84 | 0.59 |
| 34:DM:40:ARG:HB2 | 34:DM:93:VAL:CG2 | 2.32 | 0.59 |
| 36:DO:2:ASP:OD2 | 36:DO:4:LYS:HB3 | 2.03 | 0.59 |
| 37:DP:20:ARG:HB3 | 37:DP:23:ASP:OD2 | 2.02 | 0.59 |
| 39:DR:4:VAL:HG23 | 39:DR:39:LEU:H | 1.68 | 0.59 |
| 39:DR:79:ARG:CD | 39:DR:80:ARG:HH21 | 2.15 | 0.59 |
| 46:DZ:45:ARG:HE | 46:DZ:47:VAL:CG1 | 2.16 | 0.59 |
| 1:AA:1213:A:O2' | 1:AA:1214:C:H5'' | 2.03 | 0.59 |
| 1:AA:699:C:C2' | 1:AA:700:G:H5'' | 2.26 | 0.59 |
| 1:AA:746:A:H2' | 1:AA:747:A:C8 | 2.36 | 0.59 |
| 1:AA:996:A:H2' | 1:AA:997:U:C6 | 2.37 | 0.59 |
| 22:BA:32:U:H4' | 22:BA:52:A:N6 | 2.17 | 0.59 |
| 22:BA:43:C:H1' | 28:BF:91:ARG:HH21 | 1.66 | 0.59 |
| 23:BB:1326:U:H2' | 23:BB:1327:A:H8 | 1.66 | 0.59 |
| 23:BB:1550:C:H2' | 23:BB:1551:A:H8 | 1.68 | 0.59 |
| 23:BB:176:A:O2' | 23:BB:177:G:H5' | 2.02 | 0.59 |
| 23:BB:458:G:H22 | 23:BB:469:G:H2' | 1.66 | 0.59 |
| 23:BB:569:U:H2' | 23:BB:570:G:O4' | 2.03 | 0.59 |
| 23:BB:704:G:H2' | 23:BB:726:G:N2 | 2.16 | 0.59 |
| 30:BH:141:LYS:HD3 | 30:BH:141:LYS:N | 2.18 | 0.59 |
| 30:BH:73:ASN:ND2 | 30:BH:74:ALA:H | 1.95 | 0.59 |
| 30:BH:85:GLY:HA3 | 30:BH:91:PHE:HE1 | 1.67 | 0.59 |
| 34:BM:40:ARG:HB2 | 34:BM:93:VAL:CG2 | 2.32 | 0.59 |
| 34:BM:41:LEU:HB2 | 34:BM:94:ALA:HB3 | 1.84 | 0.59 |
| 35:BN:33:ILE:O | 35:BN:33:ILE:HD12 | 2.02 | 0.59 |
| 35:BN:76:VAL:HA | 35:BN:79:LEU:HD12 | 1.85 | 0.59 |
| 24:BV:42:LEU:HD11 | 24:BV:89:ILE:HD11 | 1.85 | 0.59 |
| 44:BX:45:GLN:O | 44:BX:47:ARG:N | 2.34 | 0.59 |
| 1:CA:239:U:H6 | 1:CA:239:U:C5' | 2.15 | 0.59 |
| 1:CA:499:A:H4' | 1:CA:500:G:H5' | 1.85 | 0.59 |
| 1:CA:1058:G:OP1 | 2:CC:198:LYS:HE3 | 2.03 | 0.59 |
| 8:CI:120:ALA:O | 8:CI:121:ARG:HG2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:CM:22:TYR:HB2 | 12:CM:65:GLU:HA | 1.83 | 0.59 |
| 50:D3:54:LEU:HG | 50:D3:58:ILE:HD11 | 1.84 | 0.59 |
| 23:DB:1082:U:C2 | 23:DB:1086:A:C6 | 2.90 | 0.59 |
| 23:DB:1739:A:H2' | 23:DB:1740:G:O4' | 2.02 | 0.59 |
| 23:DB:2066:C:O2' | 23:DB:2067:G:H5' | 2.02 | 0.59 |
| 23:DB:2772:C:H2' | 23:DB:2773:C:H6 | 1.68 | 0.59 |
| 23:DB:722:A:H2' | 23:DB:723:C:C6 | 2.38 | 0.59 |
| 23:DB:2598:A:H5'' | 25:DC:233:GLY:CA | 2.32 | 0.59 |
| 27:DE:111:GLU:HB3 | 33:DL:2:ARG:HH12 | 1.65 | 0.59 |
| 27:DE:29:HIS:O | 27:DE:33:VAL:HG23 | 2.03 | 0.59 |
| 27:DE:48:THR:HG22 | 27:DE:86:ALA:HB3 | 1.83 | 0.59 |
| 28:DF:111:ARG:NH2 | 28:DF:113:PHE:HB2 | 2.17 | 0.59 |
| 28:DF:34:THR:HG22 | 28:DF:89:THR:HG22 | 1.83 | 0.59 |
| 33:DL:80:SER:HA | 33:DL:115:GLU:HB2 | 1.84 | 0.59 |
| 33:DL:85:VAL:CG2 | 33:DL:94:THR:HB | 2.32 | 0.59 |
| 40:DS:28:LYS:HD2 | 40:DS:29:VAL:N | 2.18 | 0.59 |
| 42:DU:35:VAL:O | 42:DU:38:ILE:HG22 | 2.02 | 0.59 |
| 24:DV:24:ASN:O | 24:DV:44:HIS:HB2 | 2.02 | 0.59 |
| 20:AB:110:ILE:HG23 | 20:AB:151:LYS:HA | 1.84 | 0.59 |
| 20:AB:20:ARG:HA | 20:AB:38:HIS:CE1 | 2.38 | 0.59 |
| 20:AB:42:LEU:O | 20:AB:46:VAL:HG12 | 2.02 | 0.59 |
| 13:AN:41:TRP:HB3 | 13:AN:44:VAL:HB | 1.84 | 0.59 |
| 15:AP:20:VAL:HG23 | 15:AP:35:ARG:HA | 1.85 | 0.59 |
| 16:AQ:26:ARG:HG2 | 16:AQ:39:ARG:O | 2.02 | 0.59 |
| 50:B3:44:ARG:N | 50:B3:45:PRO:HD2 | 2.17 | 0.59 |
| 23:BB:1015:U:H2' | 23:BB:1016:G:C8 | 2.37 | 0.59 |
| 23:BB:2037:A:H2' | 23:BB:2038:G:C8 | 2.37 | 0.59 |
| 23:BB:2328:A:H2' | 23:BB:2329:U:H6 | 1.68 | 0.59 |
| 23:BB:2784:U:H2' | 23:BB:2785:C:C6 | 2.38 | 0.59 |
| 23:BB:345:A:H1' | 23:BB:346:A:C2 | 2.37 | 0.59 |
| 23:BB:419:U:H2' | 23:BB:420:C:H6 | 1.67 | 0.59 |
| 23:BB:233:A:N6 | 23:BB:428:A:H61 | 2.00 | 0.59 |
| 25:BC:93:VAL:HG13 | 25:BC:94:LEU:N | 2.17 | 0.59 |
| 27:BE:46:GLN:HG3 | 27:BE:87:ALA:HB3 | 1.83 | 0.59 |
| 37:BP:13:LYS:CD | 37:BP:76:HIS:HA | 2.32 | 0.59 |
| 42:BU:94:PHE:CB | 42:BU:101:THR:HA | 2.33 | 0.59 |
| 46:BZ:40:VAL:HG22 | 46:BZ:45:ARG:H | 1.67 | 0.59 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:H5' | 1.84 | 0.59 |
| 1:CA:1296:C:H4' | 1:CA:1302:C:N4 | 2.17 | 0.59 |
| 2:CC:82:ASP:HA | 2:CC:85:LYS:HB3 | 1.85 | 0.59 |
| 23:DB:1535:A:H5'' | 23:DB:1536:C:C5 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1723:G:N7 | 23:DB:1737:G:N2 | 2.51 | 0.59 |
| 23:DB:2241:A:H2' | 23:DB:2242:G:H8 | 1.68 | 0.59 |
| 23:DB:2784:U:H2' | 23:DB:2785:C:C6 | 2.37 | 0.59 |
| 23:DB:309:A:H4' | 42:DU:15:GLY:HA2 | 1.85 | 0.59 |
| 23:DB:630:G:N2 | 23:DB:632:A:H3' | 2.16 | 0.59 |
| 23:DB:65:U:H2' | 23:DB:66:C:C6 | 2.38 | 0.59 |
| 12:CM:70:ARG:NH1 | 28:DF:142:TYR:HB2 | 2.17 | 0.59 |
| 28:DF:36:ASN:HA | 28:DF:87:LYS:HA | 1.84 | 0.59 |
| 28:DF:40:GLY:HA2 | 28:DF:84:ILE:HG23 | 1.85 | 0.59 |
| 29:DG:26:LYS:HG2 | 29:DG:27:GLY:H | 1.67 | 0.59 |
| 23:DB:636:G:O5' | 33:DL:128:THR:HG22 | 2.03 | 0.59 |
| 23:DB:2394:C:OP1 | 33:DL:63:LYS:HG2 | 2.03 | 0.59 |
| 24:DV:80:HIS:HD2 | 24:DV:83:LYS:H | 1.49 | 0.59 |
| 41:DT:14:PRO:HD2 | 44:DX:33:ALA:HB3 | 1.84 | 0.59 |
| 1:AA:1007:U:H2' | 1:AA:1008:U:C6 | 2.37 | 0.59 |
| 7:AH:46:GLU:HB2 | 7:AH:61:THR:HB | 1.85 | 0.59 |
| 11:AL:35:ARG:HA | 11:AL:35:ARG:CZ | 2.33 | 0.59 |
| 1:AA:1302:C:H5' | 12:AM:16:ILE:HG13 | 1.85 | 0.59 |
| 15:AP:68:SER:OG | 15:AP:71:VAL:HG12 | 2.02 | 0.59 |
| 16:AQ:45:VAL:HG12 | 16:AQ:46:HIS:N | 2.18 | 0.59 |
| 23:BB:1219:U:H2' | 23:BB:1220:G:H8 | 1.68 | 0.59 |
| 23:BB:138:U:C4 | 23:BB:140:C:H1' | 2.37 | 0.59 |
| 23:BB:573:U:O2' | 23:BB:574:A:H3' | 2.02 | 0.59 |
| 23:BB:722:A:H2' | 23:BB:723:C:C6 | 2.38 | 0.59 |
| 31:BJ:20:ALA:HA | 31:BJ:23:LYS:HG2 | 1.85 | 0.59 |
| 23:BB:2376:A:N6 | 36:BO:94:ARG:HD3 | 2.18 | 0.59 |
| 37:BP:7:LEU:HA | 37:BP:10:GLU:HG2 | 1.85 | 0.59 |
| 37:BP:56:SER:O | 37:BP:74:GLN:HA | 2.03 | 0.59 |
| 45:BY:6:ILE:O | 45:BY:34:THR:HG23 | 2.03 | 0.59 |
| 1:CA:501:C:H2' | 1:CA:502:A:C8 | 2.37 | 0.59 |
| 1:CA:72:A:H5' | 1:CA:73:C:OP2 | 2.02 | 0.59 |
| 20:CB:16:GLY:CA | 20:CB:40:ILE:H | 2.16 | 0.59 |
| 5:CF:3:HIS:NE2 | 5:CF:95:ALA:HB2 | 2.18 | 0.59 |
| 12:CM:79:LEU:HD11 | 12:CM:86:ARG:NH2 | 2.17 | 0.59 |
| 51:D4:8:LYS:HG2 | 51:D4:9:LYS:H | 1.67 | 0.59 |
| 23:DB:2359:C:H2' | 23:DB:2360:G:C8 | 2.38 | 0.59 |
| 23:DB:2722:G:H2' | 23:DB:2723:C:C6 | 2.38 | 0.59 |
| 23:DB:967:U:H2' | 23:DB:968:C:C6 | 2.38 | 0.59 |
| 23:DB:968:C:H2' | 23:DB:969:G:H8 | 1.66 | 0.59 |
| 29:DG:137:LYS:HA | 29:DG:140:ILE:HD11 | 1.84 | 0.59 |
| 52:DI:126:ARG:HB3 | 52:DI:126:ARG:HH11 | 1.68 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DM:108:VAL:HG11 | 34:DM:112:LEU:HD12 | 1.83 | 0.59 |
| 34:DM:96:ILE:HD11 | 34:DM:126:ILE:HG12 | 1.84 | 0.59 |
| 36:DO:88:LYS:HD2 | 36:DO:89:ASP:HB2 | 1.85 | 0.59 |
| 41:DT:2:ILE:N | 41:DT:2:ILE:HD13 | 2.18 | 0.59 |
| 42:DU:80:ASP:HB3 | 42:DU:96:LYS:N | 2.06 | 0.59 |
| 1:AA:1294:G:H2' | 1:AA:1295:U:C6 | 2.38 | 0.59 |
| 1:AA:628:G:H2' | 1:AA:629:A:C8 | 2.38 | 0.59 |
| 20:AB:140:LEU:H | 20:AB:140:LEU:HD12 | 1.68 | 0.59 |
| 18:AS:30:LEU:H | 18:AS:48:ILE:HA | 1.67 | 0.59 |
| 23:BB:1245:G:OP1 | 33:BL:13:LYS:HE3 | 2.02 | 0.59 |
| 23:BB:2815:C:H2' | 23:BB:2816:G:H8 | 1.67 | 0.59 |
| 23:BB:282:A:H2' | 23:BB:283:G:C8 | 2.38 | 0.59 |
| 23:BB:395:U:H2' | 23:BB:396:G:N7 | 2.16 | 0.59 |
| 25:BC:66:PHE:HB2 | 25:BC:150:GLY:O | 2.02 | 0.59 |
| 26:BD:169:ARG:O | 26:BD:170:VAL:HG22 | 2.02 | 0.59 |
| 28:BF:90:LEU:HD12 | 28:BF:95:MET:HA | 1.84 | 0.59 |
| 28:BF:30:VAL:HG21 | 28:BF:96:TRP:NE1 | 2.18 | 0.59 |
| 30:BH:122:LEU:HD12 | 30:BH:122:LEU:H | 1.68 | 0.59 |
| 30:BH:72:ILE:HD13 | 30:BH:142:VAL:HG22 | 1.85 | 0.59 |
| 34:BM:19:GLY:N | 34:BM:38:ARG:HH22 | 2.01 | 0.59 |
| 36:BO:2:ASP:OD2 | 36:BO:4:LYS:HB3 | 2.02 | 0.59 |
| 39:BR:34:GLU:HA | 39:BR:59:ILE:O | 2.03 | 0.59 |
| 23:BB:141:G:C6 | 41:BT:2:ILE:HD12 | 2.38 | 0.59 |
| 24:BV:4:ILE:O | 24:BV:63:ILE:HA | 2.03 | 0.59 |
| 1:CA:621:A:H2' | 1:CA:622:A:C8 | 2.38 | 0.59 |
| 20:CB:32:GLY:N | 20:CB:39:ILE:HB | 2.16 | 0.59 |
| 7:CH:17:GLN:HE21 | 7:CH:62:LEU:HB3 | 1.68 | 0.59 |
| 12:CM:21:ILE:HB | 12:CM:24:VAL:CG2 | 2.27 | 0.59 |
| 18:CS:43:MET:HB2 | 18:CS:61:VAL:HG11 | 1.84 | 0.59 |
| 22:DA:6:G:H2' | 22:DA:7:G:C8 | 2.38 | 0.59 |
| 23:DB:2061:G:H5'' | 23:DB:2503:A:C2 | 2.37 | 0.59 |
| 23:DB:2179:C:C2' | 23:DB:2179:C:O2 | 2.48 | 0.59 |
| 23:DB:2384:U:H5'' | 23:DB:2386:A:OP1 | 2.03 | 0.59 |
| 23:DB:2800:A:H2' | 23:DB:2801:G:O4' | 2.02 | 0.59 |
| 23:DB:2813:A:H2' | 23:DB:2814:A:C8 | 2.38 | 0.59 |
| 23:DB:37:C:H4' | 23:DB:451:U:OP1 | 2.02 | 0.59 |
| 23:DB:856:G:C1' | 43:DW:23:LYS:HB3 | 2.33 | 0.59 |
| 25:DC:171:VAL:HB | 25:DC:183:VAL:HG12 | 1.85 | 0.59 |
| 26:DD:36:GLN:O | 26:DD:36:GLN:HG3 | 2.01 | 0.59 |
| 26:DD:92:VAL:O | 26:DD:94:GLN:N | 2.36 | 0.59 |
| 27:DE:108:ILE:HG13 | 33:DL:2:ARG:NH2 | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:43:C:H1' | 28:DF:91:ARG:HH21 | 1.68 | 0.59 |
| 30:DH:128:HIS:HB2 | 30:DH:144:VAL:HG23 | 1.85 | 0.59 |
| 30:DH:117:LEU:HD22 | 30:DH:130:VAL:HG13 | 1.85 | 0.59 |
| 31:DJ:25:LEU:HB2 | 31:DJ:62:VAL:CG2 | 2.33 | 0.59 |
| 32:DK:8:LEU:HD12 | 32:DK:8:LEU:N | 2.17 | 0.59 |
| 23:DB:825:A:H1' | 33:DL:54:GLN:HE21 | 1.68 | 0.59 |
| 41:DT:18:GLU:C | 41:DT:20:ALA:H | 2.06 | 0.59 |
| 5:AF:100:SER:HA | 17:AR:23:LYS:CE | 2.32 | 0.59 |
| 6:AG:26:VAL:HB | 6:AG:39:GLU:HG2 | 1.84 | 0.59 |
| 6:AG:62:GLU:O | 6:AG:66:GLU:HG3 | 2.03 | 0.59 |
| 10:AK:81:LEU:HD21 | 10:AK:104:PHE:HB3 | 1.85 | 0.59 |
| 51:B4:7:VAL:HG13 | 51:B4:8:LYS:N | 2.18 | 0.59 |
| 23:BB:1812:U:H2' | 23:BB:1813:G:C8 | 2.37 | 0.59 |
| 23:BB:660:C:H2' | 23:BB:661:A:H8 | 1.67 | 0.59 |
| 27:BE:33:VAL:O | 27:BE:36:ALA:HB3 | 2.02 | 0.59 |
| 30:BH:21:VAL:HG22 | 30:BH:22:LYS:H | 1.66 | 0.59 |
| 52:BI:96:LYS:N | 52:BI:96:LYS:HD2 | 2.18 | 0.59 |
| 31:BJ:124:VAL:O | 31:BJ:125:TYR:HB2 | 2.02 | 0.59 |
| 31:BJ:45:THR:OG1 | 31:BJ:48:VAL:HB | 2.03 | 0.59 |
| 36:BO:27:VAL:HG21 | 36:BO:40:ILE:HD12 | 1.85 | 0.59 |
| 36:BO:67:ASN:HB3 | 36:BO:70:ALA:HB2 | 1.83 | 0.59 |
| 1:CA:1478:U:H2' | 1:CA:1479:C:C6 | 2.38 | 0.59 |
| 1:CA:719:C:O2' | 17:CR:37:LYS:HB2 | 2.03 | 0.59 |
| 1:CA:802:A:H2' | 1:CA:803:G:O4' | 2.03 | 0.59 |
| 20:CB:99:MET:HA | 20:CB:106:VAL:HG11 | 1.85 | 0.59 |
| 12:CM:77:LYS:HG2 | 12:CM:81:ASP:OD2 | 2.02 | 0.59 |
| 16:CQ:26:ARG:HG2 | 16:CQ:39:ARG:O | 2.03 | 0.59 |
| 1:CA:332:G:OP2 | 19:CT:4:LYS:HB2 | 2.03 | 0.59 |
| 22:DA:13:G:C2' | 22:DA:14:U:H5'' | 2.32 | 0.59 |
| 23:DB:1551:A:H2' | 23:DB:1552:A:O4' | 2.03 | 0.59 |
| 23:DB:233:A:N6 | 23:DB:428:A:H61 | 2.00 | 0.59 |
| 23:DB:2354:C:H4' | 43:DW:31:LEU:CD2 | 2.32 | 0.59 |
| 23:DB:2258:C:O2' | 23:DB:2426:A:H4' | 2.02 | 0.59 |
| 23:DB:2758:A:H2' | 23:DB:2759:G:O4' | 2.03 | 0.59 |
| 23:DB:569:U:H2' | 23:DB:570:G:O4' | 2.03 | 0.59 |
| 23:DB:782:A:H5' | 23:DB:783:A:C2 | 2.38 | 0.59 |
| 34:DM:41:LEU:HB2 | 34:DM:94:ALA:HB3 | 1.85 | 0.59 |
| 23:DB:1454:C:H5' | 35:DN:63:ARG:NE | 2.18 | 0.59 |
| 23:DB:2334:U:H1' | 36:DO:13:ARG:HA | 1.85 | 0.59 |
| 38:DQ:91:ARG:NH2 | 39:DR:11:GLN:H | 2.01 | 0.59 |
| 40:DS:29:VAL:HG11 | 40:DS:55:ILE:CD1 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DT:44:LYS:O | 41:DT:48:GLN:HG2 | 2.02 | 0.59 |
| 42:DU:81:ARG:HB2 | 42:DU:96:LYS:CG | 2.33 | 0.59 |
| 45:DY:2:LYS:HD3 | 45:DY:2:LYS:H | 1.67 | 0.59 |
| 1:AA:1270:G:H2' | 1:AA:1271:A:C8 | 2.38 | 0.58 |
| 1:AA:264:C:O2' | 16:AQ:65:PRO:HG2 | 2.03 | 0.58 |
| 1:AA:922:G:H4' | 4:AE:24:VAL:HA | 1.85 | 0.58 |
| 2:AC:82:ASP:HA | 2:AC:85:LYS:HB3 | 1.84 | 0.58 |
| 17:AR:55:ALA:HA | 17:AR:58:ILE:HD13 | 1.84 | 0.58 |
| 19:AT:19:HIS:O | 19:AT:23:ARG:HG2 | 2.02 | 0.58 |
| 48:B1:34:GLU:HA | 48:B1:48:TYR:O | 2.03 | 0.58 |
| 23:BB:1406:U:H2' | 23:BB:1407:G:H8 | 1.68 | 0.58 |
| 23:BB:1557:C:H3' | 23:BB:1558:C:H5'' | 1.85 | 0.58 |
| 23:BB:2277:G:H5'' | 34:BM:86:LYS:CB | 2.33 | 0.58 |
| 26:BD:7:LYS:O | 26:BD:9:VAL:HG12 | 2.03 | 0.58 |
| 40:BS:42:LYS:O | 40:BS:45:VAL:HG22 | 2.03 | 0.58 |
| 41:BT:48:GLN:HE21 | 41:BT:48:GLN:HA | 1.68 | 0.58 |
| 41:BT:57:VAL:HG13 | 41:BT:58:VAL:N | 2.18 | 0.58 |
| 45:BY:2:LYS:HD3 | 45:BY:2:LYS:H | 1.67 | 0.58 |
| 1:CA:1249:C:H4' | 8:CI:37:TYR:OH | 2.03 | 0.58 |
| 1:CA:1270:G:H2' | 1:CA:1271:A:C8 | 2.38 | 0.58 |
| 1:CA:6:G:HO2' | 1:CA:7:A:H8 | 1.48 | 0.58 |
| 20:CB:16:GLY:HA3 | 20:CB:39:ILE:HA | 1.84 | 0.58 |
| 1:CA:545:C:H5'' | 3:CD:68:GLU:HG2 | 1.85 | 0.58 |
| 7:CH:124:ILE:HG22 | 7:CH:125:ILE:N | 2.16 | 0.58 |
| 11:CL:35:ARG:NH1 | 11:CL:35:ARG:HA | 2.18 | 0.58 |
| 23:DB:2573:C:H3' | 56:DB:3631:HOH:O | 2.03 | 0.58 |
| 23:DB:2633:G:H2' | 23:DB:2634:A:O4' | 2.02 | 0.58 |
| 23:DB:2859:G:H2' | 23:DB:2860:A:C8 | 2.38 | 0.58 |
| 26:DD:13:ARG:HD3 | 26:DD:15:PHE:HE1 | 1.67 | 0.58 |
| 27:DE:98:LYS:HZ1 | 27:DE:99:LYS:HE2 | 1.68 | 0.58 |
| 28:DF:43:ILE:HG23 | 28:DF:44:ALA:N | 2.13 | 0.58 |
| 29:DG:59:ASP:O | 29:DG:63:GLN:HB2 | 2.03 | 0.58 |
| 23:DB:1098:A:H3' | 52:DI:3:LYS:C | 2.24 | 0.58 |
| 52:DI:32:VAL:HG22 | 52:DI:60:VAL:HG21 | 1.85 | 0.58 |
| 32:DK:70:ARG:HA | 32:DK:76:VAL:HA | 1.85 | 0.58 |
| 42:DU:94:PHE:CB | 42:DU:101:THR:HA | 2.33 | 0.58 |
| 23:DB:2264:C:H41 | 43:DW:11:ASN:ND2 | 1.99 | 0.58 |
| 43:DW:9:THR:OG1 | 43:DW:10:ARG:N | 2.32 | 0.58 |
| 45:DY:37:ARG:HG2 | 45:DY:43:ILE:HD11 | 1.85 | 0.58 |
| 1:AA:1008:U:H5'' | 13:AN:23:ARG:NH2 | 2.17 | 0.58 |
| 1:AA:68:G:H5' | 1:AA:171:A:H1' | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:812:G:H2' | 1:AA:812:G:N3 | 2.18 | 0.58 |
| 20:AB:126:ASP:O | 20:AB:127:LYS:HB3 | 2.03 | 0.58 |
| 4:AE:11:GLN:HE22 | 4:AE:41:GLY:HA3 | 1.69 | 0.58 |
| 8:AI:25:GLY:HA3 | 8:AI:57:VAL:H | 1.68 | 0.58 |
| 23:BB:1171:G:H2' | 23:BB:1172:C:C6 | 2.37 | 0.58 |
| 23:BB:1320:C:H5 | 23:BB:1329:U:H5'' | 1.68 | 0.58 |
| 23:BB:1739:A:H2' | 23:BB:1740:G:O4' | 2.04 | 0.58 |
| 23:BB:2088:A:H2' | 23:BB:2089:C:C6 | 2.38 | 0.58 |
| 23:BB:2384:U:H5'' | 23:BB:2386:A:OP1 | 2.03 | 0.58 |
| 23:BB:2624:G:H1' | 47:B0:18:HIS:NE2 | 2.17 | 0.58 |
| 23:BB:782:A:N7 | 25:BC:219:VAL:HG21 | 2.18 | 0.58 |
| 25:BC:171:VAL:HB | 25:BC:183:VAL:HG12 | 1.85 | 0.58 |
| 27:BE:5:LEU:HB2 | 27:BE:11:ALA:N | 2.18 | 0.58 |
| 28:BF:102:LEU:HA | 28:BF:106:ALA:CB | 2.33 | 0.58 |
| 29:BG:39:ALA:C | 29:BG:54:ARG:HB2 | 2.24 | 0.58 |
| 34:BM:19:GLY:H | 34:BM:38:ARG:NH1 | 1.98 | 0.58 |
| 35:BN:72:ASP:OD1 | 35:BN:75:ILE:HG23 | 2.03 | 0.58 |
| 37:BP:6:GLN:O | 37:BP:9:GLN:HG2 | 2.03 | 0.58 |
| 41:BT:29:THR:CA | 41:BT:86:THR:HA | 2.30 | 0.58 |
| 42:BU:35:VAL:O | 42:BU:38:ILE:HG22 | 2.03 | 0.58 |
| 24:BV:35:GLU:OE1 | 24:BV:93:ARG:HD3 | 2.03 | 0.58 |
| 45:BY:5:LYS:HG3 | 45:BY:57:GLU:HB2 | 1.85 | 0.58 |
| 1:CA:411:A:H62 | 1:CA:413:G:H21 | 1.50 | 0.58 |
| 1:CA:451:A:H5' | 15:CP:70:ARG:NH2 | 2.17 | 0.58 |
| 1:CA:638:U:H2' | 1:CA:639:G:O4' | 2.02 | 0.58 |
| 2:CC:154:GLY:HA3 | 2:CC:162:ALA:HB1 | 1.86 | 0.58 |
| 5:CF:86:ARG:HH12 | 17:CR:63:TYR:HB3 | 1.66 | 0.58 |
| 10:CK:124:LYS:HA | 21:CU:34:ARG:CB | 2.30 | 0.58 |
| 10:CK:70:ALA:C | 10:CK:72:ALA:H | 2.05 | 0.58 |
| 13:CN:68:ARG:NH1 | 13:CN:70:HIS:HB2 | 2.17 | 0.58 |
| 22:DA:24:G:O2' | 22:DA:25:U:H5'' | 2.02 | 0.58 |
| 23:DB:1443:U:H2' | 23:DB:1444:G:H8 | 1.68 | 0.58 |
| 23:DB:2468:A:H2' | 23:DB:2476:A:C6 | 2.38 | 0.58 |
| 23:DB:674:G:H4' | 27:DE:69:ARG:HB3 | 1.85 | 0.58 |
| 23:DB:825:A:H1' | 33:DL:54:GLN:NE2 | 2.18 | 0.58 |
| 38:DQ:105:PHE:O | 38:DQ:109:VAL:HG23 | 2.03 | 0.58 |
| 39:DR:39:LEU:CA | 39:DR:49:ILE:HG12 | 2.34 | 0.58 |
| 46:DZ:70:GLU:C | 46:DZ:72:ARG:H | 2.05 | 0.58 |
| 1:AA:370:C:H2' | 1:AA:371:A:H8 | 1.67 | 0.58 |
| 1:AA:539:A:H2' | 1:AA:540:G:H8 | 1.67 | 0.58 |
| 1:AA:728:A:H2' | 1:AA:729:A:C8 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:881:G:P | 11:AL:8:ARG:HH12 | 2.26 | 0.58 |
| 6:AG:78:ARG:NH1 | 6:AG:81:GLY:H | 2.01 | 0.58 |
| 11:AL:109:ARG:HB3 | 11:AL:118:VAL:HG21 | 1.85 | 0.58 |
| 11:AL:26:CYS:SG | 11:AL:29:LYS:HE2 | 2.43 | 0.58 |
| 18:AS:11:ASP:H | 18:AS:14:LEU:HD21 | 1.67 | 0.58 |
| 18:AS:43:MET:HB2 | 18:AS:61:VAL:HG11 | 1.84 | 0.58 |
| 21:AU:3:ILE:HD12 | 21:AU:3:ILE:N | 2.18 | 0.58 |
| 22:BA:13:G:C2' | 22:BA:14:U:H5' | 2.34 | 0.58 |
| 22:BA:15:A:OP2 | 22:BA:15:A:H3' | 2.03 | 0.58 |
| 23:BB:1172:C:H3' | 23:BB:1173:U:C5 | 2.38 | 0.58 |
| 23:BB:1400:U:H2' | 23:BB:1401:G:C8 | 2.38 | 0.58 |
| 23:BB:1785:A:H2' | 23:BB:1787:A:N7 | 2.18 | 0.58 |
| 23:BB:1882:U:O2' | 23:BB:1883:U:H5' | 2.04 | 0.58 |
| 23:BB:2241:A:H2' | 23:BB:2242:G:H8 | 1.65 | 0.58 |
| 23:BB:2633:G:H2' | 23:BB:2634:A:O4' | 2.03 | 0.58 |
| 23:BB:2804:U:H2' | 23:BB:2805:C:C6 | 2.38 | 0.58 |
| 28:BF:37:MET:HB2 | 28:BF:56:LEU:HD21 | 1.85 | 0.58 |
| 29:BG:2:ARG:H | 29:BG:5:LYS:HE2 | 1.67 | 0.58 |
| 29:BG:68:ARG:HH12 | 29:BG:72:ASN:HD22 | 1.51 | 0.58 |
| 31:BJ:57:LEU:HG | 31:BJ:128:ASN:H | 1.68 | 0.58 |
| 34:BM:60:GLN:HG2 | 34:BM:108:VAL:HG23 | 1.85 | 0.58 |
| 40:BS:1:MET:SD | 40:BS:62:ASP:HB2 | 2.43 | 0.58 |
| 41:BT:44:LYS:O | 41:BT:48:GLN:HG2 | 2.02 | 0.58 |
| 41:BT:50:LEU:C | 41:BT:52:GLU:H | 2.06 | 0.58 |
| 23:BB:470:A:N6 | 41:BT:72:GLN:HE22 | 1.93 | 0.58 |
| 43:BW:24:ARG:HD2 | 43:BW:25:PHE:N | 2.18 | 0.58 |
| 43:BW:17:ALA:HB1 | 43:BW:36:ILE:HA | 1.85 | 0.58 |
| 1:CA:1218:C:H2' | 1:CA:1219:A:C8 | 2.37 | 0.58 |
| 1:CA:268:U:H2' | 1:CA:269:C:C6 | 2.38 | 0.58 |
| 1:CA:555:U:H2' | 1:CA:556:C:H6 | 1.68 | 0.58 |
| 1:CA:685:G:O2' | 1:CA:686:U:H5' | 2.02 | 0.58 |
| 1:CA:845:A:H3' | 1:CA:846:G:C8 | 2.37 | 0.58 |
| 20:CB:15:PHE:O | 20:CB:40:ILE:HD12 | 2.03 | 0.58 |
| 3:CD:123:MET:HB2 | 3:CD:126:GLY:O | 2.03 | 0.58 |
| 5:CF:67:PRO:HG2 | 5:CF:70:VAL:HG22 | 1.85 | 0.58 |
| 8:CI:32:ARG:HH21 | 8:CI:36:GLN:HG3 | 1.68 | 0.58 |
| 11:CL:109:ARG:HB3 | 11:CL:118:VAL:HG21 | 1.85 | 0.58 |
| 23:DB:1281:G:H2' | 23:DB:1282:U:C6 | 2.37 | 0.58 |
| 23:DB:2884:U:H2' | 23:DB:2885:G:C8 | 2.38 | 0.58 |
| 23:DB:2897:U:H2' | 23:DB:2898:U:C6 | 2.38 | 0.58 |
| 23:DB:360:U:H2' | 23:DB:361:G:C1' | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:57:C:H2' | 23:DB:58:G:O4' | 2.03 | 0.58 |
| 23:DB:78:U:H2' | 23:DB:79:C:C6 | 2.38 | 0.58 |
| 25:DC:103:ILE:HG22 | 25:DC:105:ALA:H | 1.68 | 0.58 |
| 25:DC:196:ASN:HD22 | 25:DC:199:HIS:HB2 | 1.69 | 0.58 |
| 25:DC:75:ALA:HB2 | 25:DC:95:TYR:HA | 1.84 | 0.58 |
| 29:DG:83:THR:HA | 29:DG:84:LYS:NZ | 2.18 | 0.58 |
| 31:DJ:23:LYS:HE2 | 31:DJ:142:ILE:HA | 1.86 | 0.58 |
| 31:DJ:45:THR:N | 31:DJ:46:PRO:HD3 | 2.18 | 0.58 |
| 32:DK:2:ILE:HA | 32:DK:33:ALA:H | 1.68 | 0.58 |
| 23:DB:309:A:H4' | 42:DU:15:GLY:HA3 | 1.86 | 0.58 |
| 45:DY:40:THR:O | 45:DY:43:ILE:HG22 | 2.03 | 0.58 |
| 1:AA:1149:C:H2' | 1:AA:1150:A:C8 | 2.38 | 0.58 |
| 1:AA:93:U:O2' | 1:AA:94:G:H5' | 2.04 | 0.58 |
| 1:AA:625:U:H4' | 15:AP:16:PHE:CZ | 2.38 | 0.58 |
| 23:BB:1082:U:C2 | 23:BB:1086:A:C6 | 2.91 | 0.58 |
| 23:BB:1097:U:H2' | 23:BB:1098:A:H5' | 1.85 | 0.58 |
| 23:BB:1203:U:O4' | 33:BL:3:LEU:HD12 | 2.03 | 0.58 |
| 23:BB:1400:U:H2' | 23:BB:1401:G:H8 | 1.67 | 0.58 |
| 23:BB:182:A:H2' | 23:BB:183:C:C6 | 2.39 | 0.58 |
| 23:BB:2054:A:H2' | 47:B0:4:GLN:OE1 | 2.04 | 0.58 |
| 23:BB:57:C:H2' | 23:BB:58:G:O4' | 2.03 | 0.58 |
| 23:BB:947:A:H2' | 23:BB:948:C:C6 | 2.38 | 0.58 |
| 26:BD:117:GLY:O | 26:BD:164:GLN:HA | 2.03 | 0.58 |
| 31:BJ:16:TYR:O | 31:BJ:55:ILE:HG12 | 2.04 | 0.58 |
| 38:BQ:91:ARG:HH22 | 39:BR:10:LYS:HB3 | 1.67 | 0.58 |
| 42:BU:71:ILE:HD11 | 42:BU:82:VAL:HG22 | 1.85 | 0.58 |
| 1:CA:472:U:H2' | 1:CA:473:U:C6 | 2.39 | 0.58 |
| 1:CA:576:C:OP2 | 1:CA:576:C:H3' | 2.03 | 0.58 |
| 1:CA:742:G:H2' | 1:CA:743:A:H8 | 1.68 | 0.58 |
| 1:CA:746:A:H2' | 1:CA:747:A:C8 | 2.38 | 0.58 |
| 20:CB:117:GLU:HA | 20:CB:140:LEU:HD21 | 1.85 | 0.58 |
| 4:CE:82:HIS:HB2 | 4:CE:83:PRO:HD2 | 1.85 | 0.58 |
| 10:CK:16:SER:HA | 10:CK:77:GLY:O | 2.03 | 0.58 |
| 11:CL:35:ARG:HA | 11:CL:35:ARG:CZ | 2.34 | 0.58 |
| 14:CO:27:GLN:O | 14:CO:31:LEU:HD23 | 2.02 | 0.58 |
| 47:D0:53:VAL:O | 47:D0:54:ILE:HB | 2.04 | 0.58 |
| 23:DB:1018:U:O2' | 23:DB:1019:U:H5' | 2.02 | 0.58 |
| 23:DB:1092:C:H2' | 23:DB:1093:G:H5' | 1.86 | 0.58 |
| 23:DB:176:A:O2' | 23:DB:177:G:H5' | 2.03 | 0.58 |
| 23:DB:2331:G:N2 | 23:DB:2336:A:H8 | 2.00 | 0.58 |
| 23:DB:2472:G:O6 | 23:DB:2476:A:H4' | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2848:G:H22 | 23:DB:2867:G:N2 | 2.02 | 0.58 |
| 34:DM:19:GLY:N | 34:DM:38:ARG:HH22 | 2.01 | 0.58 |
| 34:DM:63:ILE:HD12 | 34:DM:63:ILE:H | 1.67 | 0.58 |
| 39:DR:28:ALA:O | 39:DR:63:VAL:HG21 | 2.03 | 0.58 |
| 24:DV:30:ILE:HG13 | 24:DV:40:ILE:HD12 | 1.83 | 0.58 |
| 43:DW:17:ALA:HB1 | 43:DW:36:ILE:HA | 1.85 | 0.58 |
| 45:DY:15:ARG:N | 45:DY:15:ARG:HD2 | 2.18 | 0.58 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.39 | 0.58 |
| 1:AA:1071:C:H2' | 1:AA:1072:G:H8 | 1.69 | 0.58 |
| 20:AB:172:ILE:HG22 | 20:AB:176:ASN:HD21 | 1.69 | 0.58 |
| 6:AG:14:ASP:CB | 6:AG:19:SER:H | 2.15 | 0.58 |
| 7:AH:17:GLN:HE21 | 7:AH:62:LEU:HB3 | 1.69 | 0.58 |
| 10:AK:70:ALA:C | 10:AK:72:ALA:H | 2.07 | 0.58 |
| 13:AN:9:GLU:HB2 | 13:AN:62:ARG:CZ | 2.33 | 0.58 |
| 18:AS:11:ASP:O | 18:AS:14:LEU:HG | 2.02 | 0.58 |
| 23:BB:1443:U:H2' | 23:BB:1444:G:H8 | 1.68 | 0.58 |
| 23:BB:2291:U:H2' | 23:BB:2292:U:C6 | 2.38 | 0.58 |
| 23:BB:2370:G:H2' | 23:BB:2371:G:O4' | 2.03 | 0.58 |
| 23:BB:65:U:H2' | 23:BB:66:C:C6 | 2.38 | 0.58 |
| 26:BD:179:ARG:HB2 | 26:BD:188:LEU:HD12 | 1.86 | 0.58 |
| 27:BE:137:LYS:HE2 | 27:BE:141:MET:SD | 2.43 | 0.58 |
| 30:BH:80:ILE:HD13 | 30:BH:99:ILE:HD13 | 1.84 | 0.58 |
| 32:BK:108:ARG:O | 32:BK:113:MET:HE3 | 2.04 | 0.58 |
| 1:CA:1008:U:H5'' | 13:CN:23:ARG:HH22 | 1.69 | 0.58 |
| 1:CA:390:U:H2' | 1:CA:391:G:C8 | 2.39 | 0.58 |
| 1:CA:728:A:H2' | 1:CA:729:A:C8 | 2.38 | 0.58 |
| 1:CA:620:C:O2 | 3:CD:131:ILE:HG21 | 2.03 | 0.58 |
| 7:CH:6:ILE:HB | 7:CH:76:ARG:NH1 | 2.18 | 0.58 |
| 22:DA:95:U:H2' | 22:DA:96:G:C8 | 2.39 | 0.58 |
| 23:DB:1381:G:C2' | 23:DB:1382:G:H5' | 2.33 | 0.58 |
| 23:DB:1485:U:H2' | 23:DB:1486:U:H6 | 1.69 | 0.58 |
| 23:DB:2144:G:O2' | 23:DB:2146:C:H5'' | 2.03 | 0.58 |
| 23:DB:2649:C:H2' | 23:DB:2650:U:C6 | 2.36 | 0.58 |
| 23:DB:654:A:H2' | 23:DB:655:A:H5'' | 1.84 | 0.58 |
| 25:DC:146:LYS:HB3 | 25:DC:147:PRO:CD | 2.28 | 0.58 |
| 26:DD:176:ASP:HB2 | 26:DD:190:LYS:HG2 | 1.85 | 0.58 |
| 27:DE:46:GLN:HG3 | 27:DE:87:ALA:HB3 | 1.85 | 0.58 |
| 38:DQ:65:ASN:CB | 38:DQ:75:TYR:HB2 | 2.32 | 0.58 |
| 38:DQ:79:ILE:O | 38:DQ:82:LEU:HB2 | 2.03 | 0.58 |
| 40:DS:18:ARG:HB3 | 40:DS:76:VAL:CG2 | 2.33 | 0.58 |
| 41:DT:57:VAL:HG13 | 41:DT:58:VAL:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DT:7:LEU:HA | 41:DT:9:LYS:NZ | 2.19 | 0.58 |
| 24:DV:70:ILE:HD13 | 24:DV:70:ILE:H | 1.69 | 0.58 |
| 46:DZ:70:GLU:O | 46:DZ:71:LEU:HB3 | 2.03 | 0.58 |
| 1:AA:1461:G:H2' | 1:AA:1462:C:H6 | 1.69 | 0.58 |
| 1:AA:352:C:H4' | 1:AA:354:G:OP1 | 2.03 | 0.58 |
| 1:AA:596:A:H2' | 1:AA:597:G:H8 | 1.69 | 0.58 |
| 20:AB:93:HIS:CD2 | 20:AB:145:ASN:HB3 | 2.39 | 0.58 |
| 6:AG:72:VAL:HG12 | 6:AG:89:GLU:HA | 1.85 | 0.58 |
| 7:AH:45:ILE:HG22 | 7:AH:62:LEU:HA | 1.86 | 0.58 |
| 10:AK:124:LYS:HA | 21:AU:34:ARG:CB | 2.33 | 0.58 |
| 14:AO:27:GLN:O | 14:AO:31:LEU:HD23 | 2.03 | 0.58 |
| 50:B3:30:HIS:O | 50:B3:31:ILE:HG12 | 2.02 | 0.58 |
| 23:BB:118:A:H5' | 23:BB:119:A:H8 | 1.68 | 0.58 |
| 23:BB:1550:C:H2' | 23:BB:1551:A:C8 | 2.39 | 0.58 |
| 23:BB:15:G:O2' | 23:BB:16:C:H5' | 2.03 | 0.58 |
| 23:BB:2820:A:OP1 | 35:BN:4:ARG:HA | 2.03 | 0.58 |
| 23:BB:443:A:C5 | 27:BE:40:ARG:HD3 | 2.38 | 0.58 |
| 23:BB:712:G:H2' | 23:BB:713:G:O4' | 2.04 | 0.58 |
| 23:BB:770:G:H5'' | 49:B2:10:LEU:HD12 | 1.84 | 0.58 |
| 27:BE:48:THR:HG22 | 27:BE:86:ALA:HB3 | 1.84 | 0.58 |
| 30:BH:89:LYS:HE3 | 30:BH:89:LYS:HA | 1.85 | 0.58 |
| 52:BI:27:LEU:H | 52:BI:27:LEU:CD2 | 2.15 | 0.58 |
| 31:BJ:57:LEU:HD21 | 31:BJ:128:ASN:HA | 1.86 | 0.58 |
| 34:BM:71:LYS:HG2 | 34:BM:73:ILE:HD11 | 1.85 | 0.58 |
| 44:BX:56:LEU:C | 44:BX:58:ASN:H | 2.06 | 0.58 |
| 45:BY:40:THR:O | 45:BY:43:ILE:HG22 | 2.03 | 0.58 |
| 1:CA:1090:U:H2' | 1:CA:1091:U:C6 | 2.37 | 0.58 |
| 1:CA:1461:G:H2' | 1:CA:1462:C:H6 | 1.68 | 0.58 |
| 1:CA:628:G:H2' | 1:CA:629:A:C8 | 2.38 | 0.58 |
| 1:CA:651:C:H2' | 1:CA:652:U:C6 | 2.39 | 0.58 |
| 1:CA:777:A:H2' | 1:CA:778:G:C8 | 2.37 | 0.58 |
| 1:CA:921:U:H2' | 1:CA:922:G:C8 | 2.38 | 0.58 |
| 1:CA:950:U:H2' | 1:CA:951:G:H8 | 1.68 | 0.58 |
| 20:CB:44:LYS:C | 20:CB:47:PRO:HD2 | 2.24 | 0.58 |
| 20:CB:80:LYS:HG3 | 20:CB:81:ASP:H | 1.69 | 0.58 |
| 5:CF:79:ARG:HH21 | 5:CF:87:SER:HB3 | 1.69 | 0.58 |
| 33:DL:51:GLU:HG2 | 50:D3:56:LEU:HD21 | 1.85 | 0.58 |
| 23:DB:1042:G:H2' | 23:DB:1043:C:C6 | 2.38 | 0.58 |
| 23:DB:1429:G:O2' | 23:DB:1430:G:H5' | 2.04 | 0.58 |
| 23:DB:1450:G:H21 | 23:DB:1452:G:H1 | 1.51 | 0.58 |
| 23:DB:1678:A:H2' | 23:DB:1679:A:H8 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:2377:A:H2' | 23:DB:2378:A:C8 | 2.39 | 0.58 |
| 23:DB:572:A:H5'' | 23:DB:573:U:OP2 | 2.03 | 0.58 |
| 25:DC:93:VAL:HG13 | 25:DC:94:LEU:N | 2.18 | 0.58 |
| 52:DI:121:ILE:CD1 | 52:DI:121:ILE:H | 2.14 | 0.58 |
| 34:DM:97:GLN:HB2 | 34:DM:98:PRO:HD2 | 1.85 | 0.58 |
| 1:AA:328:C:H4' | 1:AA:329:A:H5'' | 1.84 | 0.58 |
| 1:AA:472:U:H2' | 1:AA:473:U:C6 | 2.39 | 0.58 |
| 20:AB:23:ASN:HD22 | 20:AB:24:PRO:HD2 | 1.67 | 0.58 |
| 18:AS:27:LYS:NZ | 18:AS:27:LYS:HB3 | 2.19 | 0.58 |
| 47:B0:38:LEU:HB3 | 47:B0:41:HIS:CD2 | 2.38 | 0.58 |
| 23:BB:131:A:H2' | 23:BB:132:G:H8 | 1.69 | 0.58 |
| 23:BB:142:A:H2' | 23:BB:143:C:O4' | 2.02 | 0.58 |
| 23:BB:1458:U:H2' | 23:BB:1459:G:H5'' | 1.85 | 0.58 |
| 23:BB:1747:U:H2' | 23:BB:1748:C:C6 | 2.39 | 0.58 |
| 23:BB:2700:A:H2' | 23:BB:2701:U:H6 | 1.68 | 0.58 |
| 23:BB:414:C:H2' | 23:BB:415:A:H8 | 1.67 | 0.58 |
| 23:BB:593:U:H2' | 23:BB:594:U:C6 | 2.38 | 0.58 |
| 23:BB:857:G:O2' | 23:BB:858:G:H5' | 2.04 | 0.58 |
| 23:BB:877:A:H3' | 23:BB:899:A:N1 | 2.18 | 0.58 |
| 27:BE:5:LEU:HD12 | 27:BE:10:SER:HB2 | 1.86 | 0.58 |
| 32:BK:70:ARG:CB | 32:BK:76:VAL:HG22 | 2.34 | 0.58 |
| 33:BL:85:VAL:HG21 | 33:BL:94:THR:HB | 1.84 | 0.58 |
| 38:BQ:4:LYS:HE3 | 38:BQ:8:ILE:HD11 | 1.86 | 0.58 |
| 41:BT:18:GLU:C | 41:BT:20:ALA:H | 2.07 | 0.58 |
| 24:BV:53:LYS:HA | 24:BV:53:LYS:HE2 | 1.86 | 0.58 |
| 43:BW:23:LYS:HZ3 | 43:BW:24:ARG:HG3 | 1.68 | 0.58 |
| 43:BW:35:ILE:HG13 | 43:BW:57:THR:OG1 | 2.02 | 0.58 |
| 1:CA:1054:C:O2' | 1:CA:1055:A:H5'' | 2.04 | 0.58 |
| 1:CA:16:A:O2' | 1:CA:17:U:H5' | 2.03 | 0.58 |
| 20:CB:65:LYS:H | 20:CB:158:ASP:CG | 2.07 | 0.58 |
| 20:CB:217:ALA:O | 20:CB:221:ARG:HG2 | 2.03 | 0.58 |
| 3:CD:123:MET:SD | 3:CD:145:ARG:HD2 | 2.43 | 0.58 |
| 3:CD:22:SER:H | 3:CD:109:THR:HG22 | 1.68 | 0.58 |
| 12:CM:39:ALA:HB3 | 12:CM:42:VAL:HG13 | 1.86 | 0.58 |
| 13:CN:60:ARG:NE | 13:CN:62:ARG:HG2 | 2.19 | 0.58 |
| 49:D2:3:ARG:HE | 49:D2:4:THR:HG22 | 1.69 | 0.58 |
| 23:DB:124:G:O2' | 23:DB:125:A:H5'' | 2.04 | 0.58 |
| 23:DB:1407:G:H2' | 23:DB:1408:G:C8 | 2.39 | 0.58 |
| 23:DB:1487:U:H2' | 23:DB:1488:C:C6 | 2.38 | 0.58 |
| 23:DB:2054:A:H2' | 47:D0:4:GLN:OE1 | 2.03 | 0.58 |
| 23:DB:2346:A:H3' | 23:DB:2347:C:H5'' | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:248:G:H5' | 23:DB:250:G:N7 | 2.18 | 0.58 |
| 23:DB:2718:G:H4' | 37:DP:95:LYS:HB2 | 1.85 | 0.58 |
| 23:DB:370:G:O2' | 23:DB:423:A:H3' | 2.04 | 0.58 |
| 23:DB:532:A:H4' | 23:DB:533:G:C8 | 2.38 | 0.58 |
| 23:DB:929:U:O2 | 45:DY:25:GLY:HA2 | 2.02 | 0.58 |
| 25:DC:161:VAL:HG12 | 25:DC:162:GLN:N | 2.17 | 0.58 |
| 31:DJ:16:TYR:O | 31:DJ:55:ILE:HG12 | 2.03 | 0.58 |
| 23:DB:996:A:C4' | 38:DQ:91:ARG:HD2 | 2.31 | 0.58 |
| 39:DR:78:ARG:NH2 | 39:DR:78:ARG:HG3 | 2.18 | 0.58 |
| 1:AA:1250:A:H2' | 1:AA:1251:A:C8 | 2.39 | 0.58 |
| 1:AA:1338:G:H2' | 1:AA:1339:A:C8 | 2.39 | 0.58 |
| 1:AA:190:A:O5' | 1:AA:190:A:H8 | 1.87 | 0.58 |
| 1:AA:208:U:H4' | 1:AA:209:U:C5 | 2.38 | 0.58 |
| 1:AA:265:G:H2' | 1:AA:267:C:H5 | 1.68 | 0.58 |
| 1:AA:313:A:H2' | 1:AA:314:C:C6 | 2.39 | 0.58 |
| 1:AA:621:A:H2' | 1:AA:622:A:C8 | 2.38 | 0.58 |
| 20:AB:83:ALA:CB | 20:AB:90:PHE:HB3 | 2.34 | 0.58 |
| 2:AC:154:GLY:HA3 | 2:AC:162:ALA:HB1 | 1.86 | 0.58 |
| 2:AC:18:ASN:OD1 | 2:AC:53:ARG:HD2 | 2.04 | 0.58 |
| 3:AD:123:MET:HB2 | 3:AD:126:GLY:O | 2.04 | 0.58 |
| 3:AD:7:LYS:O | 3:AD:20:LEU:HD12 | 2.04 | 0.58 |
| 6:AG:65:LEU:O | 6:AG:69:ARG:HG3 | 2.04 | 0.58 |
| 10:AK:16:SER:HA | 10:AK:77:GLY:O | 2.02 | 0.58 |
| 12:AM:79:LEU:HD21 | 12:AM:86:ARG:HH21 | 1.67 | 0.58 |
| 23:BB:1203:U:H1' | 33:BL:4:ASN:ND2 | 2.06 | 0.58 |
| 23:BB:141:G:H5'' | 23:BB:142:A:C5 | 2.38 | 0.58 |
| 23:BB:2060:A:H62 | 27:BE:69:ARG:HH12 | 1.50 | 0.58 |
| 23:BB:279:A:N6 | 23:BB:361:G:H1' | 2.19 | 0.58 |
| 26:BD:34:VAL:CG1 | 26:BD:94:GLN:H | 2.15 | 0.58 |
| 30:BH:68:ARG:HH12 | 30:BH:110:VAL:HG12 | 1.68 | 0.58 |
| 31:BJ:13:ARG:HB3 | 31:BJ:53:TYR:HD2 | 1.68 | 0.58 |
| 1:CA:328:C:H4' | 1:CA:329:A:H5'' | 1.86 | 0.58 |
| 1:CA:922:G:H4' | 4:CE:24:VAL:HA | 1.84 | 0.58 |
| 1:CA:538:G:H5'' | 11:CL:110:LYS:HG2 | 1.84 | 0.58 |
| 13:CN:79:SER:OG | 13:CN:82:LYS:HG2 | 2.04 | 0.58 |
| 18:CS:62:THR:H | 18:CS:65:MET:HB2 | 1.69 | 0.58 |
| 48:D1:8:ILE:HD12 | 48:D1:51:ALA:HA | 1.85 | 0.58 |
| 49:D2:34:ARG:HE | 49:D2:39:ARG:HG2 | 1.69 | 0.58 |
| 23:DB:1882:U:O2' | 23:DB:1883:U:H5' | 2.04 | 0.58 |
| 23:DB:2271:G:H2' | 23:DB:2272:U:C6 | 2.39 | 0.58 |
| 23:DB:30:G:H2' | 23:DB:31:C:H6 | 1.66 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:352:A:H3' | 23:DB:353:C:C6 | 2.39 | 0.58 |
| 33:DL:116:VAL:HG13 | 33:DL:117:THR:N | 2.19 | 0.58 |
| 35:DN:9:GLN:O | 35:DN:11:ASN:N | 2.37 | 0.58 |
| 36:DO:55:GLU:HB2 | 36:DO:58:ILE:HD12 | 1.86 | 0.58 |
| 38:DQ:26:ALA:HB1 | 38:DQ:30:VAL:HB | 1.85 | 0.58 |
| 1:AA:1141:C:H2' | 1:AA:1142:G:C8 | 2.39 | 0.58 |
| 1:AA:60:A:H4' | 1:AA:61:G:OP1 | 2.03 | 0.58 |
| 20:AB:32:GLY:N | 20:AB:39:ILE:HB | 2.18 | 0.58 |
| 4:AE:125:LYS:HD2 | 4:AE:126:ALA:H | 1.69 | 0.58 |
| 12:AM:95:PRO:N | 12:AM:108:ARG:HG2 | 2.18 | 0.58 |
| 12:AM:2:ARG:HB2 | 12:AM:56:ARG:NH2 | 2.18 | 0.58 |
| 1:AA:276:G:H5' | 16:AQ:16:MET:SD | 2.44 | 0.58 |
| 17:AR:25:ILE:O | 17:AR:29:LYS:HG3 | 2.02 | 0.58 |
| 23:BB:1812:U:H1' | 25:BC:43:ASN:ND2 | 2.08 | 0.58 |
| 26:BD:36:GLN:HG3 | 26:BD:36:GLN:O | 2.02 | 0.58 |
| 28:BF:155:ILE:O | 28:BF:156:THR:HB | 2.03 | 0.58 |
| 29:BG:9:VAL:HA | 29:BG:48:THR:HG22 | 1.86 | 0.58 |
| 32:BK:70:ARG:HA | 32:BK:76:VAL:HA | 1.84 | 0.58 |
| 35:BN:9:GLN:O | 35:BN:11:ASN:N | 2.37 | 0.58 |
| 39:BR:78:ARG:NH2 | 39:BR:78:ARG:HG3 | 2.18 | 0.58 |
| 45:BY:35:VAL:HG22 | 45:BY:36:GLU:N | 2.16 | 0.58 |
| 1:CA:1448:C:H2' | 1:CA:1449:C:C6 | 2.38 | 0.58 |
| 1:CA:182:A:H1' | 1:CA:183:C:C5 | 2.38 | 0.58 |
| 1:CA:501:C:H2' | 1:CA:502:A:H8 | 1.68 | 0.58 |
| 20:CB:107:ARG:HA | 20:CB:110:ILE:HD12 | 1.86 | 0.58 |
| 20:CB:172:ILE:HG22 | 20:CB:176:ASN:HD21 | 1.69 | 0.58 |
| 2:CC:31:ASN:ND2 | 2:CC:58:ARG:HE | 2.01 | 0.58 |
| 23:DB:2144:G:O2' | 23:DB:2145:C:H5' | 2.03 | 0.58 |
| 23:DB:730:A:O2' | 23:DB:731:C:H5' | 2.04 | 0.58 |
| 23:DB:753:A:H2' | 23:DB:754:U:C6 | 2.39 | 0.58 |
| 23:DB:2052:A:O4' | 26:DD:147:GLY:HA3 | 2.04 | 0.58 |
| 30:DH:133:GLN:HB3 | 30:DH:139:PHE:CA | 2.32 | 0.58 |
| 33:DL:109:LYS:O | 33:DL:111:ILE:HG12 | 2.04 | 0.58 |
| 39:DR:34:GLU:HA | 39:DR:59:ILE:O | 2.03 | 0.58 |
| 46:DZ:40:VAL:HG22 | 46:DZ:45:ARG:H | 1.67 | 0.58 |
| 1:AA:1244:G:H2' | 1:AA:1245:C:C6 | 2.38 | 0.58 |
| 1:AA:1427:C:H2' | 1:AA:1428:A:C8 | 2.38 | 0.58 |
| 1:AA:950:U:H2' | 1:AA:951:G:H8 | 1.67 | 0.58 |
| 3:AD:77:GLU:O | 3:AD:81:LEU:HG | 2.04 | 0.58 |
| 3:AD:201:GLU:OE1 | 4:AE:104:ILE:HG22 | 2.04 | 0.58 |
| 4:AE:73:VAL:HB | 4:AE:75:LEU:HD21 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:AG:72:VAL:HA | 6:AG:89:GLU:HA | 1.86 | 0.58 |
| 8:AI:9:GLY:HA3 | 8:AI:81:GLY:H | 1.69 | 0.58 |
| 11:AL:13:ARG:CD | 11:AL:13:ARG:H | 2.16 | 0.58 |
| 1:AA:668:G:O2' | 14:AO:45:HIS:HB3 | 2.03 | 0.58 |
| 18:AS:24:SER:HB2 | 18:AS:27:LYS:HE3 | 1.86 | 0.58 |
| 23:BB:1353:A:H2' | 23:BB:1354:A:H8 | 1.69 | 0.58 |
| 23:BB:1355:G:O2' | 23:BB:1356:G:H5' | 2.03 | 0.58 |
| 23:BB:2015:A:C2 | 47:B0:2:VAL:HG22 | 2.38 | 0.58 |
| 23:BB:2031:A:C6 | 23:BB:2498:C:H1' | 2.38 | 0.58 |
| 25:BC:239:PHE:O | 25:BC:241:LYS:HG3 | 2.04 | 0.58 |
| 32:BK:88:ASN:HB3 | 32:BK:92:GLU:O | 2.03 | 0.58 |
| 40:BS:81:SER:HB3 | 40:BS:99:ARG:HB3 | 1.85 | 0.58 |
| 1:CA:518:C:H2' | 1:CA:530:G:H8 | 1.69 | 0.58 |
| 1:CA:580:C:H2' | 1:CA:581:G:O4' | 2.04 | 0.58 |
| 1:CA:747:A:H2' | 1:CA:748:G:O4' | 2.04 | 0.58 |
| 2:CC:13:ILE:H | 2:CC:13:ILE:HD13 | 1.68 | 0.58 |
| 2:CC:88:LYS:O | 2:CC:88:LYS:HE3 | 2.03 | 0.58 |
| 5:CF:98:GLU:HG2 | 5:CF:99:ALA:N | 2.19 | 0.58 |
| 19:CT:43:LYS:HE2 | 19:CT:44:ALA:N | 2.18 | 0.58 |
| 51:D4:7:VAL:HG13 | 51:D4:8:LYS:N | 2.19 | 0.58 |
| 23:DB:1054:A:H2' | 23:DB:1055:G:H8 | 1.67 | 0.58 |
| 23:DB:2194:U:H2' | 23:DB:2195:U:H6 | 1.69 | 0.58 |
| 23:DB:2291:U:H2' | 23:DB:2292:U:C6 | 2.39 | 0.58 |
| 23:DB:2563:U:H2' | 23:DB:2565:A:OP2 | 2.03 | 0.58 |
| 23:DB:2636:C:O5' | 26:DD:81:GLU:HB2 | 2.03 | 0.58 |
| 23:DB:2678:C:H2' | 23:DB:2679:A:H8 | 1.69 | 0.58 |
| 23:DB:322:A:H5' | 23:DB:340:A:C1' | 2.34 | 0.58 |
| 23:DB:609:A:H2' | 23:DB:610:C:O4' | 2.04 | 0.58 |
| 25:DC:239:PHE:O | 25:DC:241:LYS:HG3 | 2.04 | 0.58 |
| 27:DE:106:LYS:HE2 | 27:DE:200:LEU:HB3 | 1.86 | 0.58 |
| 28:DF:11:VAL:HG12 | 28:DF:12:VAL:N | 2.15 | 0.58 |
| 32:DK:88:ASN:HB3 | 32:DK:92:GLU:O | 2.03 | 0.58 |
| 34:DM:35:ALA:HB3 | 34:DM:99:GLY:N | 2.19 | 0.58 |
| 36:DO:35:ILE:CG1 | 36:DO:102:ARG:HE | 2.16 | 0.58 |
| 41:DT:11:LEU:HD22 | 41:DT:11:LEU:N | 2.15 | 0.58 |
| 41:DT:48:GLN:HA | 41:DT:48:GLN:HE21 | 1.69 | 0.58 |
| 41:DT:50:LEU:C | 41:DT:52:GLU:H | 2.06 | 0.58 |
| 46:DZ:65:ASP:HA | 46:DZ:68:LEU:HB2 | 1.85 | 0.58 |
| 1:AA:791:G:C6 | 1:AA:792:A:N7 | 2.72 | 0.57 |
| 1:AA:987:G:O2' | 1:AA:988:G:H5' | 2.03 | 0.57 |
| 20:AB:117:GLU:HA | 20:AB:140:LEU:HD21 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:AB:20:ARG:HA | 20:AB:38:HIS:HE1 | 1.68 | 0.57 |
| 1:AA:1057:G:H5'' | 2:AC:153:SER:HB2 | 1.86 | 0.57 |
| 5:AF:36:ILE:HG13 | 5:AF:64:VAL:HG13 | 1.86 | 0.57 |
| 17:AR:58:ILE:HD12 | 17:AR:58:ILE:H | 1.69 | 0.57 |
| 23:BB:1647:U:H3' | 23:BB:1647:U:P | 2.42 | 0.57 |
| 23:BB:2339:C:H2' | 23:BB:2340:A:C8 | 2.39 | 0.57 |
| 23:BB:2718:G:H4' | 37:BP:95:LYS:HB2 | 1.86 | 0.57 |
| 23:BB:2801:G:H3' | 23:BB:2802:G:H8 | 1.69 | 0.57 |
| 23:BB:572:A:H5'' | 23:BB:573:U:OP2 | 2.04 | 0.57 |
| 23:BB:693:A:OP1 | 25:BC:38:LYS:HG2 | 2.04 | 0.57 |
| 23:BB:709:U:H2' | 23:BB:710:U:C6 | 2.39 | 0.57 |
| 25:BC:146:LYS:HB3 | 25:BC:147:PRO:CD | 2.28 | 0.57 |
| 26:BD:105:LYS:HE3 | 26:BD:176:ASP:OD1 | 2.03 | 0.57 |
| 28:BF:66:ILE:HA | 28:BF:86:CYS:HB3 | 1.84 | 0.57 |
| 34:BM:4:PRO:HG2 | 34:BM:70:ASP:HA | 1.85 | 0.57 |
| 37:BP:6:GLN:HA | 37:BP:9:GLN:HG2 | 1.85 | 0.57 |
| 38:BQ:91:ARG:HH12 | 39:BR:10:LYS:CB | 2.17 | 0.57 |
| 39:BR:8:GLY:HA3 | 39:BR:23:GLU:HB2 | 1.86 | 0.57 |
| 40:BS:5:ALA:HB3 | 40:BS:54:ALA:HB2 | 1.86 | 0.57 |
| 1:CA:1004:A:N7 | 1:CA:1025:U:H1' | 2.19 | 0.57 |
| 1:CA:1343:G:H2' | 1:CA:1344:C:C6 | 2.39 | 0.57 |
| 1:CA:235:C:H2' | 1:CA:236:A:H8 | 1.67 | 0.57 |
| 1:CA:285:C:H2' | 1:CA:286:C:H6 | 1.68 | 0.57 |
| 1:CA:920:U:H2' | 1:CA:921:U:H6 | 1.69 | 0.57 |
| 1:CA:1160:G:H4' | 20:CB:130:LYS:CB | 2.34 | 0.57 |
| 3:CD:24:VAL:HG13 | 3:CD:160:LEU:HB3 | 1.86 | 0.57 |
| 3:CD:44:LYS:HD2 | 3:CD:46:ARG:HG2 | 1.86 | 0.57 |
| 7:CH:10:LEU:HD22 | 7:CH:74:ILE:HD11 | 1.86 | 0.57 |
| 8:CI:22:PRO:HA | 8:CI:60:LEU:HB2 | 1.87 | 0.57 |
| 11:CL:82:ARG:HG2 | 11:CL:82:ARG:HH11 | 1.68 | 0.57 |
| 19:CT:15:LYS:HA | 19:CT:15:LYS:HE2 | 1.84 | 0.57 |
| 19:CT:24:ARG:HD2 | 19:CT:28:ARG:NH2 | 2.19 | 0.57 |
| 50:D3:30:HIS:O | 50:D3:31:ILE:HG12 | 2.04 | 0.57 |
| 23:DB:1287:A:H3' | 23:DB:1288:G:H21 | 1.66 | 0.57 |
| 23:DB:1341:G:H3' | 23:DB:1397:U:O2 | 2.03 | 0.57 |
| 23:DB:1400:U:H2' | 23:DB:1401:G:C8 | 2.37 | 0.57 |
| 23:DB:182:A:H2' | 23:DB:183:C:C6 | 2.38 | 0.57 |
| 23:DB:833:A:H2' | 23:DB:834:G:C8 | 2.39 | 0.57 |
| 26:DD:136:ASN:OD1 | 26:DD:139:SER:HB2 | 2.04 | 0.57 |
| 29:DG:84:LYS:HG2 | 29:DG:85:LYS:N | 2.18 | 0.57 |
| 41:DT:11:LEU:HA | 41:DT:34:VAL:HG12 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:DW:23:LYS:HD2 | 43:DW:24:ARG:N | 2.19 | 0.57 |
| 43:DW:50:VAL:HG23 | 43:DW:61:LYS:HE3 | 1.86 | 0.57 |
| 1:AA:1091:U:H2' | 1:AA:1093:A:OP2 | 2.03 | 0.57 |
| 1:AA:285:C:H2' | 1:AA:286:C:H6 | 1.68 | 0.57 |
| 1:AA:518:C:H2' | 1:AA:530:G:H8 | 1.69 | 0.57 |
| 1:AA:638:U:H2' | 1:AA:639:G:O4' | 2.03 | 0.57 |
| 2:AC:33:ASP:O | 2:AC:37:LYS:HG3 | 2.04 | 0.57 |
| 10:AK:58:THR:HB | 10:AK:59:PRO:HD2 | 1.86 | 0.57 |
| 11:AL:3:VAL:O | 11:AL:7:VAL:HG23 | 2.04 | 0.57 |
| 12:AM:70:ARG:HH12 | 28:BF:112:ASP:CB | 2.13 | 0.57 |
| 21:AU:36:PHE:HA | 21:AU:39:LYS:HE2 | 1.85 | 0.57 |
| 48:B1:8:ILE:HD12 | 48:B1:51:ALA:HA | 1.86 | 0.57 |
| 51:B4:13:ASN:HB3 | 51:B4:28:SER:H | 1.69 | 0.57 |
| 23:BB:1857:G:H2' | 23:BB:1884:G:N2 | 2.19 | 0.57 |
| 23:BB:2149:U:O2' | 23:BB:2150:C:H5' | 2.04 | 0.57 |
| 23:BB:2393:U:O2' | 23:BB:2394:C:H5' | 2.04 | 0.57 |
| 25:BC:131:MET:HA | 25:BC:134:ILE:HG23 | 1.86 | 0.57 |
| 27:BE:155:GLU:HA | 27:BE:158:PHE:HB3 | 1.86 | 0.57 |
| 29:BG:84:LYS:HG2 | 29:BG:85:LYS:N | 2.17 | 0.57 |
| 33:BL:4:ASN:ND2 | 33:BL:4:ASN:N | 2.51 | 0.57 |
| 33:BL:57:LEU:HA | 33:BL:60:ARG:NH2 | 2.19 | 0.57 |
| 35:BN:7:GLY:HA2 | 35:BN:46:ARG:NH1 | 2.19 | 0.57 |
| 36:BO:88:LYS:HD2 | 36:BO:89:ASP:HB2 | 1.85 | 0.57 |
| 42:BU:40:LEU:HD23 | 42:BU:59:GLU:HG2 | 1.86 | 0.57 |
| 44:BX:19:LEU:O | 44:BX:24:GLU:HB2 | 2.03 | 0.57 |
| 1:CA:1004:A:H5' | 1:CA:1024:G:N2 | 2.18 | 0.57 |
| 1:CA:769:G:H4' | 1:CA:1513:A:H4' | 1.86 | 0.57 |
| 1:CA:777:A:H2' | 1:CA:778:G:H8 | 1.68 | 0.57 |
| 20:CB:110:ILE:HG23 | 20:CB:151:LYS:HA | 1.85 | 0.57 |
| 20:CB:112:ARG:HH11 | 20:CB:116:LEU:HG | 1.69 | 0.57 |
| 4:CE:11:GLN:HE22 | 4:CE:41:GLY:HA3 | 1.69 | 0.57 |
| 8:CI:18:VAL:HA | 8:CI:64:ILE:HG13 | 1.86 | 0.57 |
| 14:CO:43:ALA:O | 14:CO:46:LYS:HE3 | 2.04 | 0.57 |
| 21:CU:36:PHE:HB3 | 21:CU:39:LYS:HB2 | 1.86 | 0.57 |
| 22:DA:2:G:H2' | 22:DA:3:C:H6 | 1.65 | 0.57 |
| 23:DB:1164:C:H2' | 23:DB:1165:A:H8 | 1.69 | 0.57 |
| 23:DB:1260:A:H2' | 23:DB:1261:C:C6 | 2.39 | 0.57 |
| 23:DB:2194:U:H2' | 23:DB:2195:U:C6 | 2.39 | 0.57 |
| 23:DB:2369:A:O2' | 23:DB:2370:G:H5' | 2.04 | 0.57 |
| 23:DB:709:U:H2' | 23:DB:710:U:C6 | 2.39 | 0.57 |
| 25:DC:71:ASP:OD2 | 25:DC:118:GLY:HA2 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DD:34:VAL:CG1 | 26:DD:94:GLN:H | 2.17 | 0.57 |
| 28:DF:37:MET:CG | 28:DF:52:ALA:HB1 | 2.35 | 0.57 |
| 52:DI:99:LYS:HD3 | 52:DI:99:LYS:H | 1.69 | 0.57 |
| 31:DJ:45:THR:HG21 | 31:DJ:50:THR:HG21 | 1.85 | 0.57 |
| 32:DK:24:VAL:HG13 | 32:DK:33:ALA:HB2 | 1.85 | 0.57 |
| 23:DB:2723:C:H5' | 35:DN:1:MET:HE2 | 1.86 | 0.57 |
| 39:DR:4:VAL:CG2 | 39:DR:39:LEU:HG | 2.34 | 0.57 |
| 24:DV:53:LYS:HE2 | 24:DV:53:LYS:HA | 1.85 | 0.57 |
| 44:DX:45:GLN:O | 44:DX:47:ARG:N | 2.36 | 0.57 |
| 1:AA:476:U:O2' | 1:AA:477:C:H5' | 2.03 | 0.57 |
| 1:AA:678:U:H2' | 1:AA:679:C:H6 | 1.67 | 0.57 |
| 3:AD:77:GLU:HA | 3:AD:80:ARG:HG2 | 1.87 | 0.57 |
| 4:AE:39:GLY:HA2 | 4:AE:45:VAL:HA | 1.86 | 0.57 |
| 5:AF:79:ARG:HH21 | 5:AF:87:SER:HB3 | 1.69 | 0.57 |
| 12:AM:48:SER:O | 12:AM:52:ILE:HG22 | 2.05 | 0.57 |
| 12:AM:79:LEU:HD11 | 12:AM:86:ARG:HH21 | 1.68 | 0.57 |
| 23:BB:1429:G:H2' | 23:BB:1430:G:H8 | 1.68 | 0.57 |
| 23:BB:2621:G:P | 26:BD:124:ARG:HH22 | 2.27 | 0.57 |
| 23:BB:2813:A:H2' | 23:BB:2814:A:C8 | 2.39 | 0.57 |
| 23:BB:609:A:H2' | 23:BB:610:C:O4' | 2.04 | 0.57 |
| 23:BB:630:G:N2 | 23:BB:632:A:H3' | 2.18 | 0.57 |
| 25:BC:221:GLY:C | 25:BC:223:ALA:H | 2.07 | 0.57 |
| 27:BE:29:HIS:HA | 27:BE:32:VAL:HG22 | 1.87 | 0.57 |
| 28:BF:106:ALA:HA | 28:BF:135:ILE:HD13 | 1.86 | 0.57 |
| 30:BH:72:ILE:HG13 | 30:BH:75:LEU:HD11 | 1.85 | 0.57 |
| 33:BL:90:VAL:HB | 33:BL:122:VAL:HG13 | 1.86 | 0.57 |
| 36:BO:62:LEU:HD11 | 36:BO:70:ALA:HA | 1.86 | 0.57 |
| 38:BQ:71:ASN:HD22 | 38:BQ:73:ILE:HG22 | 1.69 | 0.57 |
| 40:BS:18:ARG:HB3 | 40:BS:76:VAL:HG22 | 1.86 | 0.57 |
| 41:BT:7:LEU:HA | 41:BT:9:LYS:NZ | 2.19 | 0.57 |
| 1:CA:1405:G:O2' | 1:CA:1406:U:H5' | 2.04 | 0.57 |
| 20:CB:58:LYS:NZ | 20:CB:58:LYS:HB3 | 2.19 | 0.57 |
| 2:CC:183:TYR:HA | 2:CC:199:VAL:O | 2.04 | 0.57 |
| 3:CD:201:GLU:OE1 | 4:CE:104:ILE:HG22 | 2.04 | 0.57 |
| 6:CG:64:ALA:HA | 6:CG:127:ALA:HA | 1.85 | 0.57 |
| 12:CM:48:SER:O | 12:CM:52:ILE:HG22 | 2.03 | 0.57 |
| 19:CT:68:LYS:HA | 19:CT:68:LYS:NZ | 2.19 | 0.57 |
| 23:DB:1166:G:H2' | 23:DB:1167:C:H6 | 1.67 | 0.57 |
| 23:DB:1923:U:H2' | 23:DB:1924:C:C6 | 2.39 | 0.57 |
| 23:DB:2393:U:O2' | 23:DB:2394:C:H5' | 2.04 | 0.57 |
| 23:DB:2784:U:H4' | 26:DD:42:ASN:O | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:553:G:O2' | 23:DB:554:U:H5' | 2.05 | 0.57 |
| 23:DB:947:A:H2' | 23:DB:948:C:H6 | 1.69 | 0.57 |
| 26:DD:117:GLY:O | 26:DD:164:GLN:HA | 2.05 | 0.57 |
| 26:DD:133:THR:HG23 | 26:DD:134:HIS:N | 2.19 | 0.57 |
| 26:DD:53:GLY:C | 26:DD:76:GLY:HA2 | 2.24 | 0.57 |
| 28:DF:74:ALA:HB1 | 28:DF:76:PHE:CD2 | 2.39 | 0.57 |
| 31:DJ:103:ILE:HA | 31:DJ:106:LYS:HB3 | 1.86 | 0.57 |
| 4:AE:93:VAL:HG13 | 4:AE:126:ALA:HB2 | 1.85 | 0.57 |
| 8:AI:19:PHE:O | 8:AI:62:LEU:HA | 2.04 | 0.57 |
| 47:B0:53:VAL:O | 47:B0:54:ILE:HB | 2.05 | 0.57 |
| 50:B3:22:LYS:HA | 50:B3:47:ALA:O | 2.05 | 0.57 |
| 23:BB:1139:G:O2' | 23:BB:1140:C:H5' | 2.05 | 0.57 |
| 23:BB:1347:A:H2' | 23:BB:1348:C:O4' | 2.04 | 0.57 |
| 23:BB:1513:U:O2' | 23:BB:1514:G:H5' | 2.03 | 0.57 |
| 23:BB:192:C:C2' | 23:BB:193:U:H5' | 2.34 | 0.57 |
| 23:BB:2199:A:H5'' | 23:BB:2200:C:H5 | 1.69 | 0.57 |
| 23:BB:2472:G:O6 | 23:BB:2476:A:H4' | 2.03 | 0.57 |
| 23:BB:364:C:H2' | 23:BB:365:U:H6 | 1.70 | 0.57 |
| 23:BB:83:A:H5'' | 42:BU:1:ALA:N | 2.19 | 0.57 |
| 26:BD:53:GLY:C | 26:BD:76:GLY:HA2 | 2.25 | 0.57 |
| 31:BJ:23:LYS:HE3 | 31:BJ:142:ILE:HG12 | 1.87 | 0.57 |
| 31:BJ:45:THR:N | 31:BJ:46:PRO:HD3 | 2.18 | 0.57 |
| 34:BM:97:GLN:HB2 | 34:BM:98:PRO:HD2 | 1.86 | 0.57 |
| 37:BP:112:ARG:HB2 | 37:BP:112:ARG:HH11 | 1.69 | 0.57 |
| 39:BR:4:VAL:HG23 | 39:BR:39:LEU:H | 1.69 | 0.57 |
| 42:BU:85:ARG:CD | 42:BU:86:PHE:H | 2.01 | 0.57 |
| 23:BB:2261:C:N4 | 43:BW:10:ARG:HB3 | 2.19 | 0.57 |
| 1:CA:1351:U:O2' | 1:CA:1352:C:H5' | 2.05 | 0.57 |
| 1:CA:709:U:H2' | 1:CA:710:G:H8 | 1.69 | 0.57 |
| 20:CB:93:HIS:CD2 | 20:CB:145:ASN:HB3 | 2.39 | 0.57 |
| 3:CD:84:ASN:ND2 | 3:CD:86:GLY:H | 2.03 | 0.57 |
| 12:CM:86:ARG:HA | 12:CM:96:VAL:HG11 | 1.87 | 0.57 |
| 18:CS:27:LYS:NZ | 18:CS:27:LYS:HB3 | 2.20 | 0.57 |
| 48:D1:34:GLU:HA | 48:D1:48:TYR:O | 2.04 | 0.57 |
| 23:DB:1240:U:O2' | 23:DB:1241:A:H5'' | 2.03 | 0.57 |
| 23:DB:1385:A:HO2' | 23:DB:1396:U:H6 | 1.53 | 0.57 |
| 23:DB:2150:C:H2' | 23:DB:2151:U:C6 | 2.39 | 0.57 |
| 23:DB:2187:U:H2' | 23:DB:2188:U:C6 | 2.40 | 0.57 |
| 23:DB:458:G:H22 | 23:DB:469:G:H2' | 1.67 | 0.57 |
| 23:DB:654:A:H2' | 23:DB:654:A:N3 | 2.18 | 0.57 |
| 23:DB:722:A:H2' | 23:DB:723:C:H6 | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:71:A:H5'' | 23:DB:73:A:C8 | 2.40 | 0.57 |
| 23:DB:828:U:H4' | 23:DB:831:G:N1 | 2.18 | 0.57 |
| 23:DB:971:G:H2' | 23:DB:972:A:O4' | 2.05 | 0.57 |
| 27:DE:155:GLU:HA | 27:DE:158:PHE:HB3 | 1.87 | 0.57 |
| 28:DF:64:PRO:HA | 28:DF:88:VAL:CG2 | 2.35 | 0.57 |
| 52:DI:108:ILE:HG22 | 52:DI:128:ILE:HD13 | 1.87 | 0.57 |
| 33:DL:30:THR:O | 33:DL:33:ARG:HG2 | 2.04 | 0.57 |
| 40:DS:66:ILE:HG12 | 40:DS:67:ASP:N | 2.20 | 0.57 |
| 44:DX:19:LEU:O | 44:DX:24:GLU:HB2 | 2.04 | 0.57 |
| 1:AA:451:A:H5' | 15:AP:70:ARG:NH2 | 2.18 | 0.57 |
| 1:AA:600:A:H2' | 1:AA:601:G:C8 | 2.39 | 0.57 |
| 2:AC:71:ARG:O | 2:AC:74:ILE:HG22 | 2.04 | 0.57 |
| 14:AO:78:THR:HA | 14:AO:81:ILE:HD12 | 1.86 | 0.57 |
| 21:AU:36:PHE:HB3 | 21:AU:39:LYS:HB2 | 1.87 | 0.57 |
| 23:BB:2539:C:H4' | 51:B4:36:ARG:NH2 | 2.20 | 0.57 |
| 23:BB:591:U:H1' | 50:B3:1:PRO:H3 | 1.68 | 0.57 |
| 25:BC:222:THR:HA | 25:BC:231:HIS:O | 2.03 | 0.57 |
| 35:BN:24:MET:HE1 | 35:BN:40:LYS:HD2 | 1.87 | 0.57 |
| 23:BB:335:C:H5'' | 42:BU:81:ARG:NH1 | 2.19 | 0.57 |
| 43:BW:18:LYS:HG3 | 43:BW:19:ARG:NE | 2.18 | 0.57 |
| 1:CA:1006:G:H2' | 1:CA:1007:U:H6 | 1.69 | 0.57 |
| 1:CA:1007:U:H2' | 1:CA:1008:U:C6 | 2.40 | 0.57 |
| 1:CA:1152:A:H2' | 1:CA:1153:G:C8 | 2.39 | 0.57 |
| 1:CA:1162:C:H2' | 1:CA:1163:A:C8 | 2.39 | 0.57 |
| 1:CA:1253:G:N1 | 1:CA:1285:A:N6 | 2.52 | 0.57 |
| 4:CE:39:GLY:HA2 | 4:CE:45:VAL:HA | 1.85 | 0.57 |
| 5:CF:29:ILE:HG23 | 5:CF:66:ALA:HB2 | 1.85 | 0.57 |
| 6:CG:78:ARG:HH11 | 6:CG:81:GLY:H | 1.50 | 0.57 |
| 9:CJ:40:ILE:HD12 | 9:CJ:73:LEU:HD12 | 1.87 | 0.57 |
| 12:CM:2:ARG:HB2 | 12:CM:56:ARG:NH2 | 2.16 | 0.57 |
| 12:CM:89:ARG:HD3 | 12:CM:95:PRO:O | 2.05 | 0.57 |
| 13:CN:16:ALA:HB2 | 13:CN:55:SER:N | 2.19 | 0.57 |
| 15:CP:68:SER:OG | 15:CP:71:VAL:HG12 | 2.04 | 0.57 |
| 18:CS:11:ASP:O | 18:CS:14:LEU:HG | 2.04 | 0.57 |
| 23:DB:2385:C:H2' | 23:DB:2386:A:H8 | 1.69 | 0.57 |
| 23:DB:2539:C:O2' | 23:DB:2540:C:H5' | 2.03 | 0.57 |
| 23:DB:2815:C:H2' | 23:DB:2816:G:C8 | 2.39 | 0.57 |
| 23:DB:784:G:H5'' | 25:DC:225:ASN:OD1 | 2.04 | 0.57 |
| 26:DD:179:ARG:HH11 | 26:DD:179:ARG:HB3 | 1.68 | 0.57 |
| 29:DG:116:LEU:HD23 | 29:DG:120:ILE:HD13 | 1.86 | 0.57 |
| 29:DG:30:GLY:CA | 29:DG:78:VAL:HA | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:DH:112:LYS:HA | 30:DH:132:PHE:CE1 | 2.39 | 0.57 |
| 36:DO:27:VAL:HG21 | 36:DO:40:ILE:HD12 | 1.86 | 0.57 |
| 40:DS:5:ALA:HB3 | 40:DS:54:ALA:HB2 | 1.86 | 0.57 |
| 44:DX:56:LEU:C | 44:DX:58:ASN:H | 2.08 | 0.57 |
| 1:AA:272:C:H2' | 1:AA:273:U:C6 | 2.39 | 0.57 |
| 1:AA:32:A:H2' | 1:AA:33:A:C8 | 2.38 | 0.57 |
| 1:AA:580:C:H2' | 1:AA:581:G:O4' | 2.05 | 0.57 |
| 1:AA:736:C:H2' | 1:AA:737:C:C6 | 2.40 | 0.57 |
| 1:AA:860:A:H2' | 1:AA:861:G:O4' | 2.05 | 0.57 |
| 1:AA:920:U:H2' | 1:AA:921:U:H6 | 1.68 | 0.57 |
| 8:AI:6:TYR:HB2 | 8:AI:19:PHE:CE1 | 2.39 | 0.57 |
| 10:AK:34:THR:HA | 10:AK:41:LEU:HG | 1.86 | 0.57 |
| 18:AS:43:MET:O | 18:AS:61:VAL:HB | 2.05 | 0.57 |
| 19:AT:15:LYS:HA | 19:AT:15:LYS:HE2 | 1.86 | 0.57 |
| 50:B3:7:ARG:O | 50:B3:11:LYS:HG3 | 2.04 | 0.57 |
| 22:BA:106:G:H2' | 22:BA:107:G:O4' | 2.05 | 0.57 |
| 22:BA:28:C:H2' | 22:BA:29:A:O4' | 2.04 | 0.57 |
| 22:BA:95:U:H2' | 22:BA:96:G:C8 | 2.39 | 0.57 |
| 23:BB:129:C:H2' | 23:BB:130:C:C6 | 2.37 | 0.57 |
| 23:BB:1567:G:H2' | 25:BC:84:PRO:HG3 | 1.87 | 0.57 |
| 23:BB:2264:C:H41 | 43:BW:11:ASN:ND2 | 2.03 | 0.57 |
| 23:BB:2772:C:H2' | 23:BB:2773:C:C6 | 2.40 | 0.57 |
| 23:BB:654:A:N3 | 23:BB:654:A:H2' | 2.20 | 0.57 |
| 23:BB:722:A:H2' | 23:BB:723:C:H6 | 1.68 | 0.57 |
| 23:BB:782:A:H5' | 23:BB:783:A:C2 | 2.40 | 0.57 |
| 25:BC:129:LEU:HD23 | 25:BC:130:PRO:CD | 2.33 | 0.57 |
| 25:BC:143:VAL:HB | 25:BC:153:LEU:HB2 | 1.87 | 0.57 |
| 25:BC:1:ALA:HB3 | 25:BC:19:VAL:HG23 | 1.85 | 0.57 |
| 26:BD:5:VAL:H | 26:BD:32:ASN:ND2 | 1.93 | 0.57 |
| 28:BF:74:ALA:HB1 | 28:BF:76:PHE:CD2 | 2.40 | 0.57 |
| 30:BH:133:GLN:HB2 | 30:BH:139:PHE:CA | 2.35 | 0.57 |
| 24:BV:70:ILE:H | 24:BV:70:ILE:HD13 | 1.69 | 0.57 |
| 1:CA:1173:U:H2' | 1:CA:1174:G:C8 | 2.39 | 0.57 |
| 1:CA:1213:A:O2' | 1:CA:1214:C:H5'' | 2.04 | 0.57 |
| 1:CA:1446:A:H2' | 1:CA:1447:A:H5'' | 1.87 | 0.57 |
| 1:CA:194:C:O2' | 1:CA:195:A:H5' | 2.04 | 0.57 |
| 1:CA:778:G:H2' | 1:CA:779:C:C6 | 2.40 | 0.57 |
| 1:CA:928:G:H2' | 1:CA:929:G:H8 | 1.69 | 0.57 |
| 3:CD:7:LYS:O | 3:CD:20:LEU:HD12 | 2.03 | 0.57 |
| 13:CN:60:ARG:HD3 | 13:CN:62:ARG:CZ | 2.35 | 0.57 |
| 23:DB:1429:G:H2' | 23:DB:1430:G:H8 | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1831:G:H2' | 23:DB:1832:C:C6 | 2.40 | 0.57 |
| 23:DB:2199:A:H5'' | 23:DB:2200:C:H5 | 1.70 | 0.57 |
| 23:DB:2700:A:H2' | 23:DB:2701:U:H6 | 1.70 | 0.57 |
| 23:DB:770:G:H5'' | 49:D2:10:LEU:HD12 | 1.86 | 0.57 |
| 23:DB:917:A:H2' | 23:DB:918:A:O4' | 2.05 | 0.57 |
| 27:DE:161:ALA:HA | 27:DE:164:LEU:HD12 | 1.86 | 0.57 |
| 31:DJ:57:LEU:HG | 31:DJ:128:ASN:H | 1.68 | 0.57 |
| 31:DJ:58:ASN:HA | 31:DJ:127:GLY:CA | 2.27 | 0.57 |
| 32:DK:105:ARG:HD2 | 32:DK:122:VAL:CG1 | 2.34 | 0.57 |
| 23:DB:566:U:H5'' | 33:DL:29:LYS:NZ | 2.19 | 0.57 |
| 33:DL:79:LEU:HB3 | 33:DL:115:GLU:O | 2.04 | 0.57 |
| 38:DQ:93:ILE:HG23 | 38:DQ:94:LEU:HD22 | 1.86 | 0.57 |
| 40:DS:18:ARG:HB3 | 40:DS:76:VAL:HG22 | 1.87 | 0.57 |
| 44:DX:56:LEU:O | 44:DX:57:LEU:HB3 | 2.04 | 0.57 |
| 46:DZ:20:HIS:O | 46:DZ:21:ALA:HB3 | 2.05 | 0.57 |
| 1:AA:1123:U:O2' | 1:AA:1124:G:H5' | 2.04 | 0.57 |
| 1:AA:1296:C:H4' | 1:AA:1302:C:C4 | 2.38 | 0.57 |
| 1:AA:1477:U:H2' | 1:AA:1478:U:H6 | 1.69 | 0.57 |
| 7:AH:24:VAL:HG12 | 7:AH:60:LEU:O | 2.04 | 0.57 |
| 10:AK:22:ILE:HD12 | 10:AK:84:MET:O | 2.03 | 0.57 |
| 10:AK:34:THR:HB | 10:AK:40:ALA:HA | 1.86 | 0.57 |
| 16:AQ:39:ARG:HH11 | 16:AQ:39:ARG:HG3 | 1.69 | 0.57 |
| 21:AU:28:LEU:HD23 | 21:AU:29:ALA:N | 2.19 | 0.57 |
| 22:BA:88:C:H2' | 22:BA:88:C:OP1 | 2.05 | 0.57 |
| 23:BB:1082:U:O4 | 23:BB:1086:A:C2 | 2.58 | 0.57 |
| 23:BB:1262:A:N3 | 47:B0:6:LYS:HE3 | 2.20 | 0.57 |
| 23:BB:2023:C:O2' | 23:BB:2024:G:H5' | 2.05 | 0.57 |
| 23:BB:2151:U:H2' | 23:BB:2152:G:H8 | 1.67 | 0.57 |
| 23:BB:2598:A:H5'' | 25:BC:233:GLY:HA2 | 1.87 | 0.57 |
| 23:BB:2678:C:H2' | 23:BB:2679:A:H8 | 1.69 | 0.57 |
| 23:BB:2899:A:H2' | 23:BB:2900:A:C8 | 2.39 | 0.57 |
| 23:BB:856:G:H2' | 23:BB:857:G:C8 | 2.39 | 0.57 |
| 25:BC:104:LEU:O | 25:BC:105:ALA:HB3 | 2.03 | 0.57 |
| 26:BD:34:VAL:HB | 26:BD:48:ILE:HD11 | 1.85 | 0.57 |
| 29:BG:10:VAL:O | 29:BG:10:VAL:HG12 | 2.05 | 0.57 |
| 30:BH:116:ARG:CB | 30:BH:116:ARG:HH11 | 2.15 | 0.57 |
| 41:BT:65:GLY:HA3 | 41:BT:76:ARG:HH22 | 1.70 | 0.57 |
| 44:BX:57:LEU:H | 44:BX:60:LYS:HG3 | 1.68 | 0.57 |
| 1:CA:1014:A:H4' | 18:CS:13:HIS:CE1 | 2.39 | 0.57 |
| 1:CA:1057:G:H5'' | 2:CC:153:SER:HB2 | 1.87 | 0.57 |
| 1:CA:1512:U:H2' | 1:CA:1513:A:H8 | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:CB:83:ALA:CB | 20:CB:90:PHE:HB3 | 2.34 | 0.57 |
| 9:CJ:80:THR:HG21 | 9:CJ:82:LYS:HZ2 | 1.70 | 0.57 |
| 18:CS:18:VAL:CG2 | 18:CS:43:MET:HG2 | 2.32 | 0.57 |
| 23:DB:1015:U:H2' | 23:DB:1016:G:H8 | 1.70 | 0.57 |
| 23:DB:1098:A:H3' | 52:DI:3:LYS:CB | 2.35 | 0.57 |
| 23:DB:1220:G:H2' | 23:DB:1221:C:H6 | 1.69 | 0.57 |
| 23:DB:1640:A:H2' | 23:DB:1641:A:C8 | 2.39 | 0.57 |
| 23:DB:1914:C:H2' | 23:DB:1915:U:C6 | 2.39 | 0.57 |
| 23:DB:2074:U:H2' | 23:DB:2075:U:C6 | 2.39 | 0.57 |
| 23:DB:2398:U:H2' | 23:DB:2399:G:H8 | 1.70 | 0.57 |
| 23:DB:2774:C:H2' | 23:DB:2775:G:O4' | 2.04 | 0.57 |
| 23:DB:573:U:O2' | 23:DB:574:A:H3' | 2.04 | 0.57 |
| 23:DB:820:A:H1' | 23:DB:943:A:O2' | 2.04 | 0.57 |
| 28:DF:30:VAL:HG21 | 28:DF:96:TRP:NE1 | 2.20 | 0.57 |
| 40:DS:29:VAL:HG23 | 40:DS:70:LYS:HA | 1.86 | 0.57 |
| 1:AA:1004:A:N7 | 1:AA:1025:U:H1' | 2.20 | 0.57 |
| 1:AA:336:A:O2' | 1:AA:337:G:H5' | 2.05 | 0.57 |
| 1:AA:518:C:H2' | 1:AA:530:G:C8 | 2.40 | 0.57 |
| 1:AA:545:C:H5'' | 3:AD:68:GLU:HG2 | 1.86 | 0.57 |
| 1:AA:923:A:H2' | 1:AA:924:C:C6 | 2.40 | 0.57 |
| 1:AA:437:U:H4' | 3:AD:153:ARG:NH1 | 2.20 | 0.57 |
| 4:AE:18:ASN:HB2 | 4:AE:33:THR:OG1 | 2.05 | 0.57 |
| 22:BA:54:G:H21 | 28:BF:25:MET:CE | 2.17 | 0.57 |
| 23:BB:1105:U:H2' | 23:BB:1106:G:H8 | 1.68 | 0.57 |
| 23:BB:1381:G:C2' | 23:BB:1382:G:H5' | 2.35 | 0.57 |
| 23:BB:2885:G:N2 | 47:B0:31:LYS:HG2 | 2.19 | 0.57 |
| 26:BD:13:ARG:HD2 | 37:BP:55:HIS:ND1 | 2.20 | 0.57 |
| 26:BD:46:ARG:NH1 | 26:BD:85:ALA:HA | 2.20 | 0.57 |
| 23:BB:2745:C:H4' | 29:BG:141:GLY:O | 2.05 | 0.57 |
| 32:BK:60:ALA:HA | 32:BK:87:LEU:CD2 | 2.34 | 0.57 |
| 33:BL:116:VAL:HG13 | 33:BL:117:THR:N | 2.19 | 0.57 |
| 33:BL:17:LYS:HD2 | 33:BL:19:LEU:HD11 | 1.86 | 0.57 |
| 42:BU:70:ALA:HB1 | 42:BU:79:ALA:HB2 | 1.87 | 0.57 |
| 24:BV:80:HIS:HD2 | 24:BV:82:TYR:H | 1.52 | 0.57 |
| 43:BW:35:ILE:O | 43:BW:36:ILE:C | 2.43 | 0.57 |
| 1:CA:1081:A:P | 4:CE:22:LYS:HB2 | 2.44 | 0.57 |
| 1:CA:1486:G:H2' | 1:CA:1487:G:O4' | 2.05 | 0.57 |
| 1:CA:1508:A:H2' | 1:CA:1509:C:C6 | 2.39 | 0.57 |
| 1:CA:505:G:H2' | 1:CA:506:G:H8 | 1.70 | 0.57 |
| 1:CA:881:G:P | 11:CL:8:ARG:HH12 | 2.27 | 0.57 |
| 2:CC:70:ALA:HA | 2:CC:105:VAL:CG2 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1379:G:N7 | 6:CG:2:ARG:CZ | 2.68 | 0.57 |
| 8:CI:19:PHE:O | 8:CI:62:LEU:HA | 2.04 | 0.57 |
| 23:DB:1098:A:P | 52:DI:3:LYS:HG2 | 2.44 | 0.57 |
| 23:DB:1684:G:H2' | 23:DB:1685:C:H6 | 1.68 | 0.57 |
| 23:DB:1714:U:H3' | 23:DB:1715:G:C5' | 2.35 | 0.57 |
| 23:DB:2094:A:H2' | 23:DB:2095:A:C8 | 2.39 | 0.57 |
| 23:DB:2728:U:H2' | 23:DB:2729:G:H8 | 1.68 | 0.57 |
| 23:DB:2801:G:H3' | 23:DB:2802:G:H8 | 1.69 | 0.57 |
| 23:DB:5:A:H2' | 23:DB:6:A:C8 | 2.40 | 0.57 |
| 23:DB:741:U:H2' | 23:DB:742:A:C8 | 2.40 | 0.57 |
| 23:DB:1490:A:H2' | 25:DC:97:ASP:OD1 | 2.04 | 0.57 |
| 23:DB:2786:U:C5' | 26:DD:70:LYS:HG3 | 2.34 | 0.57 |
| 29:DG:155:PRO:HA | 29:DG:170:THR:HA | 1.86 | 0.57 |
| 29:DG:9:VAL:HA | 29:DG:48:THR:HG22 | 1.85 | 0.57 |
| 30:DH:94:ILE:HG13 | 30:DH:98:ASP:CB | 2.34 | 0.57 |
| 31:DJ:15:TRP:HB3 | 31:DJ:137:PRO:HG3 | 1.87 | 0.57 |
| 38:DQ:91:ARG:HH22 | 39:DR:10:LYS:HB3 | 1.70 | 0.57 |
| 40:DS:41:LYS:NZ | 40:DS:41:LYS:HB3 | 2.20 | 0.57 |
| 42:DU:35:VAL:HB | 42:DU:38:ILE:HG21 | 1.85 | 0.57 |
| 1:AA:10:A:H2' | 1:AA:11:G:H8 | 1.69 | 0.57 |
| 1:AA:373:A:H1' | 1:AA:481:G:N3 | 2.20 | 0.57 |
| 1:AA:843:U:H5' | 1:AA:844:G:N7 | 2.20 | 0.57 |
| 10:AK:27:ASN:O | 10:AK:56:LYS:HE3 | 2.05 | 0.57 |
| 10:AK:14:GLN:HA | 10:AK:77:GLY:HA3 | 1.87 | 0.57 |
| 13:AN:71:GLY:O | 13:AN:79:SER:HA | 2.05 | 0.57 |
| 18:AS:14:LEU:O | 18:AS:18:VAL:HG12 | 2.05 | 0.57 |
| 23:BB:1842:G:H2' | 23:BB:1843:C:H6 | 1.69 | 0.57 |
| 23:BB:2078:C:O2' | 23:BB:2079:U:H5' | 2.05 | 0.57 |
| 23:BB:962:G:N2 | 23:BB:2250:G:H22 | 1.95 | 0.57 |
| 23:BB:2859:G:H2' | 23:BB:2860:A:C8 | 2.40 | 0.57 |
| 23:BB:2886:A:H3' | 23:BB:2887:A:C8 | 2.39 | 0.57 |
| 23:BB:522:A:H2' | 23:BB:523:C:C6 | 2.39 | 0.57 |
| 23:BB:718:A:H3' | 23:BB:719:C:C6 | 2.40 | 0.57 |
| 23:BB:1354:A:OP1 | 25:BC:35:LYS:HE2 | 2.05 | 0.57 |
| 26:BD:133:THR:HG23 | 26:BD:134:HIS:N | 2.18 | 0.57 |
| 27:BE:58:LYS:N | 27:BE:58:LYS:HD3 | 2.14 | 0.57 |
| 29:BG:116:LEU:HD23 | 29:BG:120:ILE:HD13 | 1.85 | 0.57 |
| 30:BH:121:VAL:HG22 | 30:BH:128:HIS:NE2 | 2.19 | 0.57 |
| 30:BH:77:THR:HG22 | 30:BH:79:THR:HG23 | 1.87 | 0.57 |
| 32:BK:54:LYS:HD2 | 32:BK:54:LYS:N | 2.19 | 0.57 |
| 33:BL:111:ILE:HG22 | 33:BL:112:LEU:N | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BM:54:THR:C | 34:BM:56:ALA:H | 2.08 | 0.57 |
| 38:BQ:56:PHE:HA | 38:BQ:59:LEU:HB3 | 1.86 | 0.57 |
| 39:BR:4:VAL:HG21 | 39:BR:39:LEU:HG | 1.85 | 0.57 |
| 24:BV:44:HIS:NE2 | 24:BV:85:LYS:HB2 | 2.20 | 0.57 |
| 46:BZ:35:SER:HA | 46:BZ:50:ARG:HA | 1.86 | 0.57 |
| 1:CA:1492:A:H5' | 1:CA:1493:A:OP2 | 2.05 | 0.57 |
| 1:CA:31:G:H5' | 1:CA:306:A:C2 | 2.40 | 0.57 |
| 1:CA:430:A:OP1 | 3:CD:8:LEU:HB2 | 2.03 | 0.57 |
| 1:CA:996:A:H2' | 1:CA:997:U:C6 | 2.40 | 0.57 |
| 3:CD:12:ARG:HA | 3:CD:33:ILE:HD12 | 1.87 | 0.57 |
| 8:CI:50:PRO:HB3 | 8:CI:83:THR:HB | 1.87 | 0.57 |
| 1:CA:275:G:H5' | 16:CQ:15:LYS:HD3 | 1.85 | 0.57 |
| 47:D0:38:LEU:HB3 | 47:D0:41:HIS:CD2 | 2.39 | 0.57 |
| 22:DA:88:C:H2' | 22:DA:88:C:OP1 | 2.05 | 0.57 |
| 23:DB:2008:C:H2' | 23:DB:2009:A:H8 | 1.70 | 0.57 |
| 23:DB:2353:G:H1' | 43:DW:30:VAL:HG12 | 1.87 | 0.57 |
| 23:DB:2385:C:H2' | 23:DB:2386:A:C8 | 2.40 | 0.57 |
| 23:DB:2460:U:H2' | 23:DB:2461:A:H8 | 1.70 | 0.57 |
| 23:DB:2488:G:O2' | 23:DB:2489:U:H5' | 2.05 | 0.57 |
| 23:DB:521:U:H2' | 23:DB:522:A:H8 | 1.69 | 0.57 |
| 25:DC:77:VAL:CG2 | 25:DC:112:GLY:H | 2.07 | 0.57 |
| 27:DE:2:GLU:HA | 27:DE:13:THR:OG1 | 2.05 | 0.57 |
| 34:DM:4:PRO:HG2 | 34:DM:70:ASP:HA | 1.85 | 0.57 |
| 34:DM:54:THR:C | 34:DM:56:ALA:H | 2.08 | 0.57 |
| 35:DN:72:ASP:OD1 | 35:DN:75:ILE:HG23 | 2.04 | 0.57 |
| 45:DY:5:LYS:HG3 | 45:DY:57:GLU:HB2 | 1.85 | 0.57 |
| 1:AA:1152:A:H2' | 1:AA:1153:G:C8 | 2.38 | 0.57 |
| 1:AA:272:C:H2' | 1:AA:273:U:H6 | 1.70 | 0.57 |
| 5:AF:67:PRO:HG2 | 5:AF:70:VAL:HG22 | 1.86 | 0.57 |
| 8:AI:113:LYS:HA | 8:AI:120:ALA:HB2 | 1.87 | 0.57 |
| 10:AK:86:LYS:HA | 10:AK:113:THR:OG1 | 2.05 | 0.57 |
| 12:AM:22:TYR:HB2 | 12:AM:65:GLU:HA | 1.86 | 0.57 |
| 23:BB:2398:U:H2' | 23:BB:2399:G:H8 | 1.69 | 0.57 |
| 23:BB:2615:U:C2 | 47:B0:3:GLN:HA | 2.40 | 0.57 |
| 23:BB:2897:U:H2' | 23:BB:2898:U:C6 | 2.40 | 0.57 |
| 23:BB:688:U:O2' | 23:BB:689:A:H5' | 2.05 | 0.57 |
| 23:BB:850:U:H2' | 23:BB:851:C:C6 | 2.39 | 0.57 |
| 28:BF:11:VAL:HG21 | 28:BF:172:PHE:CE1 | 2.40 | 0.57 |
| 30:BH:3:VAL:HG12 | 30:BH:38:PRO:HA | 1.86 | 0.57 |
| 30:BH:47:PHE:HA | 30:BH:50:ARG:HE | 1.70 | 0.57 |
| 34:BM:67:VAL:HG11 | 34:BM:102:LEU:HD22 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1038:C:H2' | 1:CA:1039:G:C8 | 2.40 | 0.57 |
| 1:CA:32:A:H2' | 1:CA:33:A:C8 | 2.39 | 0.57 |
| 1:CA:600:A:H2' | 1:CA:601:G:C8 | 2.39 | 0.57 |
| 5:CF:92:THR:HG22 | 5:CF:93:LYS:N | 2.19 | 0.57 |
| 6:CG:25:PHE:HZ | 6:CG:119:LEU:HD11 | 1.70 | 0.57 |
| 7:CH:45:ILE:HG22 | 7:CH:62:LEU:HA | 1.87 | 0.57 |
| 18:CS:1:PRO:O | 18:CS:2:ARG:HB2 | 2.05 | 0.57 |
| 23:DB:1338:G:H4' | 41:DT:18:GLU:CG | 2.24 | 0.57 |
| 23:DB:2064:C:H2' | 23:DB:2065:C:H6 | 1.70 | 0.57 |
| 23:DB:2439:A:N7 | 23:DB:2586:U:H4' | 2.20 | 0.57 |
| 23:DB:2875:C:H2' | 23:DB:2876:G:H8 | 1.70 | 0.57 |
| 23:DB:523:C:H4' | 23:DB:540:C:O2 | 2.04 | 0.57 |
| 23:DB:845:A:N1 | 23:DB:847:U:H1' | 2.20 | 0.57 |
| 23:DB:850:U:H2' | 23:DB:851:C:C6 | 2.40 | 0.57 |
| 25:DC:66:PHE:HB2 | 25:DC:150:GLY:O | 2.05 | 0.57 |
| 31:DJ:13:ARG:HB3 | 31:DJ:53:TYR:HD2 | 1.68 | 0.57 |
| 42:DU:43:LYS:O | 42:DU:57:ILE:HA | 2.04 | 0.57 |
| 23:DB:2355:G:O3' | 43:DW:20:LEU:HD13 | 2.05 | 0.57 |
| 1:AA:1054:C:O2' | 1:AA:1055:A:H5'' | 2.05 | 0.56 |
| 1:AA:624:C:H2' | 1:AA:625:U:H6 | 1.70 | 0.56 |
| 2:AC:149:LYS:HB2 | 2:AC:168:ARG:HG3 | 1.87 | 0.56 |
| 11:AL:7:VAL:HG22 | 16:AQ:33:TYR:HD1 | 1.70 | 0.56 |
| 23:BB:1316:U:O2' | 23:BB:1317:G:H5' | 2.05 | 0.56 |
| 23:BB:1508:A:H5' | 23:BB:1509:A:C6 | 2.40 | 0.56 |
| 23:BB:1553:A:O2' | 23:BB:1554:U:H2' | 2.05 | 0.56 |
| 23:BB:2258:C:O2' | 23:BB:2426:A:H4' | 2.05 | 0.56 |
| 23:BB:2392:A:N3 | 23:BB:2392:A:H2' | 2.19 | 0.56 |
| 23:BB:2516:A:O2' | 23:BB:2517:C:H5' | 2.05 | 0.56 |
| 23:BB:2774:C:H2' | 23:BB:2775:G:O4' | 2.05 | 0.56 |
| 23:BB:296:U:H2' | 23:BB:297:G:H8 | 1.70 | 0.56 |
| 25:BC:75:ALA:O | 25:BC:114:GLN:HA | 2.05 | 0.56 |
| 28:BF:12:VAL:O | 28:BF:16:MET:HG2 | 2.05 | 0.56 |
| 29:BG:26:LYS:HG2 | 29:BG:27:GLY:H | 1.70 | 0.56 |
| 30:BH:79:THR:HG22 | 30:BH:145:ASN:CG | 2.25 | 0.56 |
| 32:BK:2:ILE:HA | 32:BK:33:ALA:H | 1.68 | 0.56 |
| 41:BT:54:GLU:HG3 | 41:BT:90:GLY:N | 2.20 | 0.56 |
| 23:BB:988:A:C8 | 45:BY:13:ILE:HD12 | 2.39 | 0.56 |
| 45:BY:29:ARG:H | 45:BY:33:HIS:HD2 | 1.53 | 0.56 |
| 1:CA:1294:G:H2' | 1:CA:1295:U:C6 | 2.40 | 0.56 |
| 1:CA:253:A:H2' | 1:CA:254:G:H8 | 1.69 | 0.56 |
| 1:CA:975:A:H4' | 1:CA:976:G:O5' | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:CB:140:LEU:HD12 | 20:CB:140:LEU:H | 1.68 | 0.56 |
| 2:CC:71:ARG:O | 2:CC:74:ILE:HG22 | 2.05 | 0.56 |
| 3:CD:100:VAL:O | 3:CD:104:MET:HG3 | 2.04 | 0.56 |
| 6:CG:65:LEU:O | 6:CG:69:ARG:HG3 | 2.05 | 0.56 |
| 10:CK:58:THR:HB | 10:CK:59:PRO:HD2 | 1.87 | 0.56 |
| 23:DB:1518:C:H2' | 23:DB:1519:G:H8 | 1.69 | 0.56 |
| 23:DB:2189:U:H2' | 23:DB:2190:G:O4' | 2.05 | 0.56 |
| 23:DB:548:G:C2' | 23:DB:548:G:N3 | 2.68 | 0.56 |
| 25:DC:222:THR:HA | 25:DC:231:HIS:O | 2.03 | 0.56 |
| 25:DC:226:PRO:CG | 25:DC:233:GLY:H | 2.17 | 0.56 |
| 27:DE:5:LEU:HB2 | 27:DE:11:ALA:N | 2.20 | 0.56 |
| 29:DG:25:ILE:HG22 | 29:DG:78:VAL:HG21 | 1.87 | 0.56 |
| 32:DK:13:ASN:ND2 | 32:DK:98:ARG:H | 1.99 | 0.56 |
| 46:DZ:40:VAL:CG2 | 46:DZ:43:GLU:HB3 | 2.31 | 0.56 |
| 1:AA:1417:G:H22 | 1:AA:1482:G:H2' | 1.70 | 0.56 |
| 1:AA:82:G:H1' | 1:AA:89:U:O2 | 2.06 | 0.56 |
| 1:AA:811:C:H4' | 1:AA:900:A:N6 | 2.20 | 0.56 |
| 20:AB:40:ILE:HD13 | 20:AB:201:GLY:HA2 | 1.88 | 0.56 |
| 6:AG:129:ASN:ND2 | 6:AG:137:ARG:HH22 | 2.03 | 0.56 |
| 7:AH:124:ILE:HG22 | 7:AH:125:ILE:N | 2.19 | 0.56 |
| 8:AI:50:PRO:HB3 | 8:AI:83:THR:HB | 1.86 | 0.56 |
| 22:BA:54:G:H21 | 28:BF:25:MET:HE3 | 1.69 | 0.56 |
| 23:BB:1018:U:O2' | 23:BB:1019:U:H5' | 2.05 | 0.56 |
| 23:BB:1056:G:H4' | 23:BB:1086:A:H8 | 1.69 | 0.56 |
| 23:BB:570:G:H2' | 23:BB:2030:A:N7 | 2.20 | 0.56 |
| 23:BB:2298:A:OP1 | 28:BF:70:ARG:HD3 | 2.05 | 0.56 |
| 23:BB:2303:G:H4' | 28:BF:121:PHE:O | 2.05 | 0.56 |
| 23:BB:2468:A:H2' | 23:BB:2476:A:C6 | 2.40 | 0.56 |
| 23:BB:2439:A:N7 | 23:BB:2586:U:H4' | 2.20 | 0.56 |
| 23:BB:477:A:H2' | 23:BB:478:A:C8 | 2.40 | 0.56 |
| 23:BB:974:G:OP2 | 39:BR:78:ARG:HD3 | 2.05 | 0.56 |
| 23:BB:1790:C:O2' | 25:BC:207:ALA:HB2 | 2.04 | 0.56 |
| 27:BE:192:ALA:HA | 27:BE:195:GLN:NE2 | 2.19 | 0.56 |
| 38:BQ:105:PHE:O | 38:BQ:109:VAL:HG23 | 2.05 | 0.56 |
| 24:BV:7:GLU:O | 24:BV:41:GLU:HG2 | 2.05 | 0.56 |
| 1:CA:1338:G:H2' | 1:CA:1339:A:C8 | 2.40 | 0.56 |
| 1:CA:1450:U:H2' | 1:CA:1452:C:C5 | 2.40 | 0.56 |
| 1:CA:920:U:O2' | 1:CA:1081:A:H4' | 2.05 | 0.56 |
| 2:CC:8:GLY:HA2 | 2:CC:11:LEU:HG | 1.87 | 0.56 |
| 3:CD:29:THR:HG22 | 3:CD:30:LYS:N | 2.20 | 0.56 |
| 3:CD:77:GLU:HA | 3:CD:80:ARG:HG2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:CN:50:LEU:N | 13:CN:51:PRO:HD2 | 2.20 | 0.56 |
| 16:CQ:37:ILE:HG22 | 16:CQ:38:LYS:H | 1.70 | 0.56 |
| 23:DB:1355:G:O2' | 23:DB:1356:G:H5' | 2.04 | 0.56 |
| 23:DB:1406:U:H2' | 23:DB:1407:G:H8 | 1.68 | 0.56 |
| 23:DB:1567:G:H2' | 25:DC:84:PRO:HG3 | 1.87 | 0.56 |
| 23:DB:1597:A:H5'' | 23:DB:1598:A:H5' | 1.85 | 0.56 |
| 23:DB:15:G:O2' | 23:DB:16:C:H5' | 2.04 | 0.56 |
| 23:DB:1785:A:H2' | 23:DB:1787:A:N7 | 2.20 | 0.56 |
| 23:DB:2141:G:H2' | 23:DB:2142:A:H8 | 1.69 | 0.56 |
| 23:DB:286:U:H2' | 23:DB:287:G:C8 | 2.39 | 0.56 |
| 23:DB:601:C:H2' | 23:DB:602:A:H8 | 1.70 | 0.56 |
| 25:DC:131:MET:HA | 25:DC:134:ILE:HG23 | 1.86 | 0.56 |
| 25:DC:221:GLY:C | 25:DC:223:ALA:H | 2.08 | 0.56 |
| 25:DC:243:PRO:O | 25:DC:250:GLN:HA | 2.04 | 0.56 |
| 35:DN:59:SER:O | 35:DN:63:ARG:HB2 | 2.05 | 0.56 |
| 37:DP:112:ARG:HB2 | 37:DP:112:ARG:HH11 | 1.70 | 0.56 |
| 40:DS:81:SER:HB3 | 40:DS:99:ARG:HB3 | 1.86 | 0.56 |
| 41:DT:69:ARG:HA | 41:DT:69:ARG:CZ | 2.36 | 0.56 |
| 42:DU:85:ARG:NE | 42:DU:85:ARG:HA | 2.20 | 0.56 |
| 24:DV:63:ILE:N | 24:DV:63:ILE:HD12 | 2.21 | 0.56 |
| 1:AA:1078:U:H2' | 1:AA:1079:G:O4' | 2.05 | 0.56 |
| 1:AA:1317:C:OP1 | 13:AN:56:PRO:HD2 | 2.05 | 0.56 |
| 1:AA:190:A:H2' | 1:AA:191:G:O4' | 2.05 | 0.56 |
| 1:AA:505:G:H2' | 1:AA:506:G:H8 | 1.68 | 0.56 |
| 1:AA:90:C:H2' | 1:AA:91:U:C6 | 2.40 | 0.56 |
| 4:AE:56:PRO:HG2 | 4:AE:57:ALA:H | 1.70 | 0.56 |
| 4:AE:82:HIS:CD2 | 7:AH:95:MET:HG3 | 2.41 | 0.56 |
| 51:B4:13:ASN:O | 51:B4:27:CYS:HA | 2.04 | 0.56 |
| 23:BB:1709:U:H2' | 23:BB:1710:G:H8 | 1.71 | 0.56 |
| 23:BB:1923:U:H2' | 23:BB:1924:C:C6 | 2.40 | 0.56 |
| 23:BB:2645:G:H3' | 23:BB:2646:C:C5' | 2.32 | 0.56 |
| 23:BB:2774:C:OP1 | 26:BD:169:ARG:HG3 | 2.05 | 0.56 |
| 23:BB:286:U:H2' | 23:BB:287:G:H8 | 1.69 | 0.56 |
| 23:BB:523:C:H4' | 23:BB:540:C:O2 | 2.05 | 0.56 |
| 25:BC:75:ALA:CB | 25:BC:95:TYR:HA | 2.35 | 0.56 |
| 36:BO:35:ILE:CG1 | 36:BO:102:ARG:HE | 2.17 | 0.56 |
| 40:BS:48:LYS:HE2 | 40:BS:52:GLU:OE1 | 2.05 | 0.56 |
| 42:BU:95:PHE:CE1 | 42:BU:102:ILE:HB | 2.39 | 0.56 |
| 46:BZ:65:ASP:HA | 46:BZ:68:LEU:HB2 | 1.86 | 0.56 |
| 1:CA:1320:C:H42 | 18:CS:35:ARG:HD3 | 1.70 | 0.56 |
| 1:CA:352:C:H4' | 1:CA:354:G:OP1 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CE:125:LYS:HD2 | 4:CE:126:ALA:H | 1.69 | 0.56 |
| 4:CE:140:ILE:HG22 | 4:CE:144:GLU:OE1 | 2.06 | 0.56 |
| 4:CE:61:LYS:O | 4:CE:65:LYS:HG2 | 2.05 | 0.56 |
| 9:CJ:53:ILE:CG2 | 9:CJ:61:ALA:HB1 | 2.36 | 0.56 |
| 10:CK:34:THR:HA | 10:CK:41:LEU:HG | 1.87 | 0.56 |
| 15:CP:40:ASN:ND2 | 15:CP:42:ILE:H | 2.04 | 0.56 |
| 15:CP:74:LEU:O | 15:CP:78:VAL:HG12 | 2.05 | 0.56 |
| 21:CU:24:LYS:NZ | 21:CU:25:ALA:H | 1.98 | 0.56 |
| 23:DB:1061:U:H4' | 23:DB:1070:A:O3' | 2.04 | 0.56 |
| 23:DB:53:A:N6 | 23:DB:117:G:H1' | 2.21 | 0.56 |
| 23:DB:1965:C:H5'' | 23:DB:1966:A:H2' | 1.87 | 0.56 |
| 23:DB:2088:A:H2' | 23:DB:2089:C:H6 | 1.71 | 0.56 |
| 23:DB:2137:U:O2' | 23:DB:2138:G:H5' | 2.04 | 0.56 |
| 23:DB:455:C:N3 | 23:DB:473:G:H5' | 2.21 | 0.56 |
| 26:DD:12:THR:HG22 | 26:DD:13:ARG:H | 1.69 | 0.56 |
| 28:DF:11:VAL:HG21 | 28:DF:172:PHE:CE1 | 2.40 | 0.56 |
| 52:DI:37:PHE:CZ | 52:DI:58:ILE:HD11 | 2.40 | 0.56 |
| 27:DE:117:ARG:NH1 | 33:DL:2:ARG:HB2 | 2.20 | 0.56 |
| 33:DL:3:LEU:O | 33:DL:5:THR:N | 2.39 | 0.56 |
| 35:DN:102:PHE:N | 35:DN:109:PRO:HA | 2.17 | 0.56 |
| 40:DS:48:LYS:HE2 | 40:DS:52:GLU:OE1 | 2.04 | 0.56 |
| 23:DB:483:A:H4' | 42:DU:45:GLN:O | 2.05 | 0.56 |
| 24:DV:44:HIS:NE2 | 24:DV:85:LYS:HB2 | 2.19 | 0.56 |
| 1:AA:1296:C:H4' | 1:AA:1302:C:N4 | 2.21 | 0.56 |
| 1:AA:922:G:N3 | 1:AA:1398:A:H2 | 2.03 | 0.56 |
| 1:AA:390:U:H2' | 1:AA:391:G:C8 | 2.40 | 0.56 |
| 1:AA:734:G:H21 | 17:AR:63:TYR:HE1 | 1.53 | 0.56 |
| 6:AG:145:GLU:HA | 6:AG:148:LYS:HB2 | 1.86 | 0.56 |
| 8:AI:27:ILE:HG21 | 8:AI:34:LEU:HD13 | 1.88 | 0.56 |
| 9:AJ:40:ILE:HB | 9:AJ:73:LEU:HB3 | 1.87 | 0.56 |
| 23:BB:2714:G:O2' | 23:BB:2715:C:H5' | 2.06 | 0.56 |
| 23:BB:2720:U:H5'' | 37:BP:52:ARG:NH2 | 2.20 | 0.56 |
| 23:BB:898:C:H2' | 23:BB:899:A:C4 | 2.41 | 0.56 |
| 23:BB:784:G:H5'' | 25:BC:225:ASN:OD1 | 2.05 | 0.56 |
| 23:BB:2485:G:H5'' | 34:BM:125:PRO:HG3 | 1.87 | 0.56 |
| 38:BQ:79:ILE:HD13 | 38:BQ:79:ILE:O | 2.06 | 0.56 |
| 39:BR:4:VAL:CG2 | 39:BR:39:LEU:HG | 2.35 | 0.56 |
| 24:BV:9:ARG:NH2 | 24:BV:12:GLN:HA | 2.19 | 0.56 |
| 1:CA:1512:U:H2' | 1:CA:1513:A:C8 | 2.40 | 0.56 |
| 1:CA:251:G:H1 | 1:CA:271:C:H41 | 1.53 | 0.56 |
| 1:CA:518:C:H2' | 1:CA:530:G:C8 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:6:PRO:HA | 2:CC:9:ILE:HG22 | 1.88 | 0.56 |
| 8:CI:10:ARG:HB3 | 8:CI:15:ALA:HA | 1.87 | 0.56 |
| 11:CL:20:VAL:HB | 11:CL:94:TYR:CE1 | 2.40 | 0.56 |
| 23:DB:1438:U:H2' | 23:DB:1439:A:O4' | 2.06 | 0.56 |
| 23:DB:1709:U:H2' | 23:DB:1710:G:C8 | 2.40 | 0.56 |
| 23:DB:570:G:H2' | 23:DB:2030:A:N7 | 2.19 | 0.56 |
| 23:DB:2081:U:OP1 | 46:DZ:19:SER:HB3 | 2.05 | 0.56 |
| 23:DB:21:A:H2' | 23:DB:22:C:C6 | 2.40 | 0.56 |
| 23:DB:857:G:C2' | 23:DB:858:G:H5' | 2.34 | 0.56 |
| 23:DB:899:A:H3' | 23:DB:900:A:H8 | 1.70 | 0.56 |
| 25:DC:161:VAL:O | 25:DC:162:GLN:HB2 | 2.04 | 0.56 |
| 27:DE:5:LEU:HD12 | 27:DE:10:SER:HB2 | 1.87 | 0.56 |
| 23:DB:659:G:H21 | 27:DE:30:GLN:NE2 | 2.03 | 0.56 |
| 23:DB:1080:A:H4' | 52:DI:126:ARG:CD | 2.34 | 0.56 |
| 32:DK:118:LEU:O | 32:DK:120:PRO:HD2 | 2.04 | 0.56 |
| 35:DN:96:ARG:HG2 | 35:DN:96:ARG:HH21 | 1.71 | 0.56 |
| 40:DS:1:MET:SD | 40:DS:62:ASP:HB2 | 2.45 | 0.56 |
| 43:DW:35:ILE:O | 43:DW:36:ILE:C | 2.43 | 0.56 |
| 23:DB:2336:A:H61 | 43:DW:40:ARG:CG | 2.19 | 0.56 |
| 1:AA:224:U:H2' | 1:AA:225:C:C6 | 2.39 | 0.56 |
| 1:AA:33:A:H2' | 1:AA:34:C:H6 | 1.70 | 0.56 |
| 1:AA:505:G:H4' | 1:AA:534:U:C4 | 2.40 | 0.56 |
| 1:AA:1058:G:OP1 | 2:AC:198:LYS:HE3 | 2.05 | 0.56 |
| 12:AM:43:LYS:H | 12:AM:43:LYS:HD2 | 1.70 | 0.56 |
| 13:AN:79:SER:OG | 13:AN:82:LYS:HG2 | 2.05 | 0.56 |
| 15:AP:40:ASN:ND2 | 15:AP:42:ILE:H | 2.04 | 0.56 |
| 23:BB:1291:C:O2' | 23:BB:1292:G:H5' | 2.06 | 0.56 |
| 23:BB:1579:A:H2' | 23:BB:1580:A:C8 | 2.40 | 0.56 |
| 23:BB:633:A:O5' | 23:BB:633:A:H8 | 1.89 | 0.56 |
| 23:BB:5:A:H2' | 23:BB:6:A:C8 | 2.41 | 0.56 |
| 23:BB:828:U:H4' | 23:BB:831:G:N1 | 2.19 | 0.56 |
| 25:BC:36:ASN:HD21 | 25:BC:85:ASN:HD21 | 1.53 | 0.56 |
| 25:BC:43:ASN:HB3 | 25:BC:45:ASN:HD22 | 1.70 | 0.56 |
| 25:BC:43:ASN:HB3 | 25:BC:45:ASN:ND2 | 2.21 | 0.56 |
| 29:BG:10:VAL:HG13 | 29:BG:16:VAL:HG21 | 1.87 | 0.56 |
| 29:BG:19:ASN:HB2 | 29:BG:22:VAL:HB | 1.87 | 0.56 |
| 52:BI:58:ILE:N | 52:BI:58:ILE:HD12 | 2.20 | 0.56 |
| 31:BJ:58:ASN:HA | 31:BJ:127:GLY:CA | 2.26 | 0.56 |
| 22:BA:50:A:OP1 | 36:BO:68:LYS:HG3 | 2.04 | 0.56 |
| 38:BQ:71:ASN:HD21 | 38:BQ:109:VAL:HG11 | 1.70 | 0.56 |
| 40:BS:28:LYS:HD2 | 40:BS:29:VAL:N | 2.19 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BU:81:ARG:HB2 | 42:BU:96:LYS:HG3 | 1.86 | 0.56 |
| 1:CA:1004:A:C8 | 1:CA:1025:U:H1' | 2.40 | 0.56 |
| 1:CA:1250:A:H4' | 8:CI:69:GLY:O | 2.06 | 0.56 |
| 1:CA:135:C:O2 | 15:CP:1:MET:HB2 | 2.06 | 0.56 |
| 1:CA:313:A:H2' | 1:CA:314:C:C6 | 2.41 | 0.56 |
| 2:CC:149:LYS:HB2 | 2:CC:168:ARG:HG3 | 1.87 | 0.56 |
| 2:CC:33:ASP:O | 2:CC:37:LYS:HG3 | 2.05 | 0.56 |
| 8:CI:109:GLN:NE2 | 8:CI:110:VAL:H | 2.03 | 0.56 |
| 8:CI:18:VAL:HG13 | 8:CI:64:ILE:HG13 | 1.87 | 0.56 |
| 9:CJ:55:PRO:HA | 13:CN:80:ARG:NH2 | 2.20 | 0.56 |
| 50:D3:3:ILE:HG21 | 50:D3:62:PRO:HG2 | 1.88 | 0.56 |
| 51:D4:13:ASN:O | 51:D4:27:CYS:HA | 2.06 | 0.56 |
| 51:D4:13:ASN:HB3 | 51:D4:28:SER:H | 1.69 | 0.56 |
| 23:DB:1796:U:H2' | 23:DB:1797:G:C8 | 2.40 | 0.56 |
| 23:DB:2370:G:H2' | 23:DB:2371:G:O4' | 2.05 | 0.56 |
| 23:DB:2469:A:H2' | 23:DB:2470:G:O4' | 2.04 | 0.56 |
| 23:DB:2849:U:N3 | 23:DB:2867:G:C8 | 2.74 | 0.56 |
| 31:DJ:124:VAL:O | 31:DJ:125:TYR:HB2 | 2.04 | 0.56 |
| 35:DN:7:GLY:HA2 | 35:DN:46:ARG:NH1 | 2.19 | 0.56 |
| 1:AA:1004:A:H5' | 1:AA:1024:G:N2 | 2.20 | 0.56 |
| 1:AA:555:U:H2' | 1:AA:556:C:H6 | 1.70 | 0.56 |
| 1:AA:975:A:H4' | 1:AA:976:G:O5' | 2.04 | 0.56 |
| 20:AB:58:LYS:NZ | 20:AB:58:LYS:HB3 | 2.20 | 0.56 |
| 4:AE:19:ARG:HH11 | 4:AE:28:ARG:HH22 | 1.53 | 0.56 |
| 7:AH:13:ILE:HD11 | 7:AH:60:LEU:HD21 | 1.87 | 0.56 |
| 1:AA:135:C:O2 | 15:AP:1:MET:HB2 | 2.04 | 0.56 |
| 50:B3:3:ILE:HG21 | 50:B3:62:PRO:HG2 | 1.86 | 0.56 |
| 22:BA:76:G:O2' | 22:BA:77:U:H5' | 2.06 | 0.56 |
| 23:BB:1518:C:H2' | 23:BB:1519:G:H8 | 1.70 | 0.56 |
| 23:BB:1838:C:N4 | 23:BB:1898:U:H2' | 2.21 | 0.56 |
| 23:BB:2895:G:H2' | 23:BB:2896:C:H6 | 1.68 | 0.56 |
| 23:BB:664:G:H2' | 23:BB:665:U:C6 | 2.40 | 0.56 |
| 26:BD:178:VAL:O | 26:BD:180:VAL:HG23 | 2.06 | 0.56 |
| 29:BG:146:ASP:O | 29:BG:150:TYR:HD1 | 1.89 | 0.56 |
| 30:BH:81:ALA:HA | 30:BH:147:VAL:N | 2.20 | 0.56 |
| 30:BH:31:VAL:CB | 30:BH:32:PRO:CD | 2.82 | 0.56 |
| 32:BK:10:VAL:HG21 | 32:BK:16:ALA:HA | 1.86 | 0.56 |
| 34:BM:63:ILE:H | 34:BM:63:ILE:HD12 | 1.69 | 0.56 |
| 38:BQ:71:ASN:ND2 | 38:BQ:109:VAL:HG11 | 2.20 | 0.56 |
| 1:CA:230:G:H2' | 1:CA:231:U:O4' | 2.06 | 0.56 |
| 1:CA:370:C:H2' | 1:CA:371:A:H8 | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CE:28:ARG:NH1 | 4:CE:30:PHE:HB3 | 2.21 | 0.56 |
| 13:CN:71:GLY:O | 13:CN:79:SER:HA | 2.05 | 0.56 |
| 23:DB:1098:A:C8 | 52:DI:3:LYS:HB3 | 2.40 | 0.56 |
| 23:DB:1259:G:H2' | 23:DB:1260:A:H8 | 1.69 | 0.56 |
| 23:DB:1501:G:O2' | 23:DB:1502:A:H5' | 2.05 | 0.56 |
| 28:DF:90:LEU:HD12 | 28:DF:95:MET:HA | 1.86 | 0.56 |
| 29:DG:132:LEU:HD23 | 29:DG:132:LEU:N | 2.21 | 0.56 |
| 29:DG:84:LYS:HG3 | 29:DG:132:LEU:N | 2.20 | 0.56 |
| 31:DJ:23:LYS:HE3 | 31:DJ:142:ILE:HG12 | 1.87 | 0.56 |
| 31:DJ:56:VAL:HG12 | 31:DJ:57:LEU:N | 2.21 | 0.56 |
| 33:DL:122:VAL:HG12 | 33:DL:143:GLU:OE2 | 2.06 | 0.56 |
| 38:DQ:94:LEU:C | 38:DQ:96:ASP:H | 2.09 | 0.56 |
| 1:AA:1347:G:H22 | 1:AA:1373:G:H2' | 1.71 | 0.56 |
| 1:AA:1508:A:H2' | 1:AA:1509:C:H6 | 1.70 | 0.56 |
| 1:AA:562:U:OP2 | 1:AA:562:U:H2' | 2.05 | 0.56 |
| 1:AA:672:U:H2' | 1:AA:673:A:C8 | 2.40 | 0.56 |
| 1:AA:777:A:H2' | 1:AA:778:G:C8 | 2.40 | 0.56 |
| 1:AA:824:G:O2' | 1:AA:825:A:H5' | 2.05 | 0.56 |
| 20:AB:145:ASN:N | 20:AB:145:ASN:ND2 | 2.53 | 0.56 |
| 1:AA:933:G:N7 | 6:AG:2:ARG:NH1 | 2.54 | 0.56 |
| 11:AL:122:LYS:HD2 | 11:AL:123:ALA:H | 1.69 | 0.56 |
| 19:AT:85:LEU:HD23 | 19:AT:86:ALA:N | 2.21 | 0.56 |
| 22:BA:49:C:H2' | 22:BA:50:A:H8 | 1.71 | 0.56 |
| 23:BB:2704:C:H2' | 23:BB:2705:A:O4' | 2.06 | 0.56 |
| 27:BE:3:LEU:H | 27:BE:13:THR:H | 1.53 | 0.56 |
| 52:BI:75:ALA:HB2 | 52:BI:112:LYS:HE2 | 1.85 | 0.56 |
| 32:BK:24:VAL:HG13 | 32:BK:33:ALA:HB2 | 1.88 | 0.56 |
| 35:BN:49:GLU:HA | 35:BN:94:TYR:HD2 | 1.70 | 0.56 |
| 46:BZ:77:LYS:O | 46:BZ:78:TYR:HB3 | 2.05 | 0.56 |
| 1:CA:1250:A:H2' | 1:CA:1251:A:C8 | 2.40 | 0.56 |
| 1:CA:1349:A:H2' | 1:CA:1350:A:O4' | 2.05 | 0.56 |
| 1:CA:1508:A:H2' | 1:CA:1509:C:H6 | 1.70 | 0.56 |
| 1:CA:546:A:OP1 | 3:CD:69:ARG:HB2 | 2.05 | 0.56 |
| 1:CA:811:C:H4' | 1:CA:900:A:N6 | 2.21 | 0.56 |
| 4:CE:152:VAL:O | 4:CE:156:ARG:HG2 | 2.05 | 0.56 |
| 22:DA:76:G:O2' | 22:DA:77:U:H5' | 2.05 | 0.56 |
| 23:DB:1476:U:H4' | 23:DB:1732:C:O2' | 2.05 | 0.56 |
| 23:DB:2415:G:H2' | 23:DB:2416:C:C6 | 2.40 | 0.56 |
| 23:DB:642:U:O2 | 23:DB:644:A:H3' | 2.05 | 0.56 |
| 23:DB:782:A:N3 | 25:DC:224:MET:HB3 | 2.21 | 0.56 |
| 26:DD:79:LEU:HD22 | 26:DD:79:LEU:N | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:DH:90:LEU:HD22 | 30:DH:122:LEU:O | 2.06 | 0.56 |
| 33:DL:78:ARG:HG2 | 33:DL:113:ALA:HB2 | 1.86 | 0.56 |
| 33:DL:17:LYS:HD2 | 33:DL:19:LEU:HD11 | 1.88 | 0.56 |
| 33:DL:57:LEU:HA | 33:DL:60:ARG:NH2 | 2.21 | 0.56 |
| 38:DQ:56:PHE:HA | 38:DQ:59:LEU:HB3 | 1.87 | 0.56 |
| 42:DU:12:VAL:HG22 | 42:DU:69:VAL:HG12 | 1.88 | 0.56 |
| 42:DU:17:ASP:HB3 | 42:DU:20:LYS:HE3 | 1.87 | 0.56 |
| 1:AA:1332:A:H2' | 1:AA:1333:A:H8 | 1.69 | 0.56 |
| 1:AA:1351:U:O2' | 1:AA:1352:C:H5' | 2.05 | 0.56 |
| 3:AD:40:HIS:HB3 | 3:AD:43:ARG:HG2 | 1.87 | 0.56 |
| 23:BB:1119:U:OP1 | 24:BV:83:LYS:HE3 | 2.05 | 0.56 |
| 23:BB:1640:A:H2' | 23:BB:1641:A:C8 | 2.40 | 0.56 |
| 23:BB:2567:G:H2' | 23:BB:2568:U:C6 | 2.41 | 0.56 |
| 23:BB:2815:C:H2' | 23:BB:2816:G:C8 | 2.40 | 0.56 |
| 23:BB:2841:C:H2' | 23:BB:2842:G:H8 | 1.71 | 0.56 |
| 23:BB:823:C:O2' | 23:BB:824:U:H5' | 2.05 | 0.56 |
| 23:BB:857:G:C2' | 23:BB:858:G:H5' | 2.36 | 0.56 |
| 26:BD:136:ASN:OD1 | 26:BD:139:SER:HB2 | 2.06 | 0.56 |
| 27:BE:21:ARG:HG3 | 27:BE:22:ASP:N | 2.21 | 0.56 |
| 30:BH:68:ARG:HB2 | 30:BH:134:VAL:CG2 | 2.34 | 0.56 |
| 52:BI:105:LEU:HD11 | 52:BI:139:VAL:CG1 | 2.36 | 0.56 |
| 33:BL:85:VAL:CG2 | 33:BL:94:THR:HB | 2.35 | 0.56 |
| 44:BX:23:ARG:HA | 44:BX:27:ASN:ND2 | 2.20 | 0.56 |
| 1:CA:314:C:O2' | 1:CA:315:A:H5' | 2.06 | 0.56 |
| 1:CA:474:G:H2' | 1:CA:475:C:C6 | 2.41 | 0.56 |
| 1:CA:778:G:H2' | 1:CA:779:C:H6 | 1.70 | 0.56 |
| 4:CE:148:SER:OG | 4:CE:151:MET:HB2 | 2.06 | 0.56 |
| 6:CG:78:ARG:HG2 | 6:CG:83:THR:HG22 | 1.86 | 0.56 |
| 1:CA:1329:A:OP1 | 12:CM:28:ARG:HB2 | 2.06 | 0.56 |
| 13:CN:9:GLU:HB2 | 13:CN:62:ARG:CZ | 2.35 | 0.56 |
| 18:CS:11:ASP:H | 18:CS:14:LEU:HD21 | 1.70 | 0.56 |
| 23:DB:106:C:H2' | 23:DB:107:G:C8 | 2.41 | 0.56 |
| 23:DB:1747:U:H2' | 23:DB:1748:C:C6 | 2.41 | 0.56 |
| 23:DB:184:C:H2' | 23:DB:185:G:H8 | 1.70 | 0.56 |
| 23:DB:2389:G:H5'' | 23:DB:2390:U:H5' | 1.88 | 0.56 |
| 23:DB:2412:A:H2' | 23:DB:2413:G:O4' | 2.06 | 0.56 |
| 23:DB:845:A:C2 | 23:DB:847:U:H1' | 2.41 | 0.56 |
| 23:DB:871:U:H2' | 23:DB:872:U:C6 | 2.39 | 0.56 |
| 23:DB:996:A:H4' | 38:DQ:91:ARG:CD | 2.32 | 0.56 |
| 26:DD:8:LYS:CG | 26:DD:197:THR:H | 2.19 | 0.56 |
| 27:DE:192:ALA:HA | 27:DE:195:GLN:NE2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DE:40:ARG:NH2 | 27:DE:92:HIS:NE2 | 2.54 | 0.56 |
| 36:DO:52:SER:OG | 36:DO:54:VAL:HG12 | 2.05 | 0.56 |
| 39:DR:31:GLU:H | 39:DR:63:VAL:CG2 | 2.18 | 0.56 |
| 39:DR:79:ARG:NE | 39:DR:80:ARG:HH21 | 2.04 | 0.56 |
| 43:DW:36:ILE:HB | 43:DW:39:GLN:NE2 | 2.21 | 0.56 |
| 1:AA:1171:A:H2' | 1:AA:1172:C:C6 | 2.40 | 0.56 |
| 3:AD:44:LYS:HD2 | 3:AD:46:ARG:HG2 | 1.88 | 0.56 |
| 6:AG:25:PHE:HZ | 6:AG:119:LEU:HD11 | 1.71 | 0.56 |
| 8:AI:126:PHE:O | 8:AI:128:LYS:N | 2.39 | 0.56 |
| 13:AN:63:CYS:HB3 | 13:AN:67:GLY:N | 2.20 | 0.56 |
| 49:B2:31:LEU:HD22 | 49:B2:42:LEU:HD12 | 1.88 | 0.56 |
| 23:BB:1778:U:H2' | 23:BB:1784:A:N6 | 2.20 | 0.56 |
| 23:BB:1821:A:H2' | 23:BB:1822:C:C6 | 2.41 | 0.56 |
| 23:BB:2145:C:O4' | 23:BB:2145:C:O2 | 2.23 | 0.56 |
| 23:BB:2415:G:H2' | 23:BB:2416:C:C6 | 2.40 | 0.56 |
| 23:BB:2860:A:O5' | 23:BB:2860:A:H8 | 1.87 | 0.56 |
| 23:BB:71:A:H5'' | 23:BB:73:A:C8 | 2.41 | 0.56 |
| 25:BC:196:ASN:HD22 | 25:BC:199:HIS:HB2 | 1.69 | 0.56 |
| 27:BE:97:ASN:ND2 | 27:BE:100:MET:HG3 | 2.21 | 0.56 |
| 33:BL:92:LEU:HD21 | 33:BL:123:ARG:NH1 | 2.20 | 0.56 |
| 34:BM:103:TYR:O | 34:BM:104:GLU:HG3 | 2.05 | 0.56 |
| 42:BU:43:LYS:O | 42:BU:57:ILE:HA | 2.06 | 0.56 |
| 45:BY:37:ARG:HG3 | 45:BY:38:GLU:OE1 | 2.05 | 0.56 |
| 46:BZ:70:GLU:O | 46:BZ:71:LEU:HB3 | 2.06 | 0.56 |
| 1:CA:1021:A:H2' | 1:CA:1022:A:O4' | 2.06 | 0.56 |
| 1:CA:1091:U:H2' | 1:CA:1093:A:OP2 | 2.05 | 0.56 |
| 1:CA:215:C:H2' | 1:CA:216:U:C6 | 2.41 | 0.56 |
| 1:CA:264:C:O2' | 16:CQ:65:PRO:HG2 | 2.06 | 0.56 |
| 20:CB:145:ASN:N | 20:CB:145:ASN:ND2 | 2.54 | 0.56 |
| 3:CD:88:ASN:O | 3:CD:92:LEU:HD23 | 2.05 | 0.56 |
| 4:CE:82:HIS:CD2 | 7:CH:95:MET:HG3 | 2.41 | 0.56 |
| 6:CG:144:ALA:O | 6:CG:146:ALA:N | 2.37 | 0.56 |
| 13:CN:63:CYS:HB3 | 13:CN:67:GLY:N | 2.20 | 0.56 |
| 51:D4:2:LYS:HG2 | 51:D4:3:VAL:N | 2.21 | 0.56 |
| 23:DB:1351:C:H2' | 23:DB:1352:U:O4' | 2.05 | 0.56 |
| 23:DB:1857:G:H2' | 23:DB:1884:G:N2 | 2.21 | 0.56 |
| 23:DB:2339:C:H2' | 23:DB:2340:A:C8 | 2.40 | 0.56 |
| 23:DB:781:A:OP1 | 25:DC:216:ARG:NH2 | 2.39 | 0.56 |
| 29:DG:10:VAL:HG13 | 29:DG:16:VAL:HG21 | 1.88 | 0.56 |
| 35:DN:103:ARG:CG | 35:DN:104:ALA:H | 2.19 | 0.56 |
| 46:DZ:35:SER:HA | 46:DZ:50:ARG:HA | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1534:A:H3' | 1:AA:1534:A:N3 | 2.21 | 0.56 |
| 1:AA:45:G:H2' | 1:AA:46:G:H8 | 1.71 | 0.56 |
| 1:AA:576:C:OP2 | 1:AA:576:C:H3' | 2.06 | 0.56 |
| 1:AA:715:A:H2' | 1:AA:716:A:C8 | 2.41 | 0.56 |
| 20:AB:114:LYS:HE2 | 20:AB:151:LYS:HZ1 | 1.71 | 0.56 |
| 20:AB:112:ARG:HH11 | 20:AB:116:LEU:HG | 1.71 | 0.56 |
| 20:AB:16:GLY:CA | 20:AB:40:ILE:H | 2.19 | 0.56 |
| 20:AB:15:PHE:O | 20:AB:40:ILE:HD12 | 2.05 | 0.56 |
| 20:AB:65:LYS:HG2 | 20:AB:89:PHE:HE1 | 1.71 | 0.56 |
| 3:AD:2:ARG:HH22 | 3:AD:132:ALA:HB3 | 1.71 | 0.56 |
| 3:AD:55:ARG:HG3 | 3:AD:55:ARG:HH11 | 1.70 | 0.56 |
| 8:AI:55:ASP:CB | 8:AI:59:LYS:HG3 | 2.36 | 0.56 |
| 15:AP:74:LEU:O | 15:AP:78:VAL:HG12 | 2.06 | 0.56 |
| 19:AT:49:ALA:HA | 19:AT:52:GLU:HB3 | 1.87 | 0.56 |
| 19:AT:68:LYS:HA | 19:AT:68:LYS:NZ | 2.21 | 0.56 |
| 21:AU:24:LYS:NZ | 21:AU:25:ALA:H | 1.98 | 0.56 |
| 21:AU:39:LYS:N | 21:AU:40:PRO:HD2 | 2.21 | 0.56 |
| 23:BB:1061:U:O4' | 23:BB:1070:A:H1' | 2.06 | 0.56 |
| 23:BB:1179:G:H2' | 23:BB:1180:U:O4' | 2.06 | 0.56 |
| 23:BB:1351:C:H2' | 23:BB:1352:U:O4' | 2.06 | 0.56 |
| 23:BB:1441:G:H2' | 23:BB:1442:U:C6 | 2.39 | 0.56 |
| 23:BB:2213:U:O2 | 23:BB:2213:U:C2' | 2.54 | 0.56 |
| 23:BB:222:A:N1 | 23:BB:233:A:H5" | 2.21 | 0.56 |
| 23:BB:2469:A:H2' | 23:BB:2470:G:O4' | 2.06 | 0.56 |
| 23:BB:832:U:H2' | 23:BB:833:A:C8 | 2.41 | 0.56 |
| 23:BB:2786:U:O2' | 26:BD:66:GLY:HA3 | 2.06 | 0.56 |
| 23:BB:673:C:H5" | 27:BE:76:PRO:HD2 | 1.86 | 0.56 |
| 30:BH:38:PRO:O | 30:BH:40:THR:HG23 | 2.06 | 0.56 |
| 23:BB:661:A:H1' | 33:BL:12:SER:O | 2.06 | 0.56 |
| 35:BN:102:PHE:N | 35:BN:109:PRO:HA | 2.18 | 0.56 |
| 40:BS:24:ILE:HD11 | 40:BS:36:LEU:CD1 | 2.27 | 0.56 |
| 42:BU:12:VAL:HG22 | 42:BU:69:VAL:HG12 | 1.87 | 0.56 |
| 42:BU:90:LYS:HB3 | 42:BU:92:VAL:HG23 | 1.87 | 0.56 |
| 24:BV:80:HIS:HB3 | 24:BV:83:LYS:O | 2.06 | 0.56 |
| 43:BW:37:VAL:HG13 | 43:BW:55:ASP:O | 2.05 | 0.56 |
| 1:CA:10:A:H2' | 1:CA:11:G:H8 | 1.69 | 0.56 |
| 1:CA:1488:G:O2' | 1:CA:1489:G:H5' | 2.06 | 0.56 |
| 1:CA:373:A:H1' | 1:CA:481:G:N3 | 2.21 | 0.56 |
| 1:CA:812:G:H2' | 1:CA:812:G:N3 | 2.19 | 0.56 |
| 7:CH:76:ARG:HG3 | 7:CH:77:VAL:N | 2.21 | 0.56 |
| 9:CJ:30:LYS:NZ | 9:CJ:36:VAL:HB | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:CK:86:LYS:HA | 10:CK:113:THR:OG1 | 2.05 | 0.56 |
| 1:CA:796:C:OP1 | 10:CK:127:ARG:HB3 | 2.06 | 0.56 |
| 48:D1:35:LEU:O | 48:D1:36:LYS:HB2 | 2.05 | 0.56 |
| 22:DA:13:G:H2' | 22:DA:14:U:H5'' | 1.88 | 0.56 |
| 23:DB:1082:U:O4 | 23:DB:1086:A:C2 | 2.57 | 0.56 |
| 23:DB:1320:C:H5 | 23:DB:1329:U:H5'' | 1.71 | 0.56 |
| 23:DB:1709:U:H2' | 23:DB:1710:G:H8 | 1.69 | 0.56 |
| 23:DB:2213:U:O2 | 23:DB:2213:U:C2' | 2.54 | 0.56 |
| 23:DB:643:A:H61 | 23:DB:2370:G:H1' | 1.71 | 0.56 |
| 23:DB:2600:A:O2' | 23:DB:2601:C:H5' | 2.06 | 0.56 |
| 23:DB:49:A:H5'' | 23:DB:51:G:O4' | 2.05 | 0.56 |
| 23:DB:670:A:H4' | 33:DL:42:SER:HB2 | 1.87 | 0.56 |
| 25:DC:143:VAL:HB | 25:DC:153:LEU:HB2 | 1.88 | 0.56 |
| 27:DE:137:LYS:HE2 | 27:DE:141:MET:SD | 2.46 | 0.56 |
| 29:DG:8:VAL:HG11 | 29:DG:49:LEU:CB | 2.34 | 0.56 |
| 23:DB:1099:G:C8 | 52:DI:3:LYS:CA | 2.84 | 0.56 |
| 35:DN:76:VAL:HA | 35:DN:79:LEU:HD12 | 1.88 | 0.56 |
| 38:DQ:94:LEU:HD21 | 39:DR:11:GLN:HB2 | 1.87 | 0.56 |
| 41:DT:1:MET:HB2 | 41:DT:2:ILE:HD13 | 1.88 | 0.56 |
| 1:AA:1343:G:H4' | 8:AI:123:ARG:O | 2.06 | 0.56 |
| 1:AA:1397:C:H4' | 1:AA:1398:A:OP2 | 2.05 | 0.56 |
| 1:AA:216:U:H2' | 1:AA:217:C:C6 | 2.41 | 0.56 |
| 1:AA:41:G:H2' | 1:AA:42:G:H8 | 1.71 | 0.56 |
| 1:AA:465:A:O2' | 1:AA:466:A:H5' | 2.06 | 0.56 |
| 1:AA:501:C:H2' | 1:AA:502:A:C8 | 2.41 | 0.56 |
| 1:AA:778:G:H2' | 1:AA:779:C:H6 | 1.71 | 0.56 |
| 1:AA:811:C:H4' | 1:AA:900:A:H62 | 1.72 | 0.56 |
| 20:AB:112:ARG:HA | 20:AB:115:ASP:OD2 | 2.06 | 0.56 |
| 20:AB:199:ILE:HG21 | 20:AB:212:TYR:CE2 | 2.41 | 0.56 |
| 4:AE:92:ARG:HH11 | 4:AE:92:ARG:HB3 | 1.70 | 0.56 |
| 5:AF:15:SER:HA | 5:AF:18:VAL:HG23 | 1.88 | 0.56 |
| 14:AO:28:VAL:HB | 14:AO:80:LEU:HD11 | 1.88 | 0.56 |
| 18:AS:39:ILE:HB | 18:AS:65:MET:O | 2.06 | 0.56 |
| 22:BA:91:C:H2' | 22:BA:92:C:H6 | 1.71 | 0.56 |
| 23:BB:1086:A:H4' | 23:BB:1103:A:N1 | 2.21 | 0.56 |
| 23:BB:1021:A:H62 | 23:BB:1141:U:H3 | 1.54 | 0.56 |
| 23:BB:2102:G:C2' | 23:BB:2103:C:H5' | 2.35 | 0.56 |
| 23:BB:2197:U:O2' | 23:BB:2198:A:H2' | 2.05 | 0.56 |
| 23:BB:2605:U:H2' | 23:BB:2606:C:C6 | 2.41 | 0.56 |
| 23:BB:2849:U:H4' | 23:BB:2850:A:H5' | 1.88 | 0.56 |
| 23:BB:730:A:O2' | 23:BB:731:C:H5' | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BC:89:ASN:O | 25:BC:105:ALA:HB3 | 2.06 | 0.56 |
| 52:BI:76:ALA:O | 52:BI:80:LYS:HG3 | 2.05 | 0.56 |
| 36:BO:47:VAL:HG12 | 36:BO:48:LEU:H | 1.72 | 0.56 |
| 41:BT:38:ALA:HB3 | 41:BT:81:LYS:HZ1 | 1.69 | 0.56 |
| 1:CA:1320:C:H5'' | 18:CS:2:ARG:NH2 | 2.20 | 0.56 |
| 1:CA:1430:A:H2' | 1:CA:1431:A:O4' | 2.06 | 0.56 |
| 1:CA:476:U:O2' | 1:CA:477:C:H5' | 2.06 | 0.56 |
| 1:CA:672:U:H2' | 1:CA:673:A:C8 | 2.40 | 0.56 |
| 1:CA:738:C:H2' | 1:CA:739:C:C6 | 2.41 | 0.56 |
| 1:CA:843:U:H5' | 1:CA:844:G:N7 | 2.21 | 0.56 |
| 5:CF:22:ILE:HD11 | 5:CF:60:VAL:HG11 | 1.88 | 0.56 |
| 6:CG:91:ARG:HD2 | 6:CG:91:ARG:N | 2.19 | 0.56 |
| 19:CT:53:MET:HA | 19:CT:56:ILE:HD12 | 1.88 | 0.56 |
| 21:CU:28:LEU:HD23 | 21:CU:29:ALA:N | 2.20 | 0.56 |
| 23:DB:1397:U:H5'' | 23:DB:1398:C:H5 | 1.70 | 0.56 |
| 23:DB:2666:C:O2 | 23:DB:2666:C:O4' | 2.20 | 0.56 |
| 23:DB:2860:A:H8 | 23:DB:2860:A:O5' | 1.89 | 0.56 |
| 27:DE:18:THR:O | 27:DE:110:SER:HB2 | 2.05 | 0.56 |
| 29:DG:74:MET:O | 29:DG:78:VAL:HG22 | 2.06 | 0.56 |
| 52:DI:5:GLN:O | 52:DI:6:ALA:HB3 | 2.05 | 0.56 |
| 33:DL:78:ARG:HG2 | 33:DL:113:ALA:CB | 2.36 | 0.56 |
| 37:DP:88:ARG:HB2 | 37:DP:112:ARG:CZ | 2.35 | 0.56 |
| 24:DV:80:HIS:HB3 | 24:DV:83:LYS:O | 2.06 | 0.56 |
| 43:DW:24:ARG:HD3 | 43:DW:65:LYS:CG | 2.35 | 0.56 |
| 45:DY:29:ARG:H | 45:DY:33:HIS:HD2 | 1.54 | 0.56 |
| 1:AA:182:A:H1' | 1:AA:183:C:C5 | 2.40 | 0.55 |
| 1:AA:189:A:H2' | 1:AA:190:A:C8 | 2.41 | 0.55 |
| 1:AA:332:G:OP2 | 19:AT:4:LYS:HB2 | 2.06 | 0.55 |
| 5:AF:92:THR:HG22 | 5:AF:93:LYS:N | 2.20 | 0.55 |
| 18:AS:6:LYS:O | 18:AS:8:PRO:HD3 | 2.05 | 0.55 |
| 22:BA:3:C:H2' | 22:BA:4:C:C6 | 2.41 | 0.55 |
| 23:BB:1210:G:H5' | 23:BB:1212:G:H5'' | 1.87 | 0.55 |
| 23:BB:1450:G:H21 | 23:BB:1452:G:H1 | 1.53 | 0.55 |
| 23:BB:2008:C:H2' | 23:BB:2009:A:H8 | 1.71 | 0.55 |
| 23:BB:2092:U:H4' | 23:BB:2093:G:H5'' | 1.88 | 0.55 |
| 23:BB:2186:G:H2' | 23:BB:2187:U:C6 | 2.41 | 0.55 |
| 23:BB:2722:G:H2' | 23:BB:2723:C:H6 | 1.71 | 0.55 |
| 23:BB:500:G:N2 | 23:BB:502:A:H3' | 2.21 | 0.55 |
| 28:BF:64:PRO:HA | 28:BF:88:VAL:CG2 | 2.35 | 0.55 |
| 52:BI:17:ALA:O | 52:BI:18:ASN:HB3 | 2.05 | 0.55 |
| 31:BJ:103:ILE:HA | 31:BJ:106:LYS:HB3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BP:89:GLY:HA2 | 37:BP:111:GLU:C | 2.26 | 0.55 |
| 43:BW:59:PHE:CE2 | 43:BW:61:LYS:HG3 | 2.40 | 0.55 |
| 1:CA:1504:G:H4' | 1:CA:1505:G:C4 | 2.41 | 0.55 |
| 1:CA:434:U:H3' | 1:CA:435:A:H8 | 1.71 | 0.55 |
| 20:CB:95:TRP:CH2 | 20:CB:100:LEU:HB2 | 2.40 | 0.55 |
| 9:CJ:80:THR:HG21 | 9:CJ:82:LYS:NZ | 2.21 | 0.55 |
| 17:CR:25:ILE:O | 17:CR:29:LYS:HG3 | 2.05 | 0.55 |
| 23:DB:1163:G:H4' | 39:DR:92:TRP:HE1 | 1.69 | 0.55 |
| 23:DB:2836:U:H2' | 23:DB:2837:A:C8 | 2.40 | 0.55 |
| 23:DB:2598:A:H5'' | 25:DC:233:GLY:HA2 | 1.87 | 0.55 |
| 26:DD:29:VAL:O | 26:DD:185:ASN:HB3 | 2.05 | 0.55 |
| 28:DF:177:ARG:NH1 | 28:DF:177:ARG:HA | 2.21 | 0.55 |
| 30:DH:1:MET:HB3 | 30:DH:21:VAL:O | 2.06 | 0.55 |
| 36:DO:62:LEU:HD11 | 36:DO:70:ALA:HA | 1.88 | 0.55 |
| 40:DS:10:ALA:HB3 | 40:DS:101:SER:OG | 2.06 | 0.55 |
| 24:DV:4:ILE:O | 24:DV:63:ILE:HA | 2.06 | 0.55 |
| 24:DV:31:TYR:HA | 24:DV:93:ARG:HH21 | 1.71 | 0.55 |
| 43:DW:64:GLY:HA2 | 43:DW:84:GLU:HG2 | 1.86 | 0.55 |
| 1:AA:45:G:H2' | 1:AA:46:G:C8 | 2.41 | 0.55 |
| 1:AA:490:C:H2' | 1:AA:491:G:C8 | 2.41 | 0.55 |
| 1:AA:709:U:H2' | 1:AA:710:G:H8 | 1.71 | 0.55 |
| 1:AA:778:G:H2' | 1:AA:779:C:C6 | 2.41 | 0.55 |
| 2:AC:68:HIS:HA | 2:AC:103:ALA:HB3 | 1.88 | 0.55 |
| 7:AH:11:THR:HA | 7:AH:14:ARG:CZ | 2.36 | 0.55 |
| 18:AS:41:PRO:HA | 18:AS:66:VAL:HG11 | 1.88 | 0.55 |
| 19:AT:53:MET:O | 19:AT:57:VAL:HG22 | 2.07 | 0.55 |
| 23:BB:1205:A:N1 | 27:BE:165:HIS:HB2 | 2.20 | 0.55 |
| 23:BB:2698:U:H2' | 23:BB:2699:C:C6 | 2.41 | 0.55 |
| 23:BB:2828:G:O2' | 23:BB:2829:A:H5' | 2.05 | 0.55 |
| 23:BB:948:C:H2' | 23:BB:949:G:H8 | 1.71 | 0.55 |
| 25:BC:105:ALA:HB1 | 25:BC:109:LEU:HD11 | 1.87 | 0.55 |
| 25:BC:250:GLN:O | 25:BC:250:GLN:HG2 | 2.06 | 0.55 |
| 26:BD:116:LYS:HG3 | 26:BD:165:MET:SD | 2.46 | 0.55 |
| 28:BF:37:MET:CG | 28:BF:52:ALA:HB1 | 2.36 | 0.55 |
| 30:BH:122:LEU:HD12 | 30:BH:122:LEU:N | 2.21 | 0.55 |
| 38:BQ:57:ARG:HH11 | 38:BQ:57:ARG:CB | 2.19 | 0.55 |
| 38:BQ:63:ARG:NH1 | 38:BQ:96:ASP:HA | 2.22 | 0.55 |
| 39:BR:28:ALA:O | 39:BR:63:VAL:HG21 | 2.06 | 0.55 |
| 41:BT:13:ALA:O | 41:BT:32:LEU:HB2 | 2.06 | 0.55 |
| 41:BT:69:ARG:CZ | 41:BT:69:ARG:HA | 2.36 | 0.55 |
| 1:CA:1078:U:H2' | 1:CA:1079:G:O4' | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1085:U:H3' | 1:CA:1086:U:H5 | 1.70 | 0.55 |
| 1:CA:1118:U:H2' | 1:CA:1119:C:H6 | 1.70 | 0.55 |
| 1:CA:1448:C:H2' | 1:CA:1449:C:H6 | 1.71 | 0.55 |
| 1:CA:168:G:O2' | 1:CA:169:C:H5' | 2.07 | 0.55 |
| 1:CA:555:U:H2' | 1:CA:556:C:C6 | 2.42 | 0.55 |
| 1:CA:560:A:N1 | 1:CA:566:G:H5' | 2.21 | 0.55 |
| 1:CA:663:A:O2' | 1:CA:664:G:H5' | 2.06 | 0.55 |
| 20:CB:33:ALA:HA | 20:CB:38:HIS:HA | 1.87 | 0.55 |
| 3:CD:169:TRP:HB2 | 3:CD:183:ARG:O | 2.06 | 0.55 |
| 12:CM:17:ALA:CB | 12:CM:44:ILE:HD11 | 2.36 | 0.55 |
| 18:CS:52:ASN:CG | 18:CS:53:GLY:H | 2.09 | 0.55 |
| 50:D3:55:GLY:HA2 | 50:D3:58:ILE:HD12 | 1.89 | 0.55 |
| 22:DA:49:C:H2' | 22:DA:50:A:H8 | 1.71 | 0.55 |
| 23:DB:1386:C:H2' | 23:DB:1387:A:H8 | 1.71 | 0.55 |
| 23:DB:1458:U:H2' | 23:DB:1459:G:H5'' | 1.88 | 0.55 |
| 23:DB:2450:A:O2' | 23:DB:2451:A:H5' | 2.06 | 0.55 |
| 23:DB:2788:C:H2' | 23:DB:2789:C:C6 | 2.40 | 0.55 |
| 23:DB:299:A:N6 | 23:DB:322:A:O2' | 2.39 | 0.55 |
| 25:DC:86:ARG:HB3 | 25:DC:86:ARG:CZ | 2.36 | 0.55 |
| 28:DF:106:ALA:HA | 28:DF:135:ILE:HD13 | 1.89 | 0.55 |
| 29:DG:10:VAL:HG12 | 29:DG:10:VAL:O | 2.05 | 0.55 |
| 52:DI:45:THR:CA | 52:DI:48:ILE:HG22 | 2.35 | 0.55 |
| 32:DK:11:ALA:HB3 | 32:DK:85:VAL:HG22 | 1.88 | 0.55 |
| 40:DS:6:LYS:HB2 | 40:DS:103:ILE:O | 2.06 | 0.55 |
| 42:DU:21:ARG:HG3 | 42:DU:21:ARG:HH11 | 1.71 | 0.55 |
| 24:DV:65:VAL:C | 24:DV:67:GLY:H | 2.09 | 0.55 |
| 1:AA:1021:A:H2' | 1:AA:1022:A:O4' | 2.06 | 0.55 |
| 1:AA:546:A:OP1 | 3:AD:69:ARG:HB2 | 2.07 | 0.55 |
| 1:AA:77:A:OP1 | 1:AA:88:U:H5'' | 2.06 | 0.55 |
| 9:AJ:40:ILE:HD12 | 9:AJ:73:LEU:HD12 | 1.88 | 0.55 |
| 11:AL:13:ARG:O | 11:AL:14:LYS:HB3 | 2.06 | 0.55 |
| 51:B4:2:LYS:HG2 | 51:B4:3:VAL:N | 2.20 | 0.55 |
| 51:B4:8:LYS:HG2 | 51:B4:9:LYS:H | 1.71 | 0.55 |
| 23:BB:2539:C:O2' | 23:BB:2540:C:H5' | 2.07 | 0.55 |
| 23:BB:2636:C:O2' | 23:BB:2637:U:H5' | 2.05 | 0.55 |
| 23:BB:2659:G:N2 | 23:BB:2661:G:H5'' | 2.22 | 0.55 |
| 23:BB:2795:C:H2' | 23:BB:2796:U:O4' | 2.07 | 0.55 |
| 23:BB:2901:C:H2' | 23:BB:2902:C:H5' | 1.88 | 0.55 |
| 25:BC:226:PRO:CG | 25:BC:233:GLY:H | 2.18 | 0.55 |
| 28:BF:31:GLU:O | 28:BF:32:LYS:O | 2.24 | 0.55 |
| 33:BL:122:VAL:HG12 | 33:BL:143:GLU:OE2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:BM:35:ALA:HB3 | 34:BM:99:GLY:N | 2.20 | 0.55 |
| 37:BP:1:SER:O | 37:BP:5:LYS:HB2 | 2.07 | 0.55 |
| 1:CA:1121:U:H2' | 1:CA:1122:U:O4' | 2.07 | 0.55 |
| 1:CA:1123:U:O2' | 1:CA:1124:G:H5' | 2.07 | 0.55 |
| 10:CK:30:ILE:HG22 | 10:CK:45:THR:OG1 | 2.07 | 0.55 |
| 1:CA:562:U:H1' | 11:CL:11:ARG:HD2 | 1.87 | 0.55 |
| 14:CO:63:ARG:HH12 | 14:CO:87:ARG:HH22 | 1.54 | 0.55 |
| 23:DB:2756:U:H4' | 23:DB:2757:A:OP1 | 2.06 | 0.55 |
| 23:DB:289:G:H2' | 23:DB:290:U:C6 | 2.40 | 0.55 |
| 23:DB:920:A:H2' | 23:DB:921:C:C6 | 2.41 | 0.55 |
| 25:DC:43:ASN:HB3 | 25:DC:45:ASN:ND2 | 2.21 | 0.55 |
| 27:DE:147:LEU:HD12 | 27:DE:149:ILE:HB | 1.87 | 0.55 |
| 27:DE:12:LEU:HD12 | 27:DE:14:VAL:HG22 | 1.87 | 0.55 |
| 28:DF:42:ALA:HA | 28:DF:48:LEU:CD2 | 2.33 | 0.55 |
| 30:DH:135:HIS:CG | 30:DH:136:SER:N | 2.73 | 0.55 |
| 32:DK:107:LEU:HB2 | 32:DK:116:ILE:CG2 | 2.37 | 0.55 |
| 41:DT:54:GLU:HG3 | 41:DT:90:GLY:N | 2.21 | 0.55 |
| 1:AA:1246:A:H2' | 1:AA:1247:U:O4' | 2.05 | 0.55 |
| 1:AA:1432:G:H1' | 1:AA:1468:A:H61 | 1.70 | 0.55 |
| 1:AA:168:G:O2' | 1:AA:169:C:H5' | 2.06 | 0.55 |
| 1:AA:33:A:H2' | 1:AA:34:C:C6 | 2.41 | 0.55 |
| 1:AA:484:G:H5' | 1:AA:486:U:H5' | 1.87 | 0.55 |
| 1:AA:590:U:H2' | 1:AA:591:U:H6 | 1.72 | 0.55 |
| 1:AA:692:U:O2 | 1:AA:694:A:H5'' | 2.07 | 0.55 |
| 1:AA:742:G:H2' | 1:AA:743:A:H8 | 1.71 | 0.55 |
| 2:AC:16:PRO:CG | 2:AC:53:ARG:HH12 | 2.20 | 0.55 |
| 18:AS:52:ASN:CG | 18:AS:53:GLY:H | 2.08 | 0.55 |
| 23:BB:2285:C:OP2 | 48:B1:5:ARG:HD3 | 2.06 | 0.55 |
| 23:BB:1947:C:H2' | 23:BB:1948:G:C8 | 2.42 | 0.55 |
| 23:BB:1969:A:H2' | 23:BB:1972:G:H21 | 1.71 | 0.55 |
| 23:BB:2037:A:H2' | 23:BB:2038:G:H8 | 1.70 | 0.55 |
| 23:BB:2466:C:OP1 | 51:B4:4:ARG:HB3 | 2.07 | 0.55 |
| 23:BB:2592:G:H2' | 23:BB:2593:U:O4' | 2.06 | 0.55 |
| 23:BB:2788:C:H2' | 23:BB:2789:C:C6 | 2.41 | 0.55 |
| 23:BB:845:A:N1 | 23:BB:847:U:H1' | 2.21 | 0.55 |
| 28:BF:28:PRO:HG3 | 28:BF:159:ALA:HB2 | 1.87 | 0.55 |
| 28:BF:78:ILE:HA | 28:BF:82:TYR:CE1 | 2.42 | 0.55 |
| 52:BI:109:ALA:HB1 | 52:BI:124:MET:HG3 | 1.89 | 0.55 |
| 42:BU:35:VAL:HB | 42:BU:38:ILE:HG21 | 1.87 | 0.55 |
| 42:BU:85:ARG:HA | 42:BU:85:ARG:NE | 2.22 | 0.55 |
| 43:BW:18:LYS:N | 43:BW:35:ILE:HG23 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1397:C:H4' | 1:CA:1398:A:OP2 | 2.05 | 0.55 |
| 1:CA:470:C:H2' | 1:CA:471:U:C6 | 2.41 | 0.55 |
| 2:CC:39:ARG:HG3 | 2:CC:56:ILE:HD11 | 1.88 | 0.55 |
| 3:CD:55:ARG:HG3 | 3:CD:55:ARG:HH11 | 1.72 | 0.55 |
| 12:CM:33:LEU:HD13 | 12:CM:39:ALA:O | 2.06 | 0.55 |
| 1:CA:625:U:H4' | 15:CP:16:PHE:CZ | 2.42 | 0.55 |
| 19:CT:72:ALA:HA | 19:CT:75:LYS:HD3 | 1.89 | 0.55 |
| 23:DB:2015:A:C2 | 47:D0:2:VAL:HG22 | 2.42 | 0.55 |
| 23:DB:572:A:C2 | 23:DB:2033:A:C2 | 2.94 | 0.55 |
| 23:DB:2313:C:H4' | 28:DF:87:LYS:HB3 | 1.87 | 0.55 |
| 23:DB:558:U:OP1 | 31:DJ:114:LEU:HB2 | 2.06 | 0.55 |
| 23:DB:870:U:O2' | 23:DB:871:U:H5' | 2.06 | 0.55 |
| 23:DB:936:A:H2' | 23:DB:937:C:C6 | 2.42 | 0.55 |
| 52:DI:17:ALA:O | 52:DI:18:ASN:CB | 2.53 | 0.55 |
| 37:DP:4:ILE:HG22 | 37:DP:5:LYS:N | 2.15 | 0.55 |
| 32:DK:79:PHE:HD2 | 37:DP:69:VAL:HG12 | 1.72 | 0.55 |
| 38:DQ:79:ILE:O | 38:DQ:79:ILE:HD13 | 2.06 | 0.55 |
| 1:AA:179:A:H2' | 1:AA:180:U:C6 | 2.41 | 0.55 |
| 20:AB:80:LYS:HG3 | 20:AB:81:ASP:H | 1.71 | 0.55 |
| 20:AB:95:TRP:CH2 | 20:AB:100:LEU:HB2 | 2.41 | 0.55 |
| 2:AC:6:PRO:HA | 2:AC:9:ILE:HG22 | 1.87 | 0.55 |
| 12:AM:18:LEU:HB2 | 12:AM:29:SER:OG | 2.06 | 0.55 |
| 12:AM:86:ARG:HA | 12:AM:96:VAL:HG11 | 1.88 | 0.55 |
| 1:AA:1320:C:H42 | 18:AS:35:ARG:HD3 | 1.70 | 0.55 |
| 48:B1:26:LYS:HD2 | 48:B1:30:PRO:HA | 1.89 | 0.55 |
| 48:B1:35:LEU:O | 48:B1:36:LYS:HB2 | 2.06 | 0.55 |
| 23:BB:1407:G:H2' | 23:BB:1408:G:C8 | 2.40 | 0.55 |
| 23:BB:161:A:C3' | 23:BB:162:U:H5'' | 2.37 | 0.55 |
| 23:BB:1771:C:H2' | 23:BB:1772:A:H8 | 1.70 | 0.55 |
| 23:BB:1979:U:O2' | 23:BB:1980:G:H5' | 2.07 | 0.55 |
| 23:BB:2097:A:H2' | 23:BB:2098:U:C6 | 2.41 | 0.55 |
| 23:BB:2149:U:H2' | 23:BB:2150:C:H6 | 1.71 | 0.55 |
| 23:BB:2185:U:C2 | 23:BB:2186:G:N7 | 2.74 | 0.55 |
| 23:BB:2271:G:H2' | 23:BB:2272:U:C6 | 2.41 | 0.55 |
| 23:BB:2772:C:H4' | 26:BD:171:THR:HG21 | 1.89 | 0.55 |
| 23:BB:870:U:O2' | 23:BB:871:U:H5' | 2.05 | 0.55 |
| 23:BB:729:G:C8 | 25:BC:206:LYS:HE3 | 2.42 | 0.55 |
| 25:BC:4:LYS:HD2 | 25:BC:5:CYS:H | 1.71 | 0.55 |
| 26:BD:62:LYS:HB2 | 26:BD:63:PRO:HD3 | 1.88 | 0.55 |
| 30:BH:1:MET:HB3 | 30:BH:21:VAL:O | 2.07 | 0.55 |
| 42:BU:64:ILE:HG13 | 42:BU:65:GLN:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:BU:94:PHE:HA | 42:BU:101:THR:HA | 1.89 | 0.55 |
| 45:BY:6:ILE:N | 45:BY:35:VAL:O | 2.39 | 0.55 |
| 46:BZ:40:VAL:HG22 | 46:BZ:45:ARG:O | 2.07 | 0.55 |
| 1:CA:1127:G:H5' | 1:CA:1280:A:O2' | 2.06 | 0.55 |
| 1:CA:858:G:O6 | 1:CA:869:G:H3' | 2.07 | 0.55 |
| 3:CD:77:GLU:O | 3:CD:81:LEU:HG | 2.06 | 0.55 |
| 6:CG:78:ARG:NH1 | 6:CG:81:GLY:H | 2.04 | 0.55 |
| 8:CI:113:LYS:HA | 8:CI:120:ALA:HB2 | 1.89 | 0.55 |
| 8:CI:49:GLN:N | 8:CI:50:PRO:HD2 | 2.21 | 0.55 |
| 8:CI:6:TYR:HB2 | 8:CI:19:PHE:CE1 | 2.42 | 0.55 |
| 11:CL:13:ARG:O | 11:CL:14:LYS:HB3 | 2.06 | 0.55 |
| 16:CQ:83:LEU:H | 16:CQ:83:LEU:HD13 | 1.71 | 0.55 |
| 18:CS:29:PRO:HA | 18:CS:47:THR:O | 2.05 | 0.55 |
| 51:D4:3:VAL:HG23 | 51:D4:4:ARG:H | 1.72 | 0.55 |
| 23:DB:1013:C:H2' | 23:DB:1014:A:C8 | 2.40 | 0.55 |
| 23:DB:1064:C:H5' | 52:DI:88:GLY:HA3 | 1.89 | 0.55 |
| 23:DB:138:U:H2' | 23:DB:140:C:O4' | 2.06 | 0.55 |
| 23:DB:1842:G:H2' | 23:DB:1843:C:C6 | 2.41 | 0.55 |
| 23:DB:1838:C:N4 | 23:DB:1898:U:H2' | 2.21 | 0.55 |
| 23:DB:2024:G:O2' | 23:DB:2025:C:H5' | 2.07 | 0.55 |
| 23:DB:2340:A:H2' | 23:DB:2341:G:C8 | 2.41 | 0.55 |
| 23:DB:2415:G:H2' | 23:DB:2416:C:H6 | 1.72 | 0.55 |
| 23:DB:2516:A:O2' | 23:DB:2517:C:H5' | 2.07 | 0.55 |
| 23:DB:2836:U:H2' | 23:DB:2837:A:H8 | 1.71 | 0.55 |
| 23:DB:45:G:H5' | 23:DB:46:G:OP1 | 2.07 | 0.55 |
| 23:DB:635:C:O2' | 23:DB:639:U:H5'' | 2.06 | 0.55 |
| 23:DB:6:A:O2' | 23:DB:7:G:H5' | 2.06 | 0.55 |
| 23:DB:919:U:H2' | 23:DB:920:A:H8 | 1.69 | 0.55 |
| 27:DE:110:SER:O | 27:DE:114:ARG:HG3 | 2.07 | 0.55 |
| 28:DF:7:TYR:HA | 28:DF:11:VAL:CG2 | 2.36 | 0.55 |
| 29:DG:115:GLN:H | 29:DG:115:GLN:CD | 2.10 | 0.55 |
| 29:DG:25:ILE:HD13 | 29:DG:74:MET:HE2 | 1.88 | 0.55 |
| 30:DH:53:GLU:HA | 30:DH:57:LYS:HB3 | 1.89 | 0.55 |
| 23:DB:2816:G:O3' | 35:DN:99:LYS:HE3 | 2.06 | 0.55 |
| 41:DT:7:LEU:O | 41:DT:7:LEU:HD13 | 2.07 | 0.55 |
| 46:DZ:66:THR:O | 46:DZ:69:ALA:HB3 | 2.06 | 0.55 |
| 1:AA:1085:U:H3' | 1:AA:1086:U:H5 | 1.72 | 0.55 |
| 1:AA:34:C:H2' | 1:AA:35:G:C8 | 2.42 | 0.55 |
| 8:AI:49:GLN:N | 8:AI:50:PRO:HD2 | 2.22 | 0.55 |
| 13:AN:5:MET:HE3 | 13:AN:60:ARG:HH11 | 1.70 | 0.55 |
| 15:AP:38:PHE:CD2 | 15:AP:51:ARG:HB2 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 23:BB:1841:U:H2' | 23:BB:1842:G:H8 | 1.72 | 0.55 |
| 23:BB:2080:A:H4' | 46:BZ:19:SER:OG | 2.06 | 0.55 |
| 23:BB:441:U:H2' | 23:BB:442:G:C8 | 2.41 | 0.55 |
| 23:BB:664:G:H2' | 23:BB:665:U:H6 | 1.70 | 0.55 |
| 23:BB:833:A:H2' | 23:BB:834:G:C8 | 2.42 | 0.55 |
| 23:BB:871:U:H2' | 23:BB:872:U:C6 | 2.40 | 0.55 |
| 23:BB:997:G:O2' | 23:BB:998:C:H5' | 2.07 | 0.55 |
| 23:BB:1820:U:OP1 | 25:BC:176:ARG:HD2 | 2.06 | 0.55 |
| 27:BE:166:LYS:O | 27:BE:167:VAL:HB | 2.06 | 0.55 |
| 28:BF:7:TYR:HA | 28:BF:11:VAL:CG2 | 2.37 | 0.55 |
| 35:BN:49:GLU:HB2 | 35:BN:50:PRO:HD3 | 1.89 | 0.55 |
| 42:BU:80:ASP:HB2 | 42:BU:95:PHE:HD2 | 1.72 | 0.55 |
| 24:BV:24:ASN:HB3 | 24:BV:44:HIS:HB3 | 1.89 | 0.55 |
| 24:BV:31:TYR:HA | 24:BV:93:ARG:HH21 | 1.71 | 0.55 |
| 44:BX:41:HIS:O | 44:BX:44:LYS:HB3 | 2.07 | 0.55 |
| 1:CA:252:U:H2' | 1:CA:253:A:C8 | 2.42 | 0.55 |
| 1:CA:284:C:H2' | 1:CA:285:C:H6 | 1.71 | 0.55 |
| 1:CA:393:A:O2' | 1:CA:394:G:H5' | 2.06 | 0.55 |
| 1:CA:784:A:H2' | 1:CA:785:G:C8 | 2.42 | 0.55 |
| 7:CH:31:LEU:O | 7:CH:35:ILE:HG13 | 2.06 | 0.55 |
| 8:CI:55:ASP:CB | 8:CI:59:LYS:HG3 | 2.36 | 0.55 |
| 23:DB:1139:G:O2' | 23:DB:1140:C:H5' | 2.06 | 0.55 |
| 23:DB:1335:C:H2' | 23:DB:1336:A:C8 | 2.42 | 0.55 |
| 23:DB:132:G:H2' | 23:DB:133:U:H6 | 1.70 | 0.55 |
| 23:DB:2101:A:O2' | 23:DB:2102:G:H5' | 2.07 | 0.55 |
| 23:DB:2665:A:H2' | 23:DB:2666:C:O2 | 2.06 | 0.55 |
| 23:DB:296:U:H2' | 23:DB:297:G:H8 | 1.72 | 0.55 |
| 23:DB:394:C:H2' | 23:DB:395:U:O4' | 2.07 | 0.55 |
| 23:DB:704:G:H1' | 23:DB:727:A:H61 | 1.72 | 0.55 |
| 23:DB:782:A:N7 | 25:DC:219:VAL:HG21 | 2.21 | 0.55 |
| 29:DG:30:GLY:HA3 | 29:DG:78:VAL:HA | 1.87 | 0.55 |
| 29:DG:24:THR:HA | 29:DG:33:THR:O | 2.07 | 0.55 |
| 52:DI:125:THR:O | 52:DI:129:GLU:HG3 | 2.07 | 0.55 |
| 33:DL:3:LEU:HA | 33:DL:6:LEU:HD21 | 1.88 | 0.55 |
| 36:DO:107:ALA:O | 36:DO:111:ARG:HG3 | 2.07 | 0.55 |
| 39:DR:3:ALA:O | 39:DR:13:ARG:HA | 2.07 | 0.55 |
| 39:DR:62:GLU:O | 39:DR:96:VAL:HA | 2.06 | 0.55 |
| 42:DU:90:LYS:HB3 | 42:DU:92:VAL:HG23 | 1.87 | 0.55 |
| 1:AA:1226:C:H4' | 1:AA:1227:A:OP1 | 2.06 | 0.55 |
| 1:AA:430:A:OP1 | 3:AD:8:LEU:HB2 | 2.06 | 0.55 |
| 1:AA:845:A:H3' | 1:AA:846:G:H8 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AC:171:ARG:NH1 | 2:AC:171:ARG:HB2 | 2.22 | 0.55 |
| 2:AC:2:GLN:H | 2:AC:2:GLN:HE21 | 1.55 | 0.55 |
| 1:AA:620:C:O2 | 3:AD:131:ILE:HG21 | 2.07 | 0.55 |
| 4:AE:158:LYS:NZ | 7:AH:63:LYS:HD3 | 2.22 | 0.55 |
| 5:AF:69:GLU:OE1 | 5:AF:70:VAL:HG13 | 2.07 | 0.55 |
| 6:AG:4:ARG:HG3 | 6:AG:5:VAL:N | 2.18 | 0.55 |
| 13:AN:60:ARG:HD3 | 13:AN:62:ARG:CZ | 2.37 | 0.55 |
| 22:BA:11:C:H5' | 43:BW:71:LYS:HG3 | 1.86 | 0.55 |
| 23:BB:2021:C:P | 47:B0:8:THR:HG21 | 2.47 | 0.55 |
| 23:BB:2364:C:H2' | 23:BB:2365:G:O4' | 2.06 | 0.55 |
| 23:BB:2678:C:H2' | 23:BB:2679:A:C8 | 2.42 | 0.55 |
| 23:BB:441:U:H2' | 23:BB:442:G:H8 | 1.72 | 0.55 |
| 23:BB:6:A:O2' | 23:BB:7:G:H5' | 2.06 | 0.55 |
| 23:BB:917:A:H2' | 23:BB:918:A:O4' | 2.06 | 0.55 |
| 23:BB:936:A:H2' | 23:BB:937:C:C6 | 2.42 | 0.55 |
| 25:BC:5:CYS:HB2 | 25:BC:15:VAL:O | 2.06 | 0.55 |
| 27:BE:12:LEU:HD12 | 27:BE:14:VAL:HG22 | 1.88 | 0.55 |
| 28:BF:126:ASN:HB3 | 28:BF:156:THR:CA | 2.36 | 0.55 |
| 30:BH:99:ILE:HG13 | 30:BH:130:VAL:HG11 | 1.89 | 0.55 |
| 38:BQ:86:SER:O | 39:BR:51:VAL:HA | 2.06 | 0.55 |
| 38:BQ:94:LEU:CD2 | 39:BR:11:GLN:HB2 | 2.37 | 0.55 |
| 41:BT:69:ARG:HB2 | 41:BT:75:GLY:N | 2.22 | 0.55 |
| 1:CA:1226:C:H4' | 1:CA:1227:A:OP1 | 2.06 | 0.55 |
| 1:CA:34:C:H2' | 1:CA:35:G:C8 | 2.42 | 0.55 |
| 2:CC:68:HIS:HA | 2:CC:103:ALA:HB3 | 1.88 | 0.55 |
| 3:CD:29:THR:HB | 3:CD:30:LYS:HZ3 | 1.71 | 0.55 |
| 4:CE:18:ASN:HB2 | 4:CE:33:THR:OG1 | 2.07 | 0.55 |
| 4:CE:23:THR:HA | 4:CE:28:ARG:HA | 1.88 | 0.55 |
| 4:CE:19:ARG:NH1 | 4:CE:28:ARG:HH22 | 2.04 | 0.55 |
| 6:CG:129:ASN:ND2 | 6:CG:137:ARG:HH22 | 2.04 | 0.55 |
| 10:CK:34:THR:HB | 10:CK:40:ALA:HA | 1.87 | 0.55 |
| 13:CN:20:PHE:C | 13:CN:22:LYS:H | 2.10 | 0.55 |
| 14:CO:78:THR:HA | 14:CO:81:ILE:HD12 | 1.87 | 0.55 |
| 14:CO:80:LEU:HD21 | 14:CO:84:LEU:HD22 | 1.89 | 0.55 |
| 16:CQ:83:LEU:HD22 | 16:CQ:83:LEU:N | 2.21 | 0.55 |
| 23:DB:1351:C:O2' | 23:DB:1571:A:H1' | 2.07 | 0.55 |
| 23:DB:1731:G:O2' | 23:DB:1732:C:H5'' | 2.06 | 0.55 |
| 23:DB:1774:C:H2' | 23:DB:1774:C:O2 | 2.06 | 0.55 |
| 23:DB:2008:C:H2' | 23:DB:2009:A:C8 | 2.42 | 0.55 |
| 23:DB:2648:G:H2' | 23:DB:2649:C:C6 | 2.41 | 0.55 |
| 23:DB:2674:G:H4' | 32:DK:30:ARG:HG3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:2678:C:H2' | 23:DB:2679:A:C8 | 2.42 | 0.55 |
| 23:DB:2863:C:O2' | 23:DB:2864:G:H5' | 2.07 | 0.55 |
| 23:DB:228:C:O2 | 23:DB:418:C:H4' | 2.06 | 0.55 |
| 23:DB:660:C:H2' | 23:DB:661:A:C8 | 2.41 | 0.55 |
| 25:DC:130:PRO:HG2 | 25:DC:133:ASN:ND2 | 2.22 | 0.55 |
| 29:DG:39:ALA:C | 29:DG:54:ARG:HB2 | 2.27 | 0.55 |
| 52:DI:71:LYS:HB3 | 52:DI:115:ASP:OD2 | 2.06 | 0.55 |
| 32:DK:53:LYS:HD3 | 32:DK:56:ASP:OD2 | 2.07 | 0.55 |
| 38:DQ:71:ASN:HD22 | 38:DQ:73:ILE:HG22 | 1.70 | 0.55 |
| 38:DQ:63:ARG:NH1 | 38:DQ:96:ASP:HA | 2.20 | 0.55 |
| 40:DS:24:ILE:CD1 | 40:DS:36:LEU:HD21 | 2.36 | 0.55 |
| 45:DY:6:ILE:N | 45:DY:35:VAL:O | 2.38 | 0.55 |
| 1:AA:1006:G:H2' | 1:AA:1007:U:H6 | 1.71 | 0.55 |
| 1:AA:137:U:H2' | 1:AA:138:G:C8 | 2.42 | 0.55 |
| 1:AA:1438:G:O2' | 1:AA:1439:G:H5' | 2.06 | 0.55 |
| 1:AA:1448:C:H2' | 1:AA:1449:C:C6 | 2.42 | 0.55 |
| 1:AA:16:A:O2' | 1:AA:17:U:H5' | 2.07 | 0.55 |
| 1:AA:642:A:H2' | 1:AA:643:C:H6 | 1.72 | 0.55 |
| 1:AA:692:U:C2 | 1:AA:694:A:H5'' | 2.42 | 0.55 |
| 1:AA:769:G:H4' | 1:AA:1513:A:H4' | 1.87 | 0.55 |
| 20:AB:53:LEU:HD11 | 20:AB:216:VAL:HA | 1.88 | 0.55 |
| 3:AD:29:THR:HG22 | 3:AD:30:LYS:N | 2.22 | 0.55 |
| 6:AG:78:ARG:HG2 | 6:AG:83:THR:HG22 | 1.88 | 0.55 |
| 7:AH:76:ARG:HG3 | 7:AH:77:VAL:N | 2.21 | 0.55 |
| 13:AN:11:LYS:N | 13:AN:11:LYS:HZ3 | 2.05 | 0.55 |
| 13:AN:60:ARG:NE | 13:AN:62:ARG:HG2 | 2.21 | 0.55 |
| 15:AP:59:HIS:O | 15:AP:63:GLN:HG3 | 2.07 | 0.55 |
| 16:AQ:7:LEU:O | 16:AQ:60:ILE:HD13 | 2.06 | 0.55 |
| 18:AS:62:THR:H | 18:AS:65:MET:HB2 | 1.71 | 0.55 |
| 47:B0:52:LYS:NZ | 47:B0:56:LYS:H | 2.05 | 0.55 |
| 50:B3:7:ARG:HH11 | 50:B3:7:ARG:HG3 | 1.71 | 0.55 |
| 23:BB:1021:A:H61 | 23:BB:1142:A:H61 | 1.55 | 0.55 |
| 23:BB:1152:C:O2' | 23:BB:1153:C:H5' | 2.07 | 0.55 |
| 23:BB:1210:G:N3 | 23:BB:1212:G:N2 | 2.55 | 0.55 |
| 23:BB:1260:A:H2' | 23:BB:1261:C:H6 | 1.70 | 0.55 |
| 23:BB:1549:A:H2' | 23:BB:1550:C:H6 | 1.70 | 0.55 |
| 23:BB:2537:U:H2' | 23:BB:2538:C:C6 | 2.42 | 0.55 |
| 23:BB:2868:A:H2' | 23:BB:2869:G:C8 | 2.42 | 0.55 |
| 23:BB:416:U:H2' | 23:BB:417:C:C6 | 2.42 | 0.55 |
| 23:BB:616:A:H4' | 27:BE:101:TYR:CE2 | 2.42 | 0.55 |
| 27:BE:110:SER:O | 27:BE:114:ARG:HG3 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BE:149:ILE:O | 27:BE:188:MET:HA | 2.07 | 0.55 |
| 29:BG:74:MET:O | 29:BG:78:VAL:HG22 | 2.07 | 0.55 |
| 29:BG:83:THR:HA | 29:BG:84:LYS:NZ | 2.22 | 0.55 |
| 29:BG:85:LYS:HB2 | 29:BG:164:ALA:CB | 2.37 | 0.55 |
| 52:BI:14:ALA:HB1 | 52:BI:50:LYS:HA | 1.88 | 0.55 |
| 33:BL:78:ARG:HG2 | 33:BL:113:ALA:HB2 | 1.88 | 0.55 |
| 33:BL:135:ILE:HG12 | 33:BL:140:GLY:CA | 2.36 | 0.55 |
| 38:BQ:26:ALA:HB1 | 38:BQ:30:VAL:HB | 1.88 | 0.55 |
| 38:BQ:74:SER:OG | 38:BQ:77:LYS:HD3 | 2.06 | 0.55 |
| 38:BQ:94:LEU:C | 38:BQ:96:ASP:H | 2.09 | 0.55 |
| 40:BS:83:LYS:HB3 | 40:BS:95:ARG:NH1 | 2.21 | 0.55 |
| 42:BU:17:ASP:HB3 | 42:BU:20:LYS:HE3 | 1.88 | 0.55 |
| 43:BW:37:VAL:HG12 | 43:BW:38:ARG:N | 2.22 | 0.55 |
| 1:CA:845:A:H3' | 1:CA:846:G:H8 | 1.71 | 0.55 |
| 20:CB:122:ASP:OD2 | 20:CB:125:PHE:HB2 | 2.07 | 0.55 |
| 11:CL:3:VAL:O | 11:CL:7:VAL:HG23 | 2.07 | 0.55 |
| 21:CU:3:ILE:HD13 | 21:CU:19:LYS:HA | 1.89 | 0.55 |
| 23:DB:1230:A:H2' | 23:DB:1231:U:C6 | 2.42 | 0.55 |
| 23:DB:2714:G:O2' | 23:DB:2715:C:H5' | 2.05 | 0.55 |
| 23:DB:2720:U:H2' | 23:DB:2721:A:C8 | 2.42 | 0.55 |
| 23:DB:438:G:H2' | 23:DB:439:A:H8 | 1.72 | 0.55 |
| 25:DC:75:ALA:CB | 25:DC:95:TYR:HA | 2.37 | 0.55 |
| 34:DM:21:ALA:HB2 | 34:DM:100:LYS:HG2 | 1.88 | 0.55 |
| 43:DW:18:LYS:N | 43:DW:35:ILE:HG23 | 2.22 | 0.55 |
| 1:AA:1004:A:C8 | 1:AA:1025:U:H1' | 2.42 | 0.55 |
| 1:AA:1147:C:H2' | 1:AA:1148:U:C6 | 2.42 | 0.55 |
| 1:AA:1332:A:H2' | 1:AA:1333:A:C8 | 2.42 | 0.55 |
| 1:AA:230:G:H2' | 1:AA:231:U:O4' | 2.07 | 0.55 |
| 1:AA:747:A:H2' | 1:AA:748:G:O4' | 2.07 | 0.55 |
| 1:AA:858:G:O6 | 1:AA:869:G:H3' | 2.07 | 0.55 |
| 20:AB:205:ALA:HB3 | 20:AB:208:ALA:CB | 2.37 | 0.55 |
| 20:AB:33:ALA:HA | 20:AB:38:HIS:HA | 1.87 | 0.55 |
| 3:AD:24:VAL:HG13 | 3:AD:160:LEU:HB3 | 1.87 | 0.55 |
| 4:AE:148:SER:OG | 4:AE:151:MET:HB2 | 2.07 | 0.55 |
| 8:AI:46:VAL:O | 8:AI:79:ARG:HG3 | 2.06 | 0.55 |
| 11:AL:41:PRO:HB3 | 11:AL:49:ARG:NH1 | 2.22 | 0.55 |
| 19:AT:53:MET:HA | 19:AT:56:ILE:HD12 | 1.89 | 0.55 |
| 23:BB:1714:U:H3' | 23:BB:1715:G:C5' | 2.36 | 0.55 |
| 23:BB:1831:G:H2' | 23:BB:1832:C:C6 | 2.42 | 0.55 |
| 23:BB:782:A:N3 | 25:BC:224:MET:HB3 | 2.21 | 0.55 |
| 23:BB:83:A:C6 | 23:BB:101:A:H5' | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:909:A:H2' | 23:BB:912:C:H5 | 1.71 | 0.55 |
| 25:BC:145:MET:HB2 | 25:BC:152:GLN:NE2 | 2.21 | 0.55 |
| 30:BH:73:ASN:N | 30:BH:73:ASN:HD22 | 2.04 | 0.55 |
| 52:BI:10:LEU:HD12 | 52:BI:10:LEU:O | 2.06 | 0.55 |
| 52:BI:5:GLN:HG2 | 52:BI:6:ALA:N | 2.22 | 0.55 |
| 31:BJ:89:PHE:CE1 | 31:BJ:93:ILE:HD13 | 2.40 | 0.55 |
| 24:BV:9:ARG:CZ | 24:BV:20:LEU:HD11 | 2.37 | 0.55 |
| 1:CA:189:A:H2' | 1:CA:190:A:C8 | 2.41 | 0.55 |
| 1:CA:522:C:H2' | 1:CA:523:A:O4' | 2.07 | 0.55 |
| 1:CA:782:A:H2' | 1:CA:783:C:O4' | 2.06 | 0.55 |
| 3:CD:2:ARG:HH22 | 3:CD:132:ALA:HB3 | 1.72 | 0.55 |
| 6:CG:72:VAL:HG12 | 6:CG:89:GLU:HA | 1.88 | 0.55 |
| 18:CS:63:ASP:O | 18:CS:66:VAL:HG22 | 2.07 | 0.55 |
| 21:CU:39:LYS:N | 21:CU:40:PRO:HD2 | 2.21 | 0.55 |
| 21:CU:3:ILE:HD12 | 21:CU:3:ILE:N | 2.21 | 0.55 |
| 48:D1:26:LYS:HD2 | 48:D1:30:PRO:HA | 1.89 | 0.55 |
| 22:DA:14:U:H5' | 22:DA:70:C:O2' | 2.07 | 0.55 |
| 23:DB:2037:A:H2' | 23:DB:2038:G:H8 | 1.71 | 0.55 |
| 23:DB:2106:U:H2' | 23:DB:2107:G:H8 | 1.72 | 0.55 |
| 23:DB:2216:G:H2' | 23:DB:2217:G:H8 | 1.72 | 0.55 |
| 23:DB:2247:A:H3' | 56:DB:3580:HOH:O | 2.06 | 0.55 |
| 23:DB:2547:A:H2' | 23:DB:2548:U:C6 | 2.42 | 0.55 |
| 23:DB:2704:C:H2' | 23:DB:2705:A:O4' | 2.07 | 0.55 |
| 23:DB:2803:G:H2' | 23:DB:2804:U:H6 | 1.72 | 0.55 |
| 25:DC:105:ALA:HB1 | 25:DC:109:LEU:HD11 | 1.87 | 0.55 |
| 25:DC:43:ASN:HB3 | 25:DC:45:ASN:HD22 | 1.71 | 0.55 |
| 27:DE:29:HIS:HA | 27:DE:32:VAL:HG22 | 1.89 | 0.55 |
| 30:DH:131:SER:OG | 30:DH:132:PHE:N | 2.40 | 0.55 |
| 30:DH:94:ILE:HG22 | 30:DH:122:LEU:HB3 | 1.88 | 0.55 |
| 52:DI:129:GLU:HB3 | 52:DI:133:ARG:HH12 | 1.71 | 0.55 |
| 31:DJ:55:ILE:CB | 31:DJ:123:LYS:HB2 | 2.37 | 0.55 |
| 34:DM:35:ALA:HB2 | 34:DM:100:LYS:HB2 | 1.89 | 0.55 |
| 39:DR:39:LEU:HA | 39:DR:49:ILE:HG12 | 1.89 | 0.55 |
| 39:DR:68:ARG:NH2 | 39:DR:90:ARG:HG2 | 2.22 | 0.55 |
| 23:DB:496:G:H1' | 40:DS:61:ASN:HD21 | 1.71 | 0.55 |
| 41:DT:69:ARG:HB2 | 41:DT:75:GLY:N | 2.22 | 0.55 |
| 24:DV:80:HIS:HD2 | 24:DV:82:TYR:H | 1.54 | 0.55 |
| 44:DX:23:ARG:HA | 44:DX:27:ASN:ND2 | 2.21 | 0.55 |
| 46:DZ:5:CYS:HB2 | 46:DZ:10:LYS:HB2 | 1.89 | 0.55 |
| 1:AA:1349:A:H2' | 1:AA:1350:A:O4' | 2.07 | 0.55 |
| 1:AA:153:C:H2' | 1:AA:154:U:C6 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:235:C:H2' | 1:AA:236:A:H8 | 1.69 | 0.55 |
| 1:AA:474:G:H2' | 1:AA:475:C:H6 | 1.72 | 0.55 |
| 1:AA:80:A:N3 | 1:AA:81:A:H1' | 2.22 | 0.55 |
| 2:AC:142:ARG:HH21 | 2:AC:143:LEU:HD21 | 1.72 | 0.55 |
| 9:AJ:53:ILE:CG2 | 9:AJ:61:ALA:HB1 | 2.37 | 0.55 |
| 23:BB:1133:A:H5' | 23:BB:1134:A:OP1 | 2.07 | 0.55 |
| 23:BB:126:A:O5' | 49:B2:19:ARG:HB2 | 2.07 | 0.55 |
| 23:BB:132:G:H2' | 23:BB:133:U:C6 | 2.41 | 0.55 |
| 23:BB:1709:U:H2' | 23:BB:1710:G:C8 | 2.42 | 0.55 |
| 23:BB:417:C:H2' | 23:BB:418:C:H6 | 1.71 | 0.55 |
| 23:BB:438:G:H2' | 23:BB:439:A:H8 | 1.72 | 0.55 |
| 23:BB:699:A:H4' | 23:BB:1634:A:N7 | 2.22 | 0.55 |
| 23:BB:812:C:H4' | 38:BQ:12:ARG:NH2 | 2.22 | 0.55 |
| 28:BF:106:ALA:HA | 28:BF:135:ILE:CD1 | 2.37 | 0.55 |
| 28:BF:134:GLN:C | 28:BF:136:ILE:H | 2.11 | 0.55 |
| 29:BG:34:ARG:NH1 | 29:BG:34:ARG:HG2 | 2.21 | 0.55 |
| 29:BG:25:ILE:HG22 | 29:BG:78:VAL:HG21 | 1.88 | 0.55 |
| 29:BG:84:LYS:HG3 | 29:BG:132:LEU:N | 2.21 | 0.55 |
| 31:BJ:4:PHE:CG | 31:BJ:5:THR:N | 2.75 | 0.55 |
| 40:BS:6:LYS:HB2 | 40:BS:103:ILE:O | 2.07 | 0.55 |
| 46:BZ:20:HIS:O | 46:BZ:21:ALA:HB3 | 2.07 | 0.55 |
| 1:CA:17:U:O2' | 1:CA:18:C:H5' | 2.06 | 0.55 |
| 1:CA:484:G:H5' | 1:CA:486:U:H5' | 1.88 | 0.55 |
| 1:CA:674:G:H2' | 1:CA:675:A:C8 | 2.38 | 0.55 |
| 1:CA:709:U:H2' | 1:CA:710:G:C8 | 2.41 | 0.55 |
| 1:CA:736:C:H2' | 1:CA:737:C:C6 | 2.42 | 0.55 |
| 20:CB:75:ALA:O | 20:CB:79:VAL:HG23 | 2.07 | 0.55 |
| 12:CM:18:LEU:HB2 | 12:CM:29:SER:OG | 2.05 | 0.55 |
| 18:CS:24:SER:HB2 | 18:CS:27:LYS:HE3 | 1.88 | 0.55 |
| 22:DA:49:C:H2' | 22:DA:50:A:C8 | 2.42 | 0.55 |
| 23:DB:1495:A:O2' | 23:DB:1496:A:H5' | 2.07 | 0.55 |
| 23:DB:1508:A:H5' | 23:DB:1509:A:C6 | 2.42 | 0.55 |
| 23:DB:1553:A:O2' | 23:DB:1554:U:H2' | 2.06 | 0.55 |
| 23:DB:189:G:H2' | 23:DB:205:G:H22 | 1.72 | 0.55 |
| 23:DB:2455:G:H2' | 23:DB:2456:C:C6 | 2.42 | 0.55 |
| 23:DB:596:U:H2' | 23:DB:597:G:H8 | 1.72 | 0.55 |
| 23:DB:638:G:H2' | 23:DB:639:U:C6 | 2.42 | 0.55 |
| 23:DB:2579:C:HO2' | 26:DD:136:ASN:HA | 1.72 | 0.55 |
| 26:DD:8:LYS:HG2 | 26:DD:197:THR:H | 1.72 | 0.55 |
| 28:DF:134:GLN:C | 28:DF:136:ILE:H | 2.10 | 0.55 |
| 29:DG:8:VAL:CG1 | 29:DG:49:LEU:HB3 | 2.32 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DG:85:LYS:HB2 | 29:DG:164:ALA:CB | 2.36 | 0.55 |
| 23:DB:1098:A:C2' | 52:DI:4:VAL:N | 2.70 | 0.55 |
| 33:DL:41:ARG:HG2 | 33:DL:41:ARG:HH21 | 1.73 | 0.55 |
| 33:DL:91:ASP:OD1 | 33:DL:92:LEU:HG | 2.07 | 0.55 |
| 34:DM:126:ILE:N | 34:DM:126:ILE:HD12 | 2.22 | 0.55 |
| 34:DM:67:VAL:HG11 | 34:DM:102:LEU:HD22 | 1.88 | 0.55 |
| 40:DS:95:ARG:HG3 | 40:DS:97:LEU:HD13 | 1.89 | 0.55 |
| 42:DU:66:VAL:O | 42:DU:69:VAL:HG22 | 2.07 | 0.55 |
| 43:DW:31:LEU:N | 43:DW:60:ALA:HB3 | 2.22 | 0.55 |
| 46:DZ:41:GLU:O | 46:DZ:44:LYS:HD2 | 2.06 | 0.55 |
| 1:AA:474:G:H2' | 1:AA:475:C:C6 | 2.42 | 0.54 |
| 1:AA:777:A:H2' | 1:AA:778:G:H8 | 1.72 | 0.54 |
| 3:AD:90:LEU:HD11 | 3:AD:194:ILE:CD1 | 2.37 | 0.54 |
| 3:AD:24:VAL:CG1 | 3:AD:160:LEU:HB3 | 2.37 | 0.54 |
| 7:AH:123:GLU:HG2 | 7:AH:124:ILE:O | 2.07 | 0.54 |
| 9:AJ:93:ALA:HB3 | 9:AJ:96:VAL:HG22 | 1.89 | 0.54 |
| 12:AM:89:ARG:HB3 | 12:AM:96:VAL:HG22 | 1.90 | 0.54 |
| 16:AQ:37:ILE:HG22 | 16:AQ:38:LYS:H | 1.70 | 0.54 |
| 48:B1:39:ASP:OD1 | 48:B1:42:VAL:HG23 | 2.08 | 0.54 |
| 23:BB:1438:U:H2' | 23:BB:1439:A:O4' | 2.08 | 0.54 |
| 23:BB:1570:A:H2' | 23:BB:1571:A:C8 | 2.42 | 0.54 |
| 23:BB:2135:A:C2 | 23:BB:2136:G:H1' | 2.42 | 0.54 |
| 23:BB:418:C:H2' | 23:BB:419:U:C6 | 2.42 | 0.54 |
| 23:BB:971:G:H2' | 23:BB:972:A:O4' | 2.07 | 0.54 |
| 27:BE:173:THR:HA | 27:BE:199:MET:HE1 | 1.88 | 0.54 |
| 30:BH:128:HIS:O | 30:BH:143:ILE:HA | 2.07 | 0.54 |
| 34:BM:60:GLN:H | 34:BM:60:GLN:HE21 | 1.51 | 0.54 |
| 40:BS:18:ARG:HB3 | 40:BS:76:VAL:CG2 | 2.37 | 0.54 |
| 1:CA:41:G:H2' | 1:CA:42:G:H8 | 1.72 | 0.54 |
| 20:CB:172:ILE:H | 20:CB:172:ILE:HD12 | 1.71 | 0.54 |
| 3:CD:24:VAL:CG1 | 3:CD:160:LEU:HB3 | 2.37 | 0.54 |
| 9:CJ:40:ILE:HB | 9:CJ:73:LEU:HB3 | 1.89 | 0.54 |
| 10:CK:83:VAL:HB | 10:CK:109:ILE:HG23 | 1.90 | 0.54 |
| 23:DB:1198:U:H2' | 23:DB:1199:U:H6 | 1.72 | 0.54 |
| 23:DB:1197:G:H2' | 23:DB:1198:U:H6 | 1.72 | 0.54 |
| 23:DB:1531:C:H2' | 23:DB:1532:A:C8 | 2.42 | 0.54 |
| 23:DB:2828:G:O2' | 23:DB:2829:A:H5' | 2.08 | 0.54 |
| 23:DB:321:U:OP2 | 27:DE:130:LYS:HA | 2.07 | 0.54 |
| 23:DB:823:C:O2' | 23:DB:824:U:H5' | 2.07 | 0.54 |
| 25:DC:209:ALA:O | 25:DC:213:ARG:HB2 | 2.07 | 0.54 |
| 28:DF:78:ILE:N | 28:DF:78:ILE:HD12 | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DG:34:ARG:HG2 | 29:DG:34:ARG:NH1 | 2.21 | 0.54 |
| 31:DJ:45:THR:OG1 | 31:DJ:48:VAL:HB | 2.07 | 0.54 |
| 33:DL:111:ILE:HG22 | 33:DL:112:LEU:N | 2.22 | 0.54 |
| 39:DR:14:VAL:CG2 | 39:DR:15:SER:H | 2.16 | 0.54 |
| 40:DS:96:ILE:HG23 | 40:DS:96:ILE:O | 2.06 | 0.54 |
| 1:AA:251:G:H1 | 1:AA:271:C:H41 | 1.53 | 0.54 |
| 8:AI:18:VAL:HA | 8:AI:64:ILE:HG13 | 1.88 | 0.54 |
| 8:AI:22:PRO:HA | 8:AI:60:LEU:HB2 | 1.87 | 0.54 |
| 13:AN:20:PHE:C | 13:AN:22:LYS:H | 2.10 | 0.54 |
| 15:AP:25:ARG:HD3 | 15:AP:25:ARG:N | 2.22 | 0.54 |
| 19:AT:54:GLN:N | 19:AT:55:PRO:HD2 | 2.22 | 0.54 |
| 23:BB:1930:G:H2' | 23:BB:1968:G:H1 | 1.71 | 0.54 |
| 23:BB:2196:C:O2' | 23:BB:2197:U:H5' | 2.07 | 0.54 |
| 23:BB:513:A:O5' | 23:BB:513:A:H8 | 1.91 | 0.54 |
| 23:BB:566:U:H5'' | 33:BL:29:LYS:NZ | 2.22 | 0.54 |
| 25:BC:209:ALA:O | 25:BC:213:ARG:HB2 | 2.07 | 0.54 |
| 25:BC:77:VAL:CG2 | 25:BC:113:ASP:H | 2.19 | 0.54 |
| 25:BC:78:GLU:HB2 | 25:BC:92:LEU:HD23 | 1.89 | 0.54 |
| 27:BE:188:MET:HE2 | 27:BE:193:VAL:HG22 | 1.89 | 0.54 |
| 52:BI:52:LEU:HD21 | 52:BI:81:LYS:HZ2 | 1.72 | 0.54 |
| 32:BK:8:LEU:N | 32:BK:8:LEU:HD12 | 2.22 | 0.54 |
| 33:BL:42:SER:C | 33:BL:44:GLY:H | 2.10 | 0.54 |
| 33:BL:4:ASN:N | 33:BL:4:ASN:HD22 | 2.04 | 0.54 |
| 34:BM:17:ASN:HD21 | 34:BM:95:LEU:HG | 1.72 | 0.54 |
| 35:BN:29:VAL:O | 35:BN:78:LYS:HE3 | 2.07 | 0.54 |
| 37:BP:88:ARG:HB2 | 37:BP:112:ARG:CZ | 2.37 | 0.54 |
| 39:BR:79:ARG:CD | 39:BR:80:ARG:HH21 | 2.20 | 0.54 |
| 42:BU:80:ASP:HB3 | 42:BU:96:LYS:N | 2.08 | 0.54 |
| 1:CA:17:U:H4' | 1:CA:1079:G:O2' | 2.08 | 0.54 |
| 1:CA:1053:G:HO2' | 1:CA:1199:U:H5 | 1.55 | 0.54 |
| 1:CA:1275:A:H2' | 1:CA:1276:G:O4' | 2.07 | 0.54 |
| 1:CA:490:C:H2' | 1:CA:491:G:C8 | 2.42 | 0.54 |
| 1:CA:734:G:H21 | 17:CR:63:TYR:HE1 | 1.54 | 0.54 |
| 20:CB:13:VAL:HG11 | 20:CB:207:ARG:HG2 | 1.87 | 0.54 |
| 2:CC:156:LEU:HD11 | 2:CC:165:GLU:HB2 | 1.89 | 0.54 |
| 4:CE:73:VAL:HB | 4:CE:75:LEU:HD21 | 1.88 | 0.54 |
| 12:CM:17:ALA:HB2 | 12:CM:44:ILE:HD11 | 1.89 | 0.54 |
| 1:CA:1317:C:OP1 | 13:CN:56:PRO:HD2 | 2.06 | 0.54 |
| 23:DB:1441:G:H2' | 23:DB:1442:U:C6 | 2.41 | 0.54 |
| 23:DB:1925:C:C2' | 23:DB:1926:U:H5'' | 2.34 | 0.54 |
| 23:DB:226:A:H1' | 23:DB:230:G:N2 | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:2741:A:H2' | 23:DB:2742:G:O4' | 2.06 | 0.54 |
| 23:DB:2772:C:H2' | 23:DB:2773:C:C6 | 2.42 | 0.54 |
| 23:DB:2840:C:H2' | 23:DB:2841:C:H6 | 1.72 | 0.54 |
| 23:DB:2861:U:H2' | 23:DB:2862:G:C8 | 2.42 | 0.54 |
| 23:DB:856:G:H2' | 23:DB:857:G:C8 | 2.41 | 0.54 |
| 25:DC:250:GLN:O | 25:DC:250:GLN:HG2 | 2.06 | 0.54 |
| 26:DD:62:LYS:HB2 | 26:DD:63:PRO:HD3 | 1.89 | 0.54 |
| 27:DE:21:ARG:HG3 | 27:DE:22:ASP:N | 2.21 | 0.54 |
| 28:DF:56:LEU:HD22 | 28:DF:59:ILE:HD12 | 1.88 | 0.54 |
| 29:DG:36:LEU:N | 29:DG:36:LEU:HD22 | 2.22 | 0.54 |
| 34:DM:17:ASN:HD21 | 34:DM:95:LEU:HG | 1.71 | 0.54 |
| 36:DO:100:HIS:HA | 36:DO:104:GLN:HE21 | 1.71 | 0.54 |
| 37:DP:7:LEU:HA | 37:DP:10:GLU:HG2 | 1.88 | 0.54 |
| 38:DQ:91:ARG:HB2 | 39:DR:11:GLN:OE1 | 2.07 | 0.54 |
| 46:DZ:6:GLN:NE2 | 46:DZ:50:ARG:N | 2.54 | 0.54 |
| 46:DZ:7:VAL:HG21 | 46:DZ:59:ILE:CD1 | 2.37 | 0.54 |
| 1:AA:1166:G:H2' | 1:AA:1168:U:OP2 | 2.07 | 0.54 |
| 1:AA:1524:C:H2' | 1:AA:1525:G:C8 | 2.42 | 0.54 |
| 1:AA:31:G:H5' | 1:AA:306:A:C2 | 2.42 | 0.54 |
| 1:AA:343:U:O2' | 1:AA:344:A:H2' | 2.07 | 0.54 |
| 1:AA:555:U:H2' | 1:AA:556:C:C6 | 2.42 | 0.54 |
| 12:AM:33:LEU:HD13 | 12:AM:39:ALA:O | 2.07 | 0.54 |
| 12:AM:50:GLY:O | 12:AM:54:THR:HG23 | 2.08 | 0.54 |
| 48:B1:33:LEU:HB3 | 48:B1:51:ALA:CB | 2.36 | 0.54 |
| 22:BA:30:C:H2' | 22:BA:30:C:O2 | 2.07 | 0.54 |
| 23:BB:1168:G:H2' | 23:BB:1169:A:H8 | 1.72 | 0.54 |
| 23:BB:154:U:H2' | 23:BB:155:A:H8 | 1.72 | 0.54 |
| 23:BB:528:A:C2 | 23:BB:2043:C:H4' | 2.42 | 0.54 |
| 23:BB:2547:A:H2' | 23:BB:2548:U:C6 | 2.43 | 0.54 |
| 23:BB:2665:A:H2' | 23:BB:2666:C:O2 | 2.07 | 0.54 |
| 23:BB:2741:A:H2' | 23:BB:2742:G:O4' | 2.08 | 0.54 |
| 23:BB:753:A:H2' | 23:BB:754:U:H6 | 1.70 | 0.54 |
| 23:BB:934:U:H2' | 23:BB:935:C:C6 | 2.42 | 0.54 |
| 26:BD:13:ARG:HH12 | 37:BP:74:GLN:NE2 | 2.06 | 0.54 |
| 23:BB:2746:U:H5' | 29:BG:138:GLN:HA | 1.89 | 0.54 |
| 29:BG:24:THR:HA | 29:BG:33:THR:O | 2.08 | 0.54 |
| 30:BH:83:LYS:HD2 | 30:BH:91:PHE:CG | 2.43 | 0.54 |
| 32:BK:15:GLY:HA2 | 32:BK:46:ALA:HA | 1.89 | 0.54 |
| 35:BN:97:ILE:HD12 | 35:BN:98:LEU:N | 2.20 | 0.54 |
| 37:BP:20:ARG:HB3 | 37:BP:23:ASP:CG | 2.28 | 0.54 |
| 40:BS:24:ILE:HG23 | 40:BS:32:ALA:HB1 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BV:72:VAL:HG21 | 24:BV:91:PHE:CB | 2.37 | 0.54 |
| 1:CA:1261:A:H1' | 1:CA:1275:A:C2 | 2.43 | 0.54 |
| 1:CA:1326:U:H2' | 1:CA:1327:C:H6 | 1.72 | 0.54 |
| 1:CA:1477:U:H2' | 1:CA:1478:U:C6 | 2.42 | 0.54 |
| 1:CA:179:A:H2' | 1:CA:180:U:C6 | 2.42 | 0.54 |
| 1:CA:272:C:H2' | 1:CA:273:U:C6 | 2.42 | 0.54 |
| 1:CA:596:A:H2' | 1:CA:597:G:H8 | 1.73 | 0.54 |
| 4:CE:56:PRO:HG2 | 4:CE:57:ALA:H | 1.71 | 0.54 |
| 7:CH:123:GLU:HG2 | 7:CH:124:ILE:O | 2.07 | 0.54 |
| 10:CK:22:ILE:HD12 | 10:CK:84:MET:O | 2.07 | 0.54 |
| 13:CN:60:ARG:HD3 | 13:CN:62:ARG:NH2 | 2.22 | 0.54 |
| 13:CN:5:MET:HE3 | 13:CN:60:ARG:HH11 | 1.72 | 0.54 |
| 17:CR:58:ILE:H | 17:CR:58:ILE:HD12 | 1.72 | 0.54 |
| 48:D1:25:ASN:OD1 | 48:D1:27:ARG:HB2 | 2.07 | 0.54 |
| 23:DB:2784:U:H2' | 23:DB:2785:C:H6 | 1.72 | 0.54 |
| 23:DB:416:U:H2' | 23:DB:417:C:C6 | 2.42 | 0.54 |
| 23:DB:692:C:H2' | 23:DB:693:A:H8 | 1.72 | 0.54 |
| 52:DI:2:LYS:NZ | 52:DI:2:LYS:HB3 | 2.22 | 0.54 |
| 38:DQ:78:PHE:O | 38:DQ:82:LEU:HG | 2.06 | 0.54 |
| 39:DR:8:GLY:HA3 | 39:DR:23:GLU:HB2 | 1.88 | 0.54 |
| 24:DV:42:LEU:HD11 | 24:DV:89:ILE:HD11 | 1.88 | 0.54 |
| 44:DX:6:LEU:C | 44:DX:8:GLU:H | 2.10 | 0.54 |
| 1:AA:1446:A:H2' | 1:AA:1447:A:H5'' | 1.89 | 0.54 |
| 1:AA:1450:U:H2' | 1:AA:1452:C:C5 | 2.42 | 0.54 |
| 1:AA:224:U:H2' | 1:AA:225:C:H6 | 1.71 | 0.54 |
| 1:AA:384:G:H2' | 1:AA:385:C:H6 | 1.73 | 0.54 |
| 1:AA:499:A:H4' | 1:AA:500:G:OP1 | 2.07 | 0.54 |
| 1:AA:5:U:H4' | 1:AA:6:G:H5' | 1.90 | 0.54 |
| 1:AA:90:C:H2' | 1:AA:91:U:H5 | 1.72 | 0.54 |
| 20:AB:75:ALA:O | 20:AB:79:VAL:HG23 | 2.07 | 0.54 |
| 2:AC:31:ASN:ND2 | 2:AC:58:ARG:HE | 2.05 | 0.54 |
| 23:BB:1476:U:H4' | 23:BB:1732:C:O2' | 2.08 | 0.54 |
| 23:BB:2186:G:H2' | 23:BB:2187:U:H6 | 1.73 | 0.54 |
| 23:BB:2852:G:H2' | 23:BB:2853:C:H6 | 1.69 | 0.54 |
| 23:BB:642:U:O2 | 23:BB:644:A:H3' | 2.07 | 0.54 |
| 23:BB:674:G:H1' | 27:BE:69:ARG:HE | 1.73 | 0.54 |
| 23:BB:927:A:H2' | 23:BB:928:A:C8 | 2.43 | 0.54 |
| 27:BE:161:ALA:HA | 27:BE:164:LEU:HD12 | 1.89 | 0.54 |
| 28:BF:72:SER:CA | 28:BF:80:GLN:H | 2.21 | 0.54 |
| 29:BG:132:LEU:HD23 | 29:BG:132:LEU:N | 2.22 | 0.54 |
| 30:BH:130:VAL:C | 30:BH:142:VAL:HB | 2.27 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:BH:69:ALA:O | 30:BH:140:ALA:HB2 | 2.08 | 0.54 |
| 52:BI:112:LYS:O | 52:BI:116:MET:HG3 | 2.07 | 0.54 |
| 35:BN:98:LEU:HG | 47:B0:42:ILE:HD11 | 1.89 | 0.54 |
| 36:BO:111:ARG:HD2 | 36:BO:117:PHE:O | 2.07 | 0.54 |
| 39:BR:68:ARG:NH2 | 39:BR:90:ARG:HG2 | 2.22 | 0.54 |
| 39:BR:79:ARG:NE | 39:BR:80:ARG:HH21 | 2.05 | 0.54 |
| 44:BX:6:LEU:C | 44:BX:8:GLU:H | 2.11 | 0.54 |
| 46:BZ:18:ARG:HG3 | 46:BZ:22:LEU:HA | 1.88 | 0.54 |
| 46:BZ:41:GLU:O | 46:BZ:44:LYS:HD2 | 2.07 | 0.54 |
| 1:CA:1525:G:O2' | 1:CA:1526:G:H5' | 2.07 | 0.54 |
| 1:CA:190:A:H2' | 1:CA:191:G:O4' | 2.08 | 0.54 |
| 1:CA:552:U:O2' | 1:CA:553:A:H5' | 2.07 | 0.54 |
| 20:CB:199:ILE:HG21 | 20:CB:212:TYR:CE2 | 2.42 | 0.54 |
| 1:CA:437:U:H4' | 3:CD:153:ARG:NH1 | 2.21 | 0.54 |
| 3:CD:72:ARG:HD3 | 3:CD:203:TYR:CZ | 2.42 | 0.54 |
| 10:CK:124:LYS:CA | 21:CU:34:ARG:HB3 | 2.36 | 0.54 |
| 48:D1:39:ASP:OD1 | 48:D1:42:VAL:HG23 | 2.07 | 0.54 |
| 48:D1:3:GLY:O | 48:D1:4:ILE:HG12 | 2.07 | 0.54 |
| 23:DB:1268:A:H2' | 23:DB:1269:A:O4' | 2.07 | 0.54 |
| 23:DB:2083:G:H2' | 23:DB:2084:C:H6 | 1.71 | 0.54 |
| 23:DB:2333:A:H4' | 23:DB:2334:U:C5' | 2.37 | 0.54 |
| 23:DB:2615:U:C2 | 47:D0:3:GLN:HA | 2.43 | 0.54 |
| 23:DB:285:G:H2' | 23:DB:286:U:O4' | 2.08 | 0.54 |
| 23:DB:997:G:O2' | 23:DB:998:C:H5' | 2.07 | 0.54 |
| 25:DC:77:VAL:CG2 | 25:DC:113:ASP:H | 2.20 | 0.54 |
| 25:DC:129:LEU:HD23 | 25:DC:130:PRO:CD | 2.35 | 0.54 |
| 23:DB:1657:U:O2' | 26:DD:138:LEU:HD12 | 2.07 | 0.54 |
| 28:DF:62:GLN:HG3 | 28:DF:91:ARG:HH11 | 1.72 | 0.54 |
| 52:DI:1:ALA:CB | 52:DI:2:LYS:HD2 | 2.38 | 0.54 |
| 52:DI:49:GLU:CB | 52:DI:52:LEU:HD12 | 2.38 | 0.54 |
| 31:DJ:4:PHE:CG | 31:DJ:5:THR:N | 2.76 | 0.54 |
| 32:DK:71:ARG:CG | 32:DK:105:ARG:HH21 | 2.21 | 0.54 |
| 41:DT:76:ARG:HH21 | 41:DT:77:ARG:HB2 | 1.72 | 0.54 |
| 24:DV:35:GLU:OE1 | 24:DV:93:ARG:HD3 | 2.07 | 0.54 |
| 46:DZ:63:GLY:O | 46:DZ:67:VAL:HG23 | 2.07 | 0.54 |
| 1:AA:1275:A:H2' | 1:AA:1276:G:O4' | 2.07 | 0.54 |
| 2:AC:39:ARG:HG3 | 2:AC:56:ILE:HD11 | 1.90 | 0.54 |
| 5:AF:22:ILE:HD11 | 5:AF:60:VAL:HG11 | 1.90 | 0.54 |
| 8:AI:20:ILE:HD12 | 8:AI:20:ILE:N | 2.22 | 0.54 |
| 10:AK:17:ASP:C | 10:AK:36:ARG:HH12 | 2.11 | 0.54 |
| 11:AL:98:ARG:HB2 | 11:AL:116:TYR:HA | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:B0:5:ASN:O | 47:B0:7:PRO:HD3 | 2.08 | 0.54 |
| 50:B3:55:GLY:HA2 | 50:B3:58:ILE:HD12 | 1.90 | 0.54 |
| 51:B4:10:LEU:HD22 | 51:B4:33:HIS:CD2 | 2.42 | 0.54 |
| 23:BB:1230:A:H2' | 23:BB:1231:U:C6 | 2.42 | 0.54 |
| 23:BB:1319:C:O2' | 23:BB:1320:C:H5' | 2.08 | 0.54 |
| 23:BB:2074:U:H2' | 23:BB:2075:U:C6 | 2.42 | 0.54 |
| 23:BB:2199:A:H3' | 23:BB:2200:C:H6 | 1.72 | 0.54 |
| 23:BB:2346:A:H3' | 23:BB:2347:C:H5'' | 1.87 | 0.54 |
| 23:BB:2412:A:H2' | 23:BB:2413:G:O4' | 2.07 | 0.54 |
| 23:BB:638:G:H2' | 23:BB:639:U:C6 | 2.41 | 0.54 |
| 23:BB:784:G:C6 | 25:BC:227:VAL:HG11 | 2.42 | 0.54 |
| 26:BD:165:MET:HG2 | 26:BD:166:GLY:N | 2.23 | 0.54 |
| 29:BG:122:ALA:HA | 29:BG:132:LEU:HA | 1.90 | 0.54 |
| 29:BG:8:VAL:CG1 | 29:BG:49:LEU:HB3 | 2.34 | 0.54 |
| 31:BJ:64:VAL:HG22 | 31:BJ:68:LYS:HD3 | 1.90 | 0.54 |
| 32:BK:105:ARG:HD2 | 32:BK:122:VAL:CG1 | 2.37 | 0.54 |
| 37:BP:103:THR:HG22 | 37:BP:104:GLY:H | 1.72 | 0.54 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C6 | 2.41 | 0.54 |
| 1:CA:1147:C:H2' | 1:CA:1148:U:C6 | 2.42 | 0.54 |
| 1:CA:1081:A:OP1 | 4:CE:22:LYS:HB2 | 2.06 | 0.54 |
| 11:CL:7:VAL:HG22 | 16:CQ:33:TYR:CD1 | 2.42 | 0.54 |
| 14:CO:28:VAL:HB | 14:CO:80:LEU:HD11 | 1.88 | 0.54 |
| 15:CP:6:LEU:HB3 | 15:CP:17:TYR:HB3 | 1.89 | 0.54 |
| 18:CS:41:PRO:HA | 18:CS:66:VAL:HG11 | 1.89 | 0.54 |
| 1:CA:1314:C:H3' | 18:CS:5:LYS:NZ | 2.23 | 0.54 |
| 23:DB:115:C:O2' | 23:DB:116:C:H5' | 2.08 | 0.54 |
| 23:DB:1880:U:H2' | 23:DB:1881:C:C6 | 2.42 | 0.54 |
| 23:DB:528:A:N1 | 23:DB:2042:A:H2' | 2.21 | 0.54 |
| 23:DB:2364:C:H2' | 23:DB:2365:G:O4' | 2.07 | 0.54 |
| 23:DB:2722:G:H2' | 23:DB:2723:C:H6 | 1.73 | 0.54 |
| 23:DB:497:A:H2' | 23:DB:498:G:O4' | 2.07 | 0.54 |
| 23:DB:927:A:H2' | 23:DB:928:A:C8 | 2.43 | 0.54 |
| 23:DB:931:U:H3 | 23:DB:1166:G:N2 | 2.06 | 0.54 |
| 23:DB:936:A:H2' | 23:DB:937:C:H6 | 1.72 | 0.54 |
| 27:DE:1:MET:O | 27:DE:13:THR:HA | 2.07 | 0.54 |
| 28:DF:102:LEU:O | 28:DF:103:ILE:HB | 2.07 | 0.54 |
| 32:DK:60:ALA:HB2 | 32:DK:86:LEU:HA | 1.90 | 0.54 |
| 35:DN:49:GLU:HB2 | 35:DN:50:PRO:HD3 | 1.88 | 0.54 |
| 45:DY:37:ARG:HG3 | 45:DY:38:GLU:OE1 | 2.08 | 0.54 |
| 1:AA:1014:A:H4' | 18:AS:13:HIS:CE1 | 2.42 | 0.54 |
| 1:AA:1118:U:H2' | 1:AA:1119:C:H6 | 1.69 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1324:A:H2' | 1:AA:1325:C:O4' | 2.08 | 0.54 |
| 1:AA:1437:A:H2' | 1:AA:1438:G:C8 | 2.43 | 0.54 |
| 1:AA:194:C:O2' | 1:AA:195:A:H5' | 2.07 | 0.54 |
| 1:AA:389:A:H2' | 1:AA:389:A:N3 | 2.23 | 0.54 |
| 20:AB:172:ILE:HD12 | 20:AB:172:ILE:H | 1.71 | 0.54 |
| 3:AD:84:ASN:ND2 | 3:AD:86:GLY:H | 2.05 | 0.54 |
| 4:AE:19:ARG:NH1 | 4:AE:28:ARG:HH22 | 2.05 | 0.54 |
| 6:AG:78:ARG:HD2 | 6:AG:78:ARG:C | 2.28 | 0.54 |
| 11:AL:20:VAL:HG23 | 11:AL:20:VAL:O | 2.08 | 0.54 |
| 48:B1:3:GLY:C | 48:B1:5:ARG:H | 2.11 | 0.54 |
| 23:BB:1164:C:H2' | 23:BB:1165:A:H8 | 1.71 | 0.54 |
| 23:BB:1168:G:H2' | 23:BB:1169:A:C8 | 2.43 | 0.54 |
| 23:BB:1335:C:H2' | 23:BB:1336:A:H8 | 1.72 | 0.54 |
| 23:BB:138:U:C5 | 23:BB:140:C:H1' | 2.43 | 0.54 |
| 23:BB:1401:G:H2' | 23:BB:1402:U:C6 | 2.42 | 0.54 |
| 23:BB:1857:G:O2' | 23:BB:1858:A:H8 | 1.91 | 0.54 |
| 23:BB:2570:G:H2' | 23:BB:2571:U:O4' | 2.08 | 0.54 |
| 23:BB:2751:G:H5' | 29:BG:2:ARG:CD | 2.37 | 0.54 |
| 23:BB:2808:G:HO2' | 23:BB:2809:A:H8 | 1.55 | 0.54 |
| 23:BB:2819:G:H2' | 23:BB:2821:A:N7 | 2.23 | 0.54 |
| 23:BB:545:U:H2' | 23:BB:547:A:OP1 | 2.08 | 0.54 |
| 23:BB:635:C:O2' | 23:BB:639:U:H5" | 2.08 | 0.54 |
| 25:BC:12:ARG:HA | 25:BC:15:VAL:HG23 | 1.89 | 0.54 |
| 25:BC:57:HIS:ND1 | 25:BC:58:LYS:N | 2.56 | 0.54 |
| 26:BD:114:LYS:HB2 | 26:BD:116:LYS:HE3 | 1.89 | 0.54 |
| 28:BF:78:ILE:HD12 | 28:BF:78:ILE:N | 2.22 | 0.54 |
| 22:BA:43:C:C4' | 28:BF:91:ARG:HD2 | 2.38 | 0.54 |
| 29:BG:17:LYS:O | 29:BG:23:ILE:HG23 | 2.08 | 0.54 |
| 36:BO:100:HIS:HA | 36:BO:104:GLN:HE21 | 1.72 | 0.54 |
| 39:BR:31:GLU:H | 39:BR:63:VAL:CG2 | 2.20 | 0.54 |
| 40:BS:41:LYS:HB3 | 40:BS:41:LYS:NZ | 2.23 | 0.54 |
| 23:BB:2354:C:H4' | 43:BW:31:LEU:HD23 | 1.90 | 0.54 |
| 1:CA:1171:A:H2' | 1:CA:1172:C:C6 | 2.42 | 0.54 |
| 1:CA:1332:A:H2' | 1:CA:1333:A:H8 | 1.72 | 0.54 |
| 1:CA:265:G:H2' | 1:CA:267:C:H5 | 1.72 | 0.54 |
| 1:CA:817:C:H1' | 1:CA:819:A:C5' | 2.35 | 0.54 |
| 1:CA:968:A:C8 | 1:CA:1062:U:H4' | 2.42 | 0.54 |
| 10:CK:27:ASN:O | 10:CK:56:LYS:HE3 | 2.08 | 0.54 |
| 50:D3:7:ARG:O | 50:D3:11:LYS:HG3 | 2.08 | 0.54 |
| 22:DA:43:C:C4' | 28:DF:91:ARG:HD2 | 2.38 | 0.54 |
| 23:DB:1081:U:H5' | 52:DI:126:ARG:NH1 | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:67:U:H2' | 23:DB:68:G:H8 | 1.72 | 0.54 |
| 23:DB:794:A:H2' | 23:DB:795:C:C6 | 2.43 | 0.54 |
| 23:DB:794:A:H2' | 23:DB:795:C:H6 | 1.72 | 0.54 |
| 25:DC:93:VAL:HG12 | 25:DC:101:ARG:O | 2.07 | 0.54 |
| 25:DC:89:ASN:O | 25:DC:105:ALA:HB3 | 2.07 | 0.54 |
| 25:DC:122:ALA:O | 25:DC:123:ILE:C | 2.46 | 0.54 |
| 23:DB:1820:U:OP1 | 25:DC:176:ARG:HD2 | 2.07 | 0.54 |
| 26:DD:178:VAL:O | 26:DD:180:VAL:HG23 | 2.08 | 0.54 |
| 29:DG:26:LYS:HG2 | 29:DG:27:GLY:N | 2.23 | 0.54 |
| 52:DI:79:LEU:HD11 | 52:DI:131:THR:OG1 | 2.07 | 0.54 |
| 36:DO:47:VAL:HG12 | 36:DO:48:LEU:H | 1.72 | 0.54 |
| 40:DS:83:LYS:HB3 | 40:DS:95:ARG:NH1 | 2.22 | 0.54 |
| 41:DT:13:ALA:O | 41:DT:32:LEU:HB2 | 2.07 | 0.54 |
| 1:AA:1017:U:H2' | 1:AA:1018:G:C8 | 2.42 | 0.54 |
| 1:AA:1349:A:OP1 | 8:AI:121:ARG:HB2 | 2.08 | 0.54 |
| 1:AA:1441:A:C2 | 37:BP:113:LEU:HD13 | 2.43 | 0.54 |
| 1:AA:1512:U:H2' | 1:AA:1513:A:C8 | 2.43 | 0.54 |
| 1:AA:501:C:H2' | 1:AA:502:A:H8 | 1.73 | 0.54 |
| 1:AA:95:C:H2' | 1:AA:96:U:H6 | 1.73 | 0.54 |
| 5:AF:70:VAL:HA | 5:AF:73:GLU:HG3 | 1.89 | 0.54 |
| 7:AH:94:VAL:CG2 | 7:AH:101:ALA:HB2 | 2.37 | 0.54 |
| 8:AI:18:VAL:HG13 | 8:AI:64:ILE:HG13 | 1.88 | 0.54 |
| 9:AJ:52:LEU:HB2 | 13:AN:80:ARG:HE | 1.73 | 0.54 |
| 18:AS:38:THR:HG22 | 18:AS:68:HIS:O | 2.08 | 0.54 |
| 19:AT:65:LEU:HG | 19:AT:66:ILE:HD13 | 1.90 | 0.54 |
| 21:AU:35:GLU:HB2 | 21:AU:37:TYR:CZ | 2.43 | 0.54 |
| 22:BA:13:G:H2' | 22:BA:14:U:H5'' | 1.89 | 0.54 |
| 23:BB:1013:C:H2' | 23:BB:1014:A:C8 | 2.42 | 0.54 |
| 23:BB:1320:C:C5 | 23:BB:1329:U:H5'' | 2.42 | 0.54 |
| 23:BB:2008:C:H2' | 23:BB:2009:A:C8 | 2.43 | 0.54 |
| 23:BB:2543:G:H8 | 23:BB:2543:G:H5' | 1.73 | 0.54 |
| 23:BB:2722:G:H4' | 35:BN:4:ARG:HB2 | 1.90 | 0.54 |
| 23:BB:2803:G:H2' | 23:BB:2804:U:C6 | 2.42 | 0.54 |
| 23:BB:497:A:H2' | 23:BB:498:G:O4' | 2.07 | 0.54 |
| 23:BB:854:C:O2' | 23:BB:855:G:H5' | 2.08 | 0.54 |
| 25:BC:122:ALA:O | 25:BC:123:ILE:C | 2.46 | 0.54 |
| 26:BD:121:THR:C | 26:BD:123:LYS:H | 2.11 | 0.54 |
| 26:BD:175:LEU:HD21 | 26:BD:191:GLY:O | 2.07 | 0.54 |
| 27:BE:18:THR:O | 27:BE:110:SER:HB2 | 2.06 | 0.54 |
| 23:BB:1076:C:H4' | 52:BI:94:LYS:HE3 | 1.88 | 0.54 |
| 34:BM:2:LEU:HD23 | 34:BM:46:ILE:HD11 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BP:103:THR:HG22 | 37:BP:104:GLY:N | 2.23 | 0.54 |
| 24:BV:1:MET:O | 24:BV:62:THR:HG23 | 2.08 | 0.54 |
| 1:CA:678:U:H4' | 1:CA:778:G:OP1 | 2.07 | 0.54 |
| 1:CA:715:A:H2' | 1:CA:716:A:C8 | 2.43 | 0.54 |
| 1:CA:79:G:H2' | 1:CA:80:A:C8 | 2.42 | 0.54 |
| 1:CA:961:U:O4' | 1:CA:961:U:O2 | 2.26 | 0.54 |
| 1:CA:8:A:H61 | 3:CD:53:GLN:HE22 | 1.56 | 0.54 |
| 6:CG:129:ASN:HA | 6:CG:134:VAL:HG21 | 1.90 | 0.54 |
| 8:CI:126:PHE:O | 8:CI:128:LYS:N | 2.41 | 0.54 |
| 35:DN:99:LYS:HB2 | 47:D0:41:HIS:HB3 | 1.88 | 0.54 |
| 51:D4:10:LEU:HD13 | 51:D4:33:HIS:HA | 1.90 | 0.54 |
| 22:DA:88:C:H1' | 22:DA:89:U:C6 | 2.43 | 0.54 |
| 23:DB:1347:A:H2' | 23:DB:1348:C:O4' | 2.08 | 0.54 |
| 23:DB:1425:G:H2' | 23:DB:1426:G:C8 | 2.43 | 0.54 |
| 23:DB:2360:G:H4' | 33:DL:61:LEU:HD11 | 1.89 | 0.54 |
| 23:DB:265:A:O2' | 23:DB:266:G:H4' | 2.08 | 0.54 |
| 23:DB:345:A:N3 | 23:DB:346:A:N1 | 2.56 | 0.54 |
| 28:DF:31:GLU:O | 28:DF:32:LYS:O | 2.24 | 0.54 |
| 30:DH:133:GLN:HB3 | 30:DH:139:PHE:HB3 | 1.90 | 0.54 |
| 32:DK:109:SER:C | 32:DK:111:LYS:H | 2.11 | 0.54 |
| 32:DK:15:GLY:HA2 | 32:DK:46:ALA:HA | 1.88 | 0.54 |
| 33:DL:65:GLY:O | 33:DL:66:PHE:HB3 | 2.08 | 0.54 |
| 34:DM:126:ILE:H | 34:DM:126:ILE:HD12 | 1.73 | 0.54 |
| 22:DA:50:A:OP1 | 36:DO:68:LYS:HG3 | 2.06 | 0.54 |
| 38:DQ:4:LYS:HE3 | 38:DQ:8:ILE:HD11 | 1.90 | 0.54 |
| 1:AA:1261:A:H1' | 1:AA:1275:A:C2 | 2.43 | 0.54 |
| 1:AA:1262:C:H2' | 1:AA:1263:C:C6 | 2.43 | 0.54 |
| 1:AA:443:C:H2' | 1:AA:444:G:C8 | 2.43 | 0.54 |
| 1:AA:562:U:H1' | 11:AL:11:ARG:HD2 | 1.90 | 0.54 |
| 1:AA:565:U:H3' | 1:AA:566:G:H2' | 1.90 | 0.54 |
| 4:AE:152:VAL:O | 4:AE:156:ARG:HG2 | 2.08 | 0.54 |
| 4:AE:156:ARG:HB2 | 7:AH:43:GLY:HA3 | 1.90 | 0.54 |
| 13:AN:20:PHE:HB2 | 13:AN:54:SER:OG | 2.07 | 0.54 |
| 15:AP:6:LEU:HB3 | 15:AP:17:TYR:HB3 | 1.89 | 0.54 |
| 33:BL:58:TYR:HB2 | 50:B3:9:ALA:HA | 1.90 | 0.54 |
| 23:BB:1100:C:H2' | 23:BB:1101:U:H6 | 1.72 | 0.54 |
| 23:BB:1242:U:H2' | 23:BB:1243:C:C6 | 2.42 | 0.54 |
| 23:BB:1259:G:H2' | 23:BB:1260:A:H8 | 1.72 | 0.54 |
| 23:BB:1604:C:H5'' | 56:BB:3373:HOH:O | 2.08 | 0.54 |
| 23:BB:1796:U:H2' | 23:BB:1797:G:C8 | 2.42 | 0.54 |
| 23:BB:2101:A:H2' | 23:BB:2102:G:H5'' | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2408:U:O2' | 23:BB:2409:G:H5' | 2.08 | 0.54 |
| 23:BB:278:A:H2' | 23:BB:278:A:N3 | 2.23 | 0.54 |
| 23:BB:2875:C:H2' | 23:BB:2876:G:H8 | 1.72 | 0.54 |
| 23:BB:917:A:C2 | 23:BB:918:A:H1' | 2.43 | 0.54 |
| 23:BB:1565:C:H5'' | 25:BC:17:LYS:HE2 | 1.90 | 0.54 |
| 23:BB:1828:G:O6 | 25:BC:220:ARG:HD2 | 2.08 | 0.54 |
| 29:BG:30:GLY:CA | 29:BG:78:VAL:HA | 2.38 | 0.54 |
| 52:BI:91:LYS:HB2 | 52:BI:94:LYS:HD2 | 1.87 | 0.54 |
| 33:BL:91:ASP:OD1 | 33:BL:92:LEU:HG | 2.07 | 0.54 |
| 36:BO:30:ARG:HG3 | 36:BO:30:ARG:HH11 | 1.72 | 0.54 |
| 42:BU:41:VAL:HG22 | 42:BU:60:LYS:O | 2.08 | 0.54 |
| 1:CA:1246:A:H2' | 1:CA:1247:U:O4' | 2.08 | 0.54 |
| 1:CA:1300:G:H1' | 1:CA:1301:U:H5 | 1.73 | 0.54 |
| 1:CA:1326:U:H2' | 1:CA:1327:C:C6 | 2.43 | 0.54 |
| 1:CA:238:A:C2' | 1:CA:239:U:H5'' | 2.38 | 0.54 |
| 1:CA:642:A:H2' | 1:CA:643:C:H6 | 1.73 | 0.54 |
| 1:CA:762:U:H2' | 1:CA:763:G:C8 | 2.43 | 0.54 |
| 1:CA:811:C:H4' | 1:CA:900:A:H62 | 1.73 | 0.54 |
| 2:CC:18:ASN:OD1 | 2:CC:53:ARG:HD2 | 2.07 | 0.54 |
| 4:CE:19:ARG:HH11 | 4:CE:28:ARG:HH22 | 1.56 | 0.54 |
| 4:CE:92:ARG:HB3 | 4:CE:92:ARG:HH11 | 1.73 | 0.54 |
| 6:CG:72:VAL:HA | 6:CG:89:GLU:HA | 1.89 | 0.54 |
| 6:CG:78:ARG:C | 6:CG:78:ARG:HD2 | 2.28 | 0.54 |
| 7:CH:13:ILE:HD11 | 7:CH:60:LEU:HD21 | 1.89 | 0.54 |
| 7:CH:94:VAL:CG2 | 7:CH:101:ALA:HB2 | 2.37 | 0.54 |
| 10:CK:14:GLN:HA | 10:CK:77:GLY:HA3 | 1.89 | 0.54 |
| 17:CR:35:SER:O | 17:CR:70:THR:HA | 2.08 | 0.54 |
| 21:CU:35:GLU:HB2 | 21:CU:37:TYR:CE2 | 2.42 | 0.54 |
| 23:DB:2487:G:H2' | 23:DB:2488:G:C8 | 2.42 | 0.54 |
| 23:DB:2605:U:H2' | 23:DB:2606:C:C6 | 2.43 | 0.54 |
| 23:DB:2679:A:O2' | 23:DB:2680:U:H5' | 2.08 | 0.54 |
| 23:DB:307:G:N2 | 23:DB:309:A:H3' | 2.23 | 0.54 |
| 23:DB:308:G:H2' | 23:DB:309:A:O4' | 2.08 | 0.54 |
| 23:DB:744:U:H2' | 23:DB:745:G:O4' | 2.08 | 0.54 |
| 25:DC:57:HIS:ND1 | 25:DC:58:LYS:N | 2.55 | 0.54 |
| 23:DB:1491:G:H5' | 25:DC:97:ASP:OD1 | 2.08 | 0.54 |
| 26:DD:175:LEU:HD21 | 26:DD:191:GLY:O | 2.08 | 0.54 |
| 28:DF:169:LEU:HB3 | 28:DF:174:PHE:CD1 | 2.42 | 0.54 |
| 30:DH:65:ALA:O | 30:DH:68:ARG:HB2 | 2.08 | 0.54 |
| 31:DJ:18:VAL:HG12 | 31:DJ:54:ILE:HD11 | 1.89 | 0.54 |
| 23:DB:587:C:O2' | 33:DL:19:LEU:HD13 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DN:29:VAL:O | 35:DN:78:LYS:HE3 | 2.08 | 0.54 |
| 42:DU:48:VAL:O | 42:DU:50:ALA:N | 2.41 | 0.54 |
| 42:DU:70:ALA:HB1 | 42:DU:79:ALA:HB2 | 1.90 | 0.54 |
| 43:DW:49:ASN:HA | 43:DW:61:LYS:HB2 | 1.88 | 0.54 |
| 1:AA:1124:G:H4' | 9:AJ:40:ILE:HG12 | 1.89 | 0.54 |
| 1:AA:1492:A:H5' | 1:AA:1493:A:OP2 | 2.08 | 0.54 |
| 1:AA:268:U:H2' | 1:AA:269:C:C6 | 2.42 | 0.54 |
| 1:AA:844:G:H2' | 1:AA:846:G:C8 | 2.43 | 0.54 |
| 3:AD:100:VAL:O | 3:AD:104:MET:HG3 | 2.08 | 0.54 |
| 4:AE:140:ILE:HG22 | 4:AE:144:GLU:OE1 | 2.07 | 0.54 |
| 6:AG:13:PRO:O | 6:AG:14:ASP:O | 2.26 | 0.54 |
| 6:AG:2:ARG:HG2 | 6:AG:3:ARG:HD3 | 1.90 | 0.54 |
| 11:AL:52:CYS:SG | 11:AL:66:ILE:HD11 | 2.48 | 0.54 |
| 15:AP:40:ASN:HD21 | 15:AP:42:ILE:C | 2.11 | 0.54 |
| 23:BB:1219:U:H2' | 23:BB:1220:G:C8 | 2.42 | 0.54 |
| 23:BB:1283:G:N2 | 23:BB:1285:A:H3' | 2.23 | 0.54 |
| 23:BB:1779:U:C5 | 23:BB:1784:A:N7 | 2.76 | 0.54 |
| 23:BB:2460:U:H2' | 23:BB:2461:A:H8 | 1.73 | 0.54 |
| 23:BB:475:C:H4' | 23:BB:509:C:H2' | 1.90 | 0.54 |
| 23:BB:946:C:H2' | 23:BB:947:A:C8 | 2.43 | 0.54 |
| 26:BD:12:THR:HG22 | 26:BD:13:ARG:H | 1.71 | 0.54 |
| 27:BE:46:GLN:HB3 | 27:BE:86:ALA:HA | 1.90 | 0.54 |
| 29:BG:26:LYS:CA | 29:BG:32:LEU:H | 2.17 | 0.54 |
| 29:BG:36:LEU:N | 29:BG:36:LEU:HD22 | 2.22 | 0.54 |
| 31:BJ:36:LEU:HD13 | 31:BJ:121:LYS:HE3 | 1.90 | 0.54 |
| 31:BJ:3:THR:HG21 | 38:BQ:60:TRP:HE1 | 1.73 | 0.54 |
| 33:BL:47:ARG:HB3 | 33:BL:47:ARG:HH21 | 1.73 | 0.54 |
| 38:BQ:111:LYS:HZ2 | 38:BQ:111:LYS:HB2 | 1.73 | 0.54 |
| 40:BS:95:ARG:HG3 | 40:BS:97:LEU:HD13 | 1.90 | 0.54 |
| 44:BX:56:LEU:O | 44:BX:57:LEU:HB3 | 2.06 | 0.54 |
| 1:CA:1278:G:H4' | 1:CA:1279:G:H5' | 1.89 | 0.54 |
| 1:CA:1384:C:H2' | 1:CA:1385:G:H8 | 1.72 | 0.54 |
| 1:CA:1464:U:H2' | 1:CA:1465:A:H8 | 1.73 | 0.54 |
| 1:CA:692:U:C2 | 1:CA:694:A:H5'' | 2.42 | 0.54 |
| 1:CA:692:U:O2 | 1:CA:694:A:H5'' | 2.07 | 0.54 |
| 20:CB:101:THR:HA | 20:CB:178:LEU:HD21 | 1.90 | 0.54 |
| 7:CH:11:THR:HA | 7:CH:14:ARG:CZ | 2.38 | 0.54 |
| 10:CK:124:LYS:HA | 21:CU:34:ARG:HG2 | 1.89 | 0.54 |
| 11:CL:2:THR:HG22 | 11:CL:5:GLN:NE2 | 2.23 | 0.54 |
| 13:CN:14:ALA:O | 13:CN:18:LYS:HG2 | 2.07 | 0.54 |
| 19:CT:54:GLN:N | 19:CT:55:PRO:HD2 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:2538:C:O2' | 23:DB:2539:C:H5' | 2.08 | 0.54 |
| 23:DB:2698:U:H2' | 23:DB:2699:C:C6 | 2.42 | 0.54 |
| 23:DB:303:G:H2' | 23:DB:304:U:C6 | 2.43 | 0.54 |
| 23:DB:45:G:C5' | 23:DB:46:G:H5' | 2.37 | 0.54 |
| 26:DD:51:THR:HG21 | 26:DD:76:GLY:HA3 | 1.90 | 0.54 |
| 27:DE:166:LYS:O | 27:DE:167:VAL:HB | 2.07 | 0.54 |
| 29:DG:146:ASP:O | 29:DG:150:TYR:HD1 | 1.91 | 0.54 |
| 30:DH:53:GLU:CA | 30:DH:57:LYS:HB3 | 2.38 | 0.54 |
| 31:DJ:44:TYR:CE2 | 38:DQ:59:LEU:HD11 | 2.43 | 0.54 |
| 35:DN:81:ASN:O | 35:DN:85:PRO:HD2 | 2.08 | 0.54 |
| 38:DQ:68:ALA:HA | 38:DQ:71:ASN:HB3 | 1.89 | 0.54 |
| 24:DV:9:ARG:NH2 | 24:DV:12:GLN:HA | 2.21 | 0.54 |
| 1:AA:1127:G:H5' | 1:AA:1280:A:O2' | 2.07 | 0.54 |
| 1:AA:613:C:H2' | 1:AA:614:C:C6 | 2.43 | 0.54 |
| 20:AB:107:ARG:HA | 20:AB:110:ILE:HD12 | 1.90 | 0.54 |
| 3:AD:75:TYR:HE1 | 3:AD:200:VAL:HA | 1.73 | 0.54 |
| 4:AE:100:GLU:HA | 4:AE:121:ASN:ND2 | 2.22 | 0.54 |
| 4:AE:53:ARG:NH1 | 4:AE:53:ARG:HB3 | 2.23 | 0.54 |
| 6:AG:14:ASP:OD2 | 6:AG:22:LEU:HB3 | 2.08 | 0.54 |
| 6:AG:70:PRO:O | 6:AG:95:ARG:HG3 | 2.08 | 0.54 |
| 13:AN:50:LEU:N | 13:AN:51:PRO:HD2 | 2.20 | 0.54 |
| 49:B2:34:ARG:HB3 | 49:B2:39:ARG:HB2 | 1.88 | 0.54 |
| 23:BB:2258:C:H4' | 23:BB:2259:U:OP2 | 2.07 | 0.54 |
| 23:BB:21:A:H2' | 23:BB:22:C:C6 | 2.43 | 0.54 |
| 23:BB:322:A:H5' | 23:BB:340:A:C1' | 2.33 | 0.54 |
| 23:BB:532:A:H2' | 38:BQ:27:ARG:NH2 | 2.16 | 0.54 |
| 23:BB:67:U:H2' | 23:BB:68:G:H8 | 1.73 | 0.54 |
| 30:BH:100:ALA:HB1 | 30:BH:110:VAL:O | 2.07 | 0.54 |
| 52:BI:77:VAL:HA | 52:BI:80:LYS:CE | 2.38 | 0.54 |
| 31:BJ:52:ASP:O | 31:BJ:54:ILE:HG22 | 2.07 | 0.54 |
| 31:BJ:59:ALA:C | 31:BJ:61:LYS:H | 2.10 | 0.54 |
| 32:BK:20:MET:C | 32:BK:41:ILE:HG13 | 2.29 | 0.54 |
| 33:BL:3:LEU:HA | 33:BL:6:LEU:HD21 | 1.90 | 0.54 |
| 36:BO:18:LEU:HD23 | 36:BO:25:ARG:HD2 | 1.91 | 0.54 |
| 40:BS:15:GLN:HA | 40:BS:18:ARG:CG | 2.38 | 0.54 |
| 24:BV:70:ILE:HD13 | 24:BV:70:ILE:N | 2.23 | 0.54 |
| 43:BW:36:ILE:HB | 43:BW:39:GLN:NE2 | 2.23 | 0.54 |
| 43:BW:36:ILE:O | 43:BW:39:GLN:HB3 | 2.08 | 0.54 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:H6 | 1.72 | 0.54 |
| 1:CA:1438:G:O2' | 1:CA:1439:G:H5' | 2.08 | 0.54 |
| 1:CA:193:C:H2' | 1:CA:194:C:H6 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:89:U:H2' | 1:CA:90:C:O4' | 2.08 | 0.54 |
| 10:CK:17:ASP:C | 10:CK:36:ARG:HH12 | 2.11 | 0.54 |
| 15:CP:40:ASN:HD21 | 15:CP:42:ILE:C | 2.11 | 0.54 |
| 23:DB:1150:C:H2' | 23:DB:1151:A:H8 | 1.73 | 0.54 |
| 23:DB:181:A:H2' | 23:DB:182:A:H8 | 1.73 | 0.54 |
| 23:DB:2258:C:H4' | 23:DB:2259:U:OP2 | 2.06 | 0.54 |
| 23:DB:2803:G:H2' | 23:DB:2804:U:C6 | 2.42 | 0.54 |
| 23:DB:305:C:H2' | 23:DB:306:U:C6 | 2.43 | 0.54 |
| 23:DB:633:A:O5' | 23:DB:633:A:H8 | 1.89 | 0.54 |
| 25:DC:18:VAL:O | 25:DC:18:VAL:HG13 | 2.08 | 0.54 |
| 27:DE:97:ASN:ND2 | 27:DE:100:MET:HG3 | 2.23 | 0.54 |
| 27:DE:4:VAL:HG12 | 27:DE:6:LYS:H | 1.73 | 0.54 |
| 31:DJ:59:ALA:C | 31:DJ:61:LYS:H | 2.12 | 0.54 |
| 31:DJ:84:ILE:HG23 | 31:DJ:84:ILE:O | 2.08 | 0.54 |
| 31:DJ:96:ARG:O | 31:DJ:99:ARG:HG3 | 2.07 | 0.54 |
| 34:DM:103:TYR:O | 34:DM:104:GLU:HG3 | 2.08 | 0.54 |
| 37:DP:103:THR:HG22 | 37:DP:104:GLY:H | 1.72 | 0.54 |
| 32:DK:120:PRO:HA | 37:DP:65:ASN:ND2 | 2.23 | 0.54 |
| 37:DP:89:GLY:HA2 | 37:DP:111:GLU:C | 2.29 | 0.54 |
| 41:DT:10:VAL:HG21 | 41:DT:42:GLU:HG3 | 1.89 | 0.54 |
| 42:DU:41:VAL:O | 42:DU:59:GLU:HA | 2.08 | 0.54 |
| 46:DZ:18:ARG:HG3 | 46:DZ:22:LEU:HA | 1.90 | 0.54 |
| 46:DZ:53:ALA:O | 46:DZ:55:GLY:N | 2.37 | 0.54 |
| 1:AA:1253:G:N1 | 1:AA:1285:A:N6 | 2.56 | 0.53 |
| 1:AA:560:A:H4' | 1:AA:561:U:H5'' | 1.88 | 0.53 |
| 20:AB:186:VAL:HB | 20:AB:190:SER:HB2 | 1.88 | 0.53 |
| 2:AC:70:ALA:HA | 2:AC:105:VAL:CG2 | 2.33 | 0.53 |
| 8:AI:10:ARG:HB3 | 8:AI:15:ALA:HA | 1.89 | 0.53 |
| 9:AJ:28:THR:O | 9:AJ:31:ARG:HG2 | 2.09 | 0.53 |
| 22:BA:49:C:H2' | 22:BA:50:A:C8 | 2.42 | 0.53 |
| 22:BA:88:C:H1' | 22:BA:89:U:C6 | 2.43 | 0.53 |
| 23:BB:1138:G:H2' | 23:BB:1139:G:O4' | 2.08 | 0.53 |
| 23:BB:1244:A:O2' | 23:BB:1245:G:H5' | 2.08 | 0.53 |
| 23:BB:1351:C:O2' | 23:BB:1571:A:H1' | 2.08 | 0.53 |
| 23:BB:2193:G:H2' | 23:BB:2194:U:H6 | 1.73 | 0.53 |
| 23:BB:41:C:O2' | 23:BB:42:A:H5' | 2.08 | 0.53 |
| 23:BB:3:U:H2' | 23:BB:4:U:H6 | 1.72 | 0.53 |
| 23:BB:643:A:H61 | 23:BB:2370:G:H1' | 1.74 | 0.53 |
| 23:BB:845:A:C2 | 23:BB:847:U:H1' | 2.42 | 0.53 |
| 23:BB:1257:C:O2' | 27:BE:79:ARG:HB2 | 2.08 | 0.53 |
| 28:BF:131:VAL:O | 28:BF:132:ARG:HB2 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BF:40:GLY:HA2 | 28:BF:84:ILE:HG23 | 1.89 | 0.53 |
| 34:BM:35:ALA:HB2 | 34:BM:100:LYS:HB2 | 1.90 | 0.53 |
| 37:BP:89:GLY:HA2 | 37:BP:112:ARG:N | 2.23 | 0.53 |
| 39:BR:39:LEU:CA | 39:BR:49:ILE:HG12 | 2.37 | 0.53 |
| 40:BS:10:ALA:HB3 | 40:BS:101:SER:OG | 2.08 | 0.53 |
| 40:BS:96:ILE:HG23 | 40:BS:96:ILE:O | 2.08 | 0.53 |
| 43:BW:9:THR:OG1 | 43:BW:10:ARG:N | 2.34 | 0.53 |
| 46:BZ:67:VAL:O | 46:BZ:70:GLU:HG3 | 2.07 | 0.53 |
| 1:CA:1141:C:H2' | 1:CA:1142:G:C8 | 2.42 | 0.53 |
| 1:CA:1262:C:H2' | 1:CA:1263:C:C6 | 2.43 | 0.53 |
| 1:CA:208:U:H4' | 1:CA:209:U:C5 | 2.42 | 0.53 |
| 1:CA:474:G:H2' | 1:CA:475:C:H6 | 1.72 | 0.53 |
| 1:CA:624:C:H2' | 1:CA:625:U:H6 | 1.73 | 0.53 |
| 20:CB:53:LEU:HD11 | 20:CB:216:VAL:HA | 1.88 | 0.53 |
| 3:CD:40:HIS:HB3 | 3:CD:43:ARG:HG2 | 1.88 | 0.53 |
| 17:CR:52:ARG:O | 17:CR:56:ARG:HG3 | 2.08 | 0.53 |
| 12:CM:82:LEU:HD11 | 18:CS:64:GLU:HB2 | 1.90 | 0.53 |
| 48:D1:6:GLU:CD | 48:D1:6:GLU:H | 2.12 | 0.53 |
| 49:D2:34:ARG:HB3 | 49:D2:39:ARG:HB2 | 1.89 | 0.53 |
| 23:DB:1178:C:H2' | 23:DB:1179:G:C8 | 2.42 | 0.53 |
| 23:DB:1495:A:H2' | 23:DB:1496:A:C8 | 2.43 | 0.53 |
| 23:DB:2096:C:H2' | 23:DB:2097:A:C8 | 2.43 | 0.53 |
| 23:DB:275:C:H2' | 23:DB:276:U:C6 | 2.42 | 0.53 |
| 23:DB:2841:C:H2' | 23:DB:2842:G:H8 | 1.73 | 0.53 |
| 23:DB:365:U:H2' | 23:DB:366:C:H6 | 1.73 | 0.53 |
| 23:DB:419:U:H2' | 23:DB:420:C:H6 | 1.71 | 0.53 |
| 23:DB:41:C:O2' | 23:DB:42:A:H5' | 2.08 | 0.53 |
| 23:DB:972:A:OP2 | 23:DB:974:G:H5'' | 2.08 | 0.53 |
| 25:DC:209:ALA:HA | 25:DC:212:TRP:NE1 | 2.23 | 0.53 |
| 25:DC:261:ARG:O | 25:DC:261:ARG:HG2 | 2.08 | 0.53 |
| 30:DH:31:VAL:O | 30:DH:32:PRO:C | 2.47 | 0.53 |
| 30:DH:95:GLY:H | 30:DH:98:ASP:HB2 | 1.72 | 0.53 |
| 34:DM:31:PHE:O | 34:DM:131:VAL:HG23 | 2.08 | 0.53 |
| 35:DN:37:THR:HB | 35:DN:40:LYS:HG3 | 1.91 | 0.53 |
| 37:DP:89:GLY:HA2 | 37:DP:112:ARG:N | 2.23 | 0.53 |
| 38:DQ:78:PHE:CE2 | 38:DQ:82:LEU:HD11 | 2.43 | 0.53 |
| 39:DR:16:GLU:HA | 39:DR:98:ILE:O | 2.08 | 0.53 |
| 46:DZ:77:LYS:O | 46:DZ:78:TYR:HB3 | 2.07 | 0.53 |
| 1:AA:1162:C:H2' | 1:AA:1163:A:C8 | 2.43 | 0.53 |
| 1:AA:1273:C:H2' | 1:AA:1274:A:O4' | 2.09 | 0.53 |
| 1:AA:453:G:H2' | 1:AA:454:G:C8 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:590:U:H2' | 1:AA:591:U:C6 | 2.43 | 0.53 |
| 1:AA:961:U:O2 | 1:AA:961:U:O4' | 2.26 | 0.53 |
| 20:AB:18:GLN:O | 20:AB:37:VAL:HG23 | 2.07 | 0.53 |
| 20:AB:44:LYS:C | 20:AB:47:PRO:HD2 | 2.27 | 0.53 |
| 7:AH:10:LEU:HD22 | 7:AH:74:ILE:HD11 | 1.90 | 0.53 |
| 11:AL:20:VAL:HB | 11:AL:94:TYR:CE1 | 2.43 | 0.53 |
| 16:AQ:75:VAL:HG23 | 16:AQ:76:ARG:N | 2.23 | 0.53 |
| 23:BB:1442:U:H2' | 23:BB:1443:U:C6 | 2.44 | 0.53 |
| 23:BB:1684:G:H2' | 23:BB:1685:C:H6 | 1.74 | 0.53 |
| 23:BB:2306:C:C3' | 23:BB:2307:G:H5' | 2.36 | 0.53 |
| 23:BB:2340:A:H2' | 23:BB:2341:G:C8 | 2.41 | 0.53 |
| 23:BB:2840:C:H2' | 23:BB:2841:C:H6 | 1.72 | 0.53 |
| 23:BB:2840:C:H2' | 23:BB:2841:C:C6 | 2.43 | 0.53 |
| 23:BB:329:G:N1 | 42:BU:16:LYS:HG2 | 2.23 | 0.53 |
| 23:BB:660:C:H2' | 23:BB:661:A:C8 | 2.42 | 0.53 |
| 23:BB:83:A:N6 | 23:BB:101:A:H5' | 2.24 | 0.53 |
| 25:BC:209:ALA:HA | 25:BC:212:TRP:CE2 | 2.44 | 0.53 |
| 27:BE:40:ARG:NH2 | 27:BE:92:HIS:NE2 | 2.56 | 0.53 |
| 31:BJ:56:VAL:HG12 | 31:BJ:57:LEU:N | 2.23 | 0.53 |
| 33:BL:65:GLY:O | 33:BL:66:PHE:HB3 | 2.09 | 0.53 |
| 36:BO:107:ALA:O | 36:BO:111:ARG:HG3 | 2.07 | 0.53 |
| 36:BO:36:TYR:HA | 36:BO:52:SER:HB3 | 1.90 | 0.53 |
| 37:BP:50:ARG:HB3 | 37:BP:57:ALA:H | 1.72 | 0.53 |
| 44:BX:23:ARG:O | 44:BX:27:ASN:N | 2.42 | 0.53 |
| 1:CA:1352:C:H2' | 1:CA:1353:G:C8 | 2.43 | 0.53 |
| 1:CA:1530:G:HO2' | 1:CA:1531:A:H8 | 1.56 | 0.53 |
| 1:CA:343:U:O2' | 1:CA:344:A:H2' | 2.07 | 0.53 |
| 1:CA:512:U:O2' | 1:CA:513:C:H5' | 2.08 | 0.53 |
| 1:CA:590:U:H2' | 1:CA:591:U:C6 | 2.43 | 0.53 |
| 1:CA:734:G:H2' | 1:CA:735:C:H6 | 1.72 | 0.53 |
| 1:CA:95:C:O2 | 1:CA:95:C:H2' | 2.06 | 0.53 |
| 3:CD:7:LYS:HB2 | 3:CD:21:LYS:HE2 | 1.91 | 0.53 |
| 3:CD:90:LEU:HD11 | 3:CD:194:ILE:CD1 | 2.38 | 0.53 |
| 8:CI:33:SER:CB | 8:CI:36:GLN:HB2 | 2.37 | 0.53 |
| 51:D4:27:CYS:SG | 51:D4:29:ALA:HB3 | 2.48 | 0.53 |
| 23:DB:126:A:H5' | 49:D2:19:ARG:CG | 2.37 | 0.53 |
| 23:DB:1841:U:H2' | 23:DB:1842:G:H8 | 1.74 | 0.53 |
| 23:DB:1930:G:H2' | 23:DB:1968:G:H1 | 1.73 | 0.53 |
| 23:DB:2840:C:H2' | 23:DB:2841:C:C6 | 2.44 | 0.53 |
| 23:DB:477:A:H2' | 23:DB:478:A:C8 | 2.43 | 0.53 |
| 23:DB:545:U:H3' | 23:DB:546:U:O3' | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:62:U:C2' | 23:DB:63:A:H5' | 2.39 | 0.53 |
| 23:DB:819:A:H5' | 23:DB:973:A:N1 | 2.23 | 0.53 |
| 23:DB:839:U:H2' | 23:DB:840:C:C6 | 2.42 | 0.53 |
| 23:DB:853:C:O2' | 23:DB:854:C:H5' | 2.09 | 0.53 |
| 23:DB:899:A:H3' | 23:DB:900:A:C8 | 2.43 | 0.53 |
| 23:DB:2512:C:OP2 | 26:DD:128:ARG:HD2 | 2.09 | 0.53 |
| 27:DE:149:ILE:O | 27:DE:188:MET:HA | 2.07 | 0.53 |
| 27:DE:181:ILE:HG13 | 33:DL:2:ARG:HB3 | 1.90 | 0.53 |
| 27:DE:4:VAL:HG12 | 27:DE:5:LEU:N | 2.23 | 0.53 |
| 28:DF:78:ILE:HA | 28:DF:82:TYR:CE1 | 2.43 | 0.53 |
| 31:DJ:18:VAL:HG22 | 31:DJ:19:ASP:N | 2.21 | 0.53 |
| 33:DL:119:PRO:HA | 33:DL:138:ALA:O | 2.08 | 0.53 |
| 39:DR:28:ALA:HB3 | 39:DR:31:GLU:HB2 | 1.90 | 0.53 |
| 40:DS:24:ILE:HD11 | 40:DS:36:LEU:HD21 | 1.90 | 0.53 |
| 23:DB:470:A:H61 | 41:DT:72:GLN:NE2 | 2.06 | 0.53 |
| 41:DT:32:LEU:O | 41:DT:83:ALA:HB2 | 2.09 | 0.53 |
| 24:DV:7:GLU:O | 24:DV:41:GLU:HG2 | 2.09 | 0.53 |
| 24:DV:77:VAL:CG1 | 34:DM:136:MET:HB3 | 2.37 | 0.53 |
| 44:DX:41:HIS:O | 44:DX:44:LYS:HB3 | 2.07 | 0.53 |
| 1:AA:205:A:H2' | 1:AA:206:C:C6 | 2.43 | 0.53 |
| 1:AA:301:G:H2' | 1:AA:302:G:H8 | 1.73 | 0.53 |
| 1:AA:505:G:H2' | 1:AA:506:G:C8 | 2.43 | 0.53 |
| 20:AB:13:VAL:HG11 | 20:AB:207:ARG:HG2 | 1.89 | 0.53 |
| 20:AB:27:LYS:HB3 | 20:AB:28:PRO:HD3 | 1.91 | 0.53 |
| 2:AC:190:THR:HG22 | 2:AC:191:THR:N | 2.23 | 0.53 |
| 4:AE:28:ARG:CZ | 4:AE:30:PHE:HB3 | 2.39 | 0.53 |
| 1:AA:734:G:O2' | 17:AR:59:LYS:HD3 | 2.08 | 0.53 |
| 18:AS:44:ILE:HG13 | 18:AS:62:THR:HA | 1.89 | 0.53 |
| 23:BB:1429:G:O2' | 23:BB:1430:G:H5' | 2.08 | 0.53 |
| 23:BB:1531:C:H2' | 23:BB:1532:A:C8 | 2.44 | 0.53 |
| 23:BB:2861:U:H2' | 23:BB:2862:G:C8 | 2.41 | 0.53 |
| 23:BB:4:U:H2' | 23:BB:5:A:C8 | 2.43 | 0.53 |
| 23:BB:972:A:OP2 | 23:BB:974:G:H5' | 2.08 | 0.53 |
| 25:BC:261:ARG:HG2 | 25:BC:261:ARG:O | 2.08 | 0.53 |
| 26:BD:149:ASN:O | 26:BD:152:PRO:HD2 | 2.09 | 0.53 |
| 26:BD:172:VAL:HG12 | 26:BD:173:GLN:N | 2.24 | 0.53 |
| 26:BD:79:LEU:N | 26:BD:79:LEU:HD22 | 2.23 | 0.53 |
| 32:BK:53:LYS:HD3 | 32:BK:56:ASP:OD2 | 2.09 | 0.53 |
| 33:BL:119:PRO:HA | 33:BL:138:ALA:O | 2.09 | 0.53 |
| 34:BM:134:THR:HG22 | 34:BM:136:MET:H | 1.71 | 0.53 |
| 41:BT:28:ASN:CA | 41:BT:91:GLN:HE22 | 2.19 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BZ:5:CYS:HB2 | 46:BZ:10:LYS:HB2 | 1.90 | 0.53 |
| 1:CA:254:G:H4' | 16:CQ:19:SER:OG | 2.07 | 0.53 |
| 1:CA:465:A:O2' | 1:CA:466:A:H5' | 2.07 | 0.53 |
| 30:BH:8:LYS:HE3 | 1:CA:494:G:O3' | 2.07 | 0.53 |
| 1:CA:860:A:H2' | 1:CA:861:G:O4' | 2.07 | 0.53 |
| 2:CC:146:LYS:HD3 | 2:CC:204:GLY:HA2 | 1.91 | 0.53 |
| 3:CD:10:LEU:HD12 | 3:CD:20:LEU:HD11 | 1.89 | 0.53 |
| 1:CA:9:G:OP2 | 4:CE:125:LYS:HD3 | 2.07 | 0.53 |
| 7:CH:17:GLN:NE2 | 7:CH:62:LEU:HB3 | 2.23 | 0.53 |
| 7:CH:9:MET:O | 7:CH:13:ILE:HG13 | 2.08 | 0.53 |
| 8:CI:78:ILE:O | 8:CI:82:ILE:HG13 | 2.08 | 0.53 |
| 10:CK:81:LEU:HD23 | 10:CK:81:LEU:N | 2.23 | 0.53 |
| 11:CL:24:GLU:HB2 | 11:CL:26:CYS:SG | 2.48 | 0.53 |
| 23:DB:1917:U:C2' | 23:DB:1918:A:H5' | 2.39 | 0.53 |
| 23:DB:2023:C:O2' | 23:DB:2024:G:H5' | 2.08 | 0.53 |
| 23:DB:2508:G:H2' | 23:DB:2509:G:H8 | 1.73 | 0.53 |
| 23:DB:2869:G:H2' | 23:DB:2870:C:O4' | 2.09 | 0.53 |
| 23:DB:2885:G:N2 | 47:D0:31:LYS:HG2 | 2.24 | 0.53 |
| 23:DB:433:C:H2' | 23:DB:434:U:C6 | 2.43 | 0.53 |
| 23:DB:564:C:O2' | 23:DB:565:C:H5' | 2.08 | 0.53 |
| 23:DB:598:U:H2' | 23:DB:599:A:H8 | 1.73 | 0.53 |
| 23:DB:783:A:H2' | 23:DB:784:G:O5' | 2.08 | 0.53 |
| 28:DF:126:ASN:HB3 | 28:DF:156:THR:CA | 2.37 | 0.53 |
| 30:DH:31:VAL:CB | 30:DH:32:PRO:CD | 2.81 | 0.53 |
| 52:DI:52:LEU:HD22 | 52:DI:81:LYS:HD3 | 1.90 | 0.53 |
| 37:DP:1:SER:O | 37:DP:5:LYS:HB2 | 2.09 | 0.53 |
| 37:DP:88:ARG:HB2 | 37:DP:112:ARG:HH12 | 1.74 | 0.53 |
| 41:DT:27:SER:O | 41:DT:28:ASN:HB3 | 2.09 | 0.53 |
| 1:AA:1018:G:H2' | 1:AA:1019:A:C8 | 2.43 | 0.53 |
| 1:AA:1258:G:O2' | 1:AA:1259:C:H5' | 2.09 | 0.53 |
| 1:AA:1277:C:O2' | 1:AA:1279:G:H1' | 2.08 | 0.53 |
| 1:AA:1278:G:H4' | 1:AA:1279:G:H5' | 1.89 | 0.53 |
| 1:AA:978:A:HO2' | 1:AA:1322:C:H5 | 1.53 | 0.53 |
| 1:AA:1511:G:O2' | 1:AA:1512:U:H5' | 2.08 | 0.53 |
| 1:AA:1525:G:O2' | 1:AA:1526:G:H5' | 2.08 | 0.53 |
| 1:AA:284:C:H2' | 1:AA:285:C:H6 | 1.73 | 0.53 |
| 1:AA:470:C:H2' | 1:AA:471:U:C6 | 2.43 | 0.53 |
| 2:AC:13:ILE:H | 2:AC:13:ILE:HD13 | 1.74 | 0.53 |
| 6:AG:91:ARG:N | 6:AG:91:ARG:HD2 | 2.22 | 0.53 |
| 15:AP:54:LEU:HD13 | 15:AP:80:LYS:HG3 | 1.90 | 0.53 |
| 18:AS:43:MET:O | 18:AS:46:LEU:HB2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:B4:3:VAL:HG23 | 51:B4:4:ARG:H | 1.74 | 0.53 |
| 23:BB:1015:U:H2' | 23:BB:1016:G:H8 | 1.73 | 0.53 |
| 23:BB:1046:A:H3' | 23:BB:1047:G:H5'' | 1.90 | 0.53 |
| 23:BB:1623:G:O2' | 23:BB:1624:U:H5' | 2.08 | 0.53 |
| 23:BB:2152:G:H2' | 23:BB:2152:G:N3 | 2.23 | 0.53 |
| 23:BB:2239:G:O2' | 23:BB:2240:U:H5' | 2.08 | 0.53 |
| 23:BB:2333:A:H4' | 23:BB:2334:U:C5' | 2.39 | 0.53 |
| 23:BB:2882:A:C3' | 23:BB:2883:A:H5'' | 2.38 | 0.53 |
| 23:BB:346:A:H5' | 23:BB:346:A:N3 | 2.23 | 0.53 |
| 23:BB:490:C:H3' | 23:BB:491:G:H5'' | 1.91 | 0.53 |
| 25:BC:239:PHE:HD1 | 25:BC:241:LYS:H | 1.57 | 0.53 |
| 27:BE:1:MET:HB2 | 27:BE:16:GLU:HB2 | 1.89 | 0.53 |
| 31:BJ:25:LEU:O | 31:BJ:27:ARG:N | 2.41 | 0.53 |
| 39:BR:49:ILE:HB | 39:BR:53:PHE:O | 2.08 | 0.53 |
| 39:BR:72:VAL:HG23 | 39:BR:89:HIS:O | 2.08 | 0.53 |
| 23:BB:138:U:O4' | 41:BT:1:MET:N | 2.39 | 0.53 |
| 42:BU:66:VAL:O | 42:BU:69:VAL:HG22 | 2.07 | 0.53 |
| 45:BY:15:ARG:HD2 | 45:BY:15:ARG:N | 2.22 | 0.53 |
| 1:CA:106:C:O2' | 1:CA:107:G:H5' | 2.08 | 0.53 |
| 1:CA:499:A:H4' | 1:CA:500:G:OP1 | 2.08 | 0.53 |
| 1:CA:652:U:H1' | 1:CA:653:U:C5 | 2.43 | 0.53 |
| 1:CA:90:C:H2' | 1:CA:91:U:C6 | 2.44 | 0.53 |
| 1:CA:928:G:H2' | 1:CA:929:G:C8 | 2.44 | 0.53 |
| 3:CD:94:GLU:HG3 | 3:CD:99:ASN:HD21 | 1.73 | 0.53 |
| 5:CF:15:SER:HA | 5:CF:18:VAL:HG23 | 1.90 | 0.53 |
| 6:CG:113:LYS:HB3 | 6:CG:113:LYS:HZ2 | 1.73 | 0.53 |
| 8:CI:46:VAL:O | 8:CI:79:ARG:HG3 | 2.08 | 0.53 |
| 11:CL:20:VAL:O | 11:CL:20:VAL:HG23 | 2.07 | 0.53 |
| 12:CM:15:VAL:O | 12:CM:19:THR:HG23 | 2.09 | 0.53 |
| 15:CP:38:PHE:CD2 | 15:CP:51:ARG:HB2 | 2.43 | 0.53 |
| 17:CR:60:ARG:O | 17:CR:64:LEU:HD13 | 2.08 | 0.53 |
| 18:CS:44:ILE:HG13 | 18:CS:62:THR:HA | 1.90 | 0.53 |
| 22:DA:35:C:H3' | 22:DA:35:C:O2 | 2.08 | 0.53 |
| 22:DA:32:U:C4' | 22:DA:52:A:H62 | 2.21 | 0.53 |
| 23:DB:1149:G:H2' | 23:DB:1150:C:H6 | 1.73 | 0.53 |
| 23:DB:1210:G:H5' | 23:DB:1212:G:H5'' | 1.91 | 0.53 |
| 23:DB:2239:G:O2' | 23:DB:2240:U:H5' | 2.07 | 0.53 |
| 23:DB:2439:A:H4' | 23:DB:2440:C:O5' | 2.08 | 0.53 |
| 23:DB:2537:U:H2' | 23:DB:2538:C:C6 | 2.44 | 0.53 |
| 23:DB:596:U:H2' | 23:DB:597:G:C8 | 2.44 | 0.53 |
| 23:DB:69:C:H2' | 23:DB:70:G:C8 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:948:C:H2' | 23:DB:949:G:H8 | 1.73 | 0.53 |
| 33:DL:4:ASN:HD22 | 33:DL:4:ASN:N | 2.04 | 0.53 |
| 37:DP:98:TYR:C | 37:DP:100:ARG:H | 2.11 | 0.53 |
| 23:DB:812:C:H4' | 38:DQ:12:ARG:NH1 | 2.24 | 0.53 |
| 1:AA:1060:U:H5'' | 9:AJ:53:ILE:HG12 | 1.90 | 0.53 |
| 1:AA:796:C:OP1 | 10:AK:127:ARG:HB3 | 2.08 | 0.53 |
| 3:AD:169:TRP:HB2 | 3:AD:183:ARG:O | 2.09 | 0.53 |
| 5:AF:74:LEU:HG | 5:AF:78:PHE:CE1 | 2.43 | 0.53 |
| 5:AF:37:HIS:O | 5:AF:97:THR:HG23 | 2.09 | 0.53 |
| 8:AI:32:ARG:HH21 | 8:AI:36:GLN:HG3 | 1.73 | 0.53 |
| 9:AJ:8:ILE:HD11 | 9:AJ:76:ILE:HG13 | 1.91 | 0.53 |
| 10:AK:30:ILE:HG22 | 10:AK:45:THR:OG1 | 2.08 | 0.53 |
| 13:AN:26:LEU:HD12 | 13:AN:44:VAL:HG13 | 1.89 | 0.53 |
| 13:AN:60:ARG:HD3 | 13:AN:62:ARG:NH2 | 2.22 | 0.53 |
| 16:AQ:24:ILE:O | 16:AQ:40:THR:HA | 2.09 | 0.53 |
| 21:AU:10:PRO:HB2 | 2:CC:71:ARG:NE | 2.19 | 0.53 |
| 23:BB:2742:G:P | 51:B4:24:ARG:HH12 | 2.31 | 0.53 |
| 22:BA:14:U:H5' | 22:BA:70:C:O2' | 2.09 | 0.53 |
| 23:BB:100:U:O2 | 23:BB:100:U:C2' | 2.54 | 0.53 |
| 23:BB:1061:U:H5' | 52:BI:9:LYS:HZ1 | 1.73 | 0.53 |
| 23:BB:1847:A:H4' | 23:BB:1848:A:H8 | 1.73 | 0.53 |
| 23:BB:1930:G:H2' | 23:BB:1968:G:N1 | 2.23 | 0.53 |
| 23:BB:2455:G:H2' | 23:BB:2456:C:C6 | 2.44 | 0.53 |
| 23:BB:2512:C:OP2 | 26:BD:128:ARG:HD2 | 2.08 | 0.53 |
| 23:BB:2728:U:H2' | 23:BB:2729:G:C8 | 2.44 | 0.53 |
| 23:BB:2809:A:H2' | 23:BB:2810:A:C8 | 2.44 | 0.53 |
| 23:BB:2846:G:H2' | 23:BB:2847:U:C6 | 2.44 | 0.53 |
| 23:BB:819:A:H5' | 23:BB:973:A:N1 | 2.23 | 0.53 |
| 25:BC:183:VAL:HG22 | 25:BC:184:GLU:H | 1.74 | 0.53 |
| 25:BC:86:ARG:HB3 | 25:BC:86:ARG:CZ | 2.39 | 0.53 |
| 26:BD:8:LYS:CG | 26:BD:197:THR:H | 2.22 | 0.53 |
| 27:BE:153:LEU:HG | 27:BE:154:ASP:N | 2.24 | 0.53 |
| 27:BE:4:VAL:HG12 | 27:BE:5:LEU:N | 2.23 | 0.53 |
| 23:BB:1061:U:H5' | 52:BI:9:LYS:NZ | 2.24 | 0.53 |
| 31:BJ:130:HIS:HD2 | 31:BJ:132:HIS:HB2 | 1.73 | 0.53 |
| 31:BJ:25:LEU:HB2 | 31:BJ:62:VAL:HG22 | 1.89 | 0.53 |
| 32:BK:105:ARG:HD2 | 32:BK:105:ARG:H | 1.72 | 0.53 |
| 22:BA:51:G:OP1 | 36:BO:63:LYS:HE3 | 2.08 | 0.53 |
| 37:BP:26:GLU:HB3 | 37:BP:84:SER:HB3 | 1.90 | 0.53 |
| 43:BW:9:THR:O | 43:BW:10:ARG:HB2 | 2.09 | 0.53 |
| 1:CA:188:C:H2' | 1:CA:189:A:O4' | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:620:C:C2 | 3:CD:131:ILE:HG21 | 2.44 | 0.53 |
| 1:CA:627:G:H2' | 1:CA:628:G:C8 | 2.42 | 0.53 |
| 1:CA:82:G:H2' | 1:CA:83:C:O4' | 2.08 | 0.53 |
| 20:CB:142:LYS:HA | 20:CB:145:ASN:OD1 | 2.09 | 0.53 |
| 9:CJ:8:ILE:N | 9:CJ:8:ILE:HD12 | 2.24 | 0.53 |
| 11:CL:98:ARG:HB2 | 11:CL:116:TYR:HA | 1.89 | 0.53 |
| 13:CN:2:LYS:O | 13:CN:6:LYS:HG3 | 2.09 | 0.53 |
| 13:CN:5:MET:HB3 | 13:CN:62:ARG:HH12 | 1.73 | 0.53 |
| 23:DB:2284:A:OP2 | 48:D1:5:ARG:HG3 | 2.09 | 0.53 |
| 50:D3:32:LEU:HA | 50:D3:35:LYS:HD2 | 1.90 | 0.53 |
| 23:DB:1031:G:H4' | 51:D4:6:SER:OG | 2.08 | 0.53 |
| 23:DB:1022:G:N2 | 23:DB:1142:A:C2 | 2.76 | 0.53 |
| 23:DB:1320:C:C5 | 23:DB:1329:U:H5'' | 2.44 | 0.53 |
| 23:DB:1526:C:H2' | 23:DB:1527:G:O4' | 2.08 | 0.53 |
| 23:DB:2852:G:H2' | 23:DB:2853:C:H6 | 1.70 | 0.53 |
| 23:DB:598:U:H2' | 23:DB:599:A:C8 | 2.44 | 0.53 |
| 23:DB:81:G:H2' | 23:DB:82:U:O4' | 2.08 | 0.53 |
| 23:DB:93:G:H2' | 23:DB:94:A:O4' | 2.09 | 0.53 |
| 25:DC:2:VAL:HG23 | 25:DC:3:VAL:H | 1.74 | 0.53 |
| 22:DA:43:C:H4' | 28:DF:91:ARG:HD2 | 1.90 | 0.53 |
| 29:DG:17:LYS:O | 29:DG:23:ILE:HG23 | 2.09 | 0.53 |
| 30:DH:88:GLY:O | 30:DH:124:THR:HA | 2.08 | 0.53 |
| 52:DI:54:ILE:HD13 | 52:DI:55:PRO:N | 2.23 | 0.53 |
| 33:DL:90:VAL:HB | 33:DL:122:VAL:HG13 | 1.89 | 0.53 |
| 34:DM:71:LYS:HG2 | 34:DM:73:ILE:HD11 | 1.90 | 0.53 |
| 34:DM:71:LYS:HG2 | 34:DM:93:VAL:HG12 | 1.89 | 0.53 |
| 43:DW:49:ASN:O | 43:DW:50:VAL:HG13 | 2.07 | 0.53 |
| 46:DZ:17:ASN:HB2 | 46:DZ:25:THR:OG1 | 2.08 | 0.53 |
| 46:DZ:39:TRP:HB2 | 46:DZ:46:PHE:CE2 | 2.44 | 0.53 |
| 1:AA:1020:G:H2' | 1:AA:1021:A:H5' | 1.90 | 0.53 |
| 1:AA:1326:U:H2' | 1:AA:1327:C:H6 | 1.74 | 0.53 |
| 1:AA:652:U:H1' | 1:AA:653:U:C5 | 2.44 | 0.53 |
| 2:AC:19:SER:HB2 | 2:AC:39:ARG:HH22 | 1.74 | 0.53 |
| 3:AD:96:ARG:NH1 | 3:AD:133:SER:HA | 2.24 | 0.53 |
| 5:AF:6:ILE:HG23 | 5:AF:62:MET:HB3 | 1.91 | 0.53 |
| 13:AN:50:LEU:HG | 13:AN:51:PRO:HD3 | 1.91 | 0.53 |
| 18:AS:35:ARG:HB3 | 18:AS:50:VAL:HG13 | 1.90 | 0.53 |
| 49:B2:10:LEU:HD11 | 49:B2:14:ARG:NH1 | 2.23 | 0.53 |
| 23:BB:2478:A:OP1 | 51:B4:32:LYS:HE2 | 2.08 | 0.53 |
| 22:BA:43:C:H4' | 28:BF:91:ARG:HD2 | 1.89 | 0.53 |
| 23:BB:1495:A:O2' | 23:BB:1496:A:H5' | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:182:A:H2' | 23:BB:183:C:H6 | 1.74 | 0.53 |
| 23:BB:1948:G:O2' | 23:BB:1949:G:H5' | 2.09 | 0.53 |
| 23:BB:2329:U:H2' | 23:BB:2330:G:C8 | 2.44 | 0.53 |
| 23:BB:296:U:H2' | 23:BB:297:G:C8 | 2.43 | 0.53 |
| 23:BB:370:G:O2' | 23:BB:423:A:H3' | 2.09 | 0.53 |
| 26:BD:164:GLN:HG3 | 26:BD:165:MET:N | 2.23 | 0.53 |
| 28:BF:56:LEU:HD22 | 28:BF:59:ILE:HD12 | 1.89 | 0.53 |
| 33:BL:110:VAL:HB | 33:BL:127:VAL:HG23 | 1.89 | 0.53 |
| 23:BB:2366:A:H4' | 43:BW:61:LYS:HE2 | 1.90 | 0.53 |
| 44:BX:17:GLU:HB3 | 44:BX:53:VAL:CG1 | 2.36 | 0.53 |
| 1:CA:1097:C:H2' | 1:CA:1098:C:C6 | 2.44 | 0.53 |
| 1:CA:922:G:N3 | 1:CA:1398:A:H2 | 2.06 | 0.53 |
| 1:CA:153:C:H2' | 1:CA:154:U:C6 | 2.43 | 0.53 |
| 1:CA:33:A:H2' | 1:CA:34:C:C6 | 2.44 | 0.53 |
| 23:DB:1442:U:H2' | 23:DB:1443:U:C6 | 2.43 | 0.53 |
| 23:DB:1849:G:H2' | 23:DB:1850:G:H8 | 1.74 | 0.53 |
| 23:DB:1872:A:H8 | 23:DB:1872:A:O5' | 1.92 | 0.53 |
| 23:DB:192:C:C2' | 23:DB:193:U:H5' | 2.37 | 0.53 |
| 23:DB:1131:G:N2 | 23:DB:2024:G:H21 | 2.06 | 0.53 |
| 23:DB:2395:C:H2' | 23:DB:2396:G:O4' | 2.08 | 0.53 |
| 23:DB:2795:C:H2' | 23:DB:2796:U:O4' | 2.08 | 0.53 |
| 23:DB:2819:G:H2' | 23:DB:2821:A:N7 | 2.24 | 0.53 |
| 23:DB:591:U:H1' | 50:D3:1:PRO:H3 | 1.72 | 0.53 |
| 23:DB:633:A:OP1 | 33:DL:68:SER:HB2 | 2.08 | 0.53 |
| 26:DD:121:THR:C | 26:DD:123:LYS:H | 2.09 | 0.53 |
| 29:DG:25:ILE:CG2 | 29:DG:78:VAL:HG21 | 2.39 | 0.53 |
| 29:DG:15:ASP:CB | 29:DG:26:LYS:H | 2.16 | 0.53 |
| 31:DJ:130:HIS:HD2 | 31:DJ:132:HIS:HB2 | 1.73 | 0.53 |
| 32:DK:70:ARG:CB | 32:DK:76:VAL:HG22 | 2.38 | 0.53 |
| 33:DL:110:VAL:HB | 33:DL:127:VAL:HG23 | 1.91 | 0.53 |
| 38:DQ:63:ARG:CZ | 38:DQ:96:ASP:HA | 2.39 | 0.53 |
| 39:DR:6:GLN:HE22 | 39:DR:9:GLY:CA | 2.22 | 0.53 |
| 8:AI:33:SER:CB | 8:AI:36:GLN:HB2 | 2.38 | 0.53 |
| 21:AU:35:GLU:HB2 | 21:AU:37:TYR:CE2 | 2.43 | 0.53 |
| 22:BA:35:C:H3' | 22:BA:35:C:O2 | 2.08 | 0.53 |
| 23:BB:123:G:H2' | 23:BB:124:G:H8 | 1.74 | 0.53 |
| 23:BB:543:G:H2' | 23:BB:544:C:H5'' | 1.91 | 0.53 |
| 23:BB:757:G:H2' | 23:BB:758:C:H5' | 1.90 | 0.53 |
| 23:BB:813:U:H2' | 23:BB:814:C:H6 | 1.74 | 0.53 |
| 26:BD:13:ARG:HD3 | 26:BD:15:PHE:CE1 | 2.44 | 0.53 |
| 27:BE:147:LEU:HD12 | 27:BE:149:ILE:HB | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BH:1:MET:HE3 | 30:BH:26:ALA:HB3 | 1.90 | 0.53 |
| 52:BI:18:ASN:N | 52:BI:19:PRO:CD | 2.71 | 0.53 |
| 32:BK:35:VAL:CG2 | 32:BK:36:GLY:H | 2.08 | 0.53 |
| 35:BN:37:THR:HB | 35:BN:40:LYS:HG3 | 1.91 | 0.53 |
| 37:BP:31:VAL:HG12 | 37:BP:38:ARG:O | 2.09 | 0.53 |
| 41:BT:7:LEU:O | 41:BT:7:LEU:HD13 | 2.08 | 0.53 |
| 24:BV:44:HIS:CE1 | 24:BV:85:LYS:HB2 | 2.43 | 0.53 |
| 1:CA:1238:A:H2 | 1:CA:1241:G:N3 | 2.06 | 0.53 |
| 1:CA:1291:U:H2' | 1:CA:1292:G:C8 | 2.44 | 0.53 |
| 1:CA:1432:G:H1' | 1:CA:1468:A:H61 | 1.72 | 0.53 |
| 1:CA:33:A:H2' | 1:CA:34:C:H6 | 1.72 | 0.53 |
| 1:CA:707:U:H2' | 1:CA:708:C:H6 | 1.71 | 0.53 |
| 1:CA:98:A:H2' | 1:CA:99:C:H6 | 1.74 | 0.53 |
| 20:CB:102:ASN:ND2 | 20:CB:105:THR:HB | 2.22 | 0.53 |
| 2:CC:50:SER:HB2 | 2:CC:70:ALA:HB3 | 1.91 | 0.53 |
| 18:CS:14:LEU:O | 18:CS:18:VAL:HG12 | 2.08 | 0.53 |
| 18:CS:43:MET:O | 18:CS:61:VAL:HB | 2.08 | 0.53 |
| 19:CT:53:MET:O | 19:CT:57:VAL:HG22 | 2.08 | 0.53 |
| 21:CU:3:ILE:HB | 21:CU:19:LYS:HD2 | 1.90 | 0.53 |
| 22:DA:89:U:O2 | 23:DB:958:U:H2' | 2.08 | 0.53 |
| 23:DB:1549:A:H2' | 23:DB:1550:C:H6 | 1.74 | 0.53 |
| 23:DB:1381:G:H1' | 23:DB:1571:A:N1 | 2.24 | 0.53 |
| 23:DB:1733:G:H2' | 23:DB:1734:G:C8 | 2.43 | 0.53 |
| 23:DB:2306:C:C3' | 23:DB:2307:G:H5' | 2.35 | 0.53 |
| 23:DB:2415:G:C4' | 33:DL:66:PHE:HB2 | 2.38 | 0.53 |
| 23:DB:2740:A:H2' | 23:DB:2741:A:C8 | 2.43 | 0.53 |
| 23:DB:276:U:H2' | 23:DB:278:A:N7 | 2.24 | 0.53 |
| 23:DB:291:G:H2' | 23:DB:292:U:H6 | 1.74 | 0.53 |
| 25:DC:5:CYS:HB2 | 25:DC:15:VAL:O | 2.09 | 0.53 |
| 29:DG:106:LEU:O | 29:DG:108:PHE:N | 2.41 | 0.53 |
| 29:DG:122:ALA:HA | 29:DG:132:LEU:HA | 1.90 | 0.53 |
| 52:DI:79:LEU:HD12 | 52:DI:135:MET:SD | 2.48 | 0.53 |
| 52:DI:99:LYS:HD3 | 52:DI:99:LYS:N | 2.24 | 0.53 |
| 34:DM:2:LEU:HD23 | 34:DM:46:ILE:HD11 | 1.90 | 0.53 |
| 38:DQ:104:ALA:O | 38:DQ:105:PHE:HB3 | 2.09 | 0.53 |
| 42:DU:40:LEU:HD23 | 42:DU:59:GLU:HG2 | 1.91 | 0.53 |
| 43:DW:30:VAL:O | 43:DW:30:VAL:HG13 | 2.08 | 0.53 |
| 46:DZ:67:VAL:O | 46:DZ:70:GLU:HG3 | 2.09 | 0.53 |
| 1:AA:370:C:H2' | 1:AA:371:A:C8 | 2.44 | 0.53 |
| 1:AA:738:C:H2' | 1:AA:739:C:C6 | 2.44 | 0.53 |
| 1:AA:787:A:O2' | 1:AA:788:U:H5' | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1101:A:C8 | 20:AB:170:ILE:HD12 | 2.43 | 0.53 |
| 14:AO:80:LEU:HD21 | 14:AO:84:LEU:HD22 | 1.91 | 0.53 |
| 23:BB:143:C:H2' | 23:BB:144:A:H8 | 1.73 | 0.53 |
| 23:BB:1526:C:H2' | 23:BB:1527:G:O4' | 2.09 | 0.53 |
| 23:BB:1731:G:O2' | 23:BB:1732:C:H5'' | 2.09 | 0.53 |
| 23:BB:1854:A:N6 | 23:BB:1888:G:H1' | 2.24 | 0.53 |
| 23:BB:2022:U:O2' | 23:BB:2617:U:H5' | 2.09 | 0.53 |
| 23:BB:2216:G:H2' | 23:BB:2217:G:C8 | 2.43 | 0.53 |
| 23:BB:564:C:O2' | 23:BB:565:C:H5' | 2.09 | 0.53 |
| 23:BB:947:A:O2' | 23:BB:984:A:H2 | 1.92 | 0.53 |
| 25:BC:2:VAL:HG23 | 25:BC:3:VAL:H | 1.73 | 0.53 |
| 28:BF:46:LYS:NZ | 28:BF:83:PRO:HD2 | 2.24 | 0.53 |
| 29:BG:30:GLY:HA3 | 29:BG:78:VAL:HA | 1.90 | 0.53 |
| 31:BJ:18:VAL:HG22 | 31:BJ:19:ASP:N | 2.24 | 0.53 |
| 33:BL:18:ARG:C | 33:BL:19:LEU:HD12 | 2.29 | 0.53 |
| 27:BE:181:ILE:HD13 | 33:BL:3:LEU:HD23 | 1.90 | 0.53 |
| 39:BR:43:ASN:HD21 | 39:BR:45:GLU:HG2 | 1.74 | 0.53 |
| 43:BW:31:LEU:N | 43:BW:60:ALA:HB3 | 2.24 | 0.53 |
| 1:CA:1221:G:O2' | 1:CA:1222:G:H5' | 2.09 | 0.53 |
| 1:CA:384:G:H2' | 1:CA:385:C:H6 | 1.73 | 0.53 |
| 2:CC:2:GLN:H | 2:CC:2:GLN:HE21 | 1.55 | 0.53 |
| 4:CE:158:LYS:NZ | 7:CH:63:LYS:HD3 | 2.23 | 0.53 |
| 23:DB:1032:A:H1' | 51:D4:23:ILE:HD13 | 1.91 | 0.53 |
| 23:DB:1063:G:C5' | 52:DI:135:MET:HG2 | 2.39 | 0.53 |
| 23:DB:1570:A:H2' | 23:DB:1571:A:C8 | 2.44 | 0.53 |
| 23:DB:1576:U:O2' | 23:DB:1577:C:H5' | 2.09 | 0.53 |
| 23:DB:1821:A:H2' | 23:DB:1822:C:C6 | 2.43 | 0.53 |
| 23:DB:1846:G:H2' | 23:DB:1847:A:O4' | 2.08 | 0.53 |
| 23:DB:1973:G:H2' | 23:DB:1974:C:C6 | 2.44 | 0.53 |
| 23:DB:2199:A:H3' | 23:DB:2200:C:H6 | 1.73 | 0.53 |
| 23:DB:2305:U:H2' | 23:DB:2306:C:C6 | 2.44 | 0.53 |
| 23:DB:256:A:H2' | 23:DB:257:C:C6 | 2.44 | 0.53 |
| 23:DB:2821:A:OP2 | 26:DD:115:GLY:HA3 | 2.08 | 0.53 |
| 23:DB:417:C:H2' | 23:DB:418:C:H6 | 1.72 | 0.53 |
| 23:DB:854:C:O2' | 23:DB:855:G:H5' | 2.08 | 0.53 |
| 23:DB:934:U:H2' | 23:DB:935:C:C6 | 2.44 | 0.53 |
| 23:DB:2621:G:P | 26:DD:124:ARG:HH22 | 2.31 | 0.53 |
| 27:DE:149:ILE:HG23 | 27:DE:188:MET:CA | 2.39 | 0.53 |
| 27:DE:176:ASP:OD1 | 27:DE:178:VAL:HG12 | 2.09 | 0.53 |
| 28:DF:106:ALA:HA | 28:DF:135:ILE:CD1 | 2.39 | 0.53 |
| 28:DF:122:ASP:OD2 | 28:DF:126:ASN:HB2 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2277:G:H5'' | 34:DM:86:LYS:HB2 | 1.91 | 0.53 |
| 34:DM:94:ALA:O | 34:DM:96:ILE:HG23 | 2.09 | 0.53 |
| 24:DV:24:ASN:HB3 | 24:DV:44:HIS:HB3 | 1.91 | 0.53 |
| 1:AA:312:C:H2' | 1:AA:313:A:C8 | 2.43 | 0.53 |
| 1:AA:678:U:H4' | 1:AA:778:G:OP1 | 2.09 | 0.53 |
| 1:AA:820:U:H4' | 1:AA:821:G:OP2 | 2.09 | 0.53 |
| 4:AE:23:THR:HA | 4:AE:28:ARG:HA | 1.90 | 0.53 |
| 6:AG:131:GLY:O | 6:AG:134:VAL:HG22 | 2.09 | 0.53 |
| 8:AI:61:ASP:C | 8:AI:62:LEU:HD13 | 2.29 | 0.53 |
| 1:AA:1250:A:H4' | 8:AI:69:GLY:O | 2.08 | 0.53 |
| 48:B1:3:GLY:O | 48:B1:4:ILE:HG12 | 2.08 | 0.53 |
| 23:BB:1747:U:H2' | 23:BB:1748:C:H6 | 1.72 | 0.53 |
| 23:BB:2078:C:H2' | 23:BB:2079:U:C6 | 2.43 | 0.53 |
| 23:BB:2186:G:H2' | 23:BB:2187:U:O4' | 2.09 | 0.53 |
| 23:BB:2508:G:H2' | 23:BB:2509:G:H8 | 1.73 | 0.53 |
| 23:BB:256:A:H2' | 23:BB:257:C:C6 | 2.43 | 0.53 |
| 23:BB:2784:U:H2' | 23:BB:2785:C:H6 | 1.72 | 0.53 |
| 25:BC:140:VAL:HG12 | 25:BC:141:HIS:N | 2.20 | 0.53 |
| 25:BC:159:THR:O | 25:BC:194:VAL:HG12 | 2.09 | 0.53 |
| 26:BD:187:LEU:HD12 | 26:BD:188:LEU:H | 1.74 | 0.53 |
| 26:BD:56:LYS:HG3 | 26:BD:58:ASN:HB2 | 1.91 | 0.53 |
| 29:BG:25:ILE:CG2 | 29:BG:78:VAL:HG21 | 2.39 | 0.53 |
| 31:BJ:123:LYS:HG2 | 31:BJ:132:HIS:NE2 | 2.23 | 0.53 |
| 31:BJ:38:GLY:HA3 | 31:BJ:50:THR:O | 2.09 | 0.53 |
| 31:BJ:96:ARG:O | 31:BJ:99:ARG:HG3 | 2.09 | 0.53 |
| 32:BK:107:LEU:HB2 | 32:BK:116:ILE:CG2 | 2.39 | 0.53 |
| 33:BL:41:ARG:HH21 | 33:BL:41:ARG:HG2 | 1.74 | 0.53 |
| 39:BR:28:ALA:HB3 | 39:BR:31:GLU:HB2 | 1.90 | 0.53 |
| 41:BT:57:VAL:HG12 | 41:BT:86:THR:OG1 | 2.09 | 0.53 |
| 41:BT:81:LYS:HG3 | 41:BT:82:LYS:N | 2.23 | 0.53 |
| 1:CA:1168:U:H4' | 1:CA:1169:A:OP2 | 2.08 | 0.53 |
| 1:CA:1277:C:O2' | 1:CA:1279:G:H1' | 2.09 | 0.53 |
| 1:CA:1332:A:H2' | 1:CA:1333:A:C8 | 2.44 | 0.53 |
| 1:CA:590:U:H2' | 1:CA:591:U:H6 | 1.72 | 0.53 |
| 20:CB:23:ASN:HD22 | 20:CB:24:PRO:CD | 2.21 | 0.53 |
| 3:CD:22:SER:HB2 | 3:CD:109:THR:HG22 | 1.91 | 0.53 |
| 5:CF:4:TYR:CE2 | 5:CF:71:ILE:HD13 | 2.44 | 0.53 |
| 7:CH:100:ILE:HG13 | 7:CH:128:VAL:O | 2.08 | 0.53 |
| 13:CN:50:LEU:CD2 | 13:CN:51:PRO:HD3 | 2.39 | 0.53 |
| 21:CU:35:GLU:HB2 | 21:CU:37:TYR:CZ | 2.43 | 0.53 |
| 51:D4:7:VAL:HG13 | 51:D4:8:LYS:H | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1210:G:N3 | 23:DB:1212:G:N2 | 2.56 | 0.53 |
| 23:DB:1244:A:O2' | 23:DB:1245:G:H5' | 2.09 | 0.53 |
| 23:DB:1623:G:O2' | 23:DB:1624:U:H5' | 2.08 | 0.53 |
| 23:DB:1792:G:O2' | 23:DB:1793:C:H5' | 2.09 | 0.53 |
| 23:DB:2846:G:H2' | 23:DB:2847:U:C6 | 2.43 | 0.53 |
| 23:DB:513:A:O5' | 23:DB:513:A:H8 | 1.92 | 0.53 |
| 26:DD:165:MET:HG2 | 26:DD:166:GLY:N | 2.24 | 0.53 |
| 26:DD:172:VAL:HG12 | 26:DD:173:GLN:N | 2.23 | 0.53 |
| 27:DE:150:THR:HG21 | 27:DE:153:LEU:HA | 1.91 | 0.53 |
| 23:DB:1099:G:H4' | 52:DI:4:VAL:CG1 | 2.39 | 0.53 |
| 32:DK:19:VAL:HG12 | 32:DK:41:ILE:CG1 | 2.39 | 0.53 |
| 34:DM:19:GLY:N | 34:DM:38:ARG:HH12 | 2.02 | 0.53 |
| 36:DO:111:ARG:HD2 | 36:DO:117:PHE:C | 2.29 | 0.53 |
| 38:DQ:68:ALA:O | 38:DQ:71:ASN:HB3 | 2.09 | 0.53 |
| 40:DS:57:ASN:O | 40:DS:61:ASN:HB2 | 2.09 | 0.53 |
| 42:DU:41:VAL:HG22 | 42:DU:60:LYS:O | 2.09 | 0.53 |
| 42:DU:64:ILE:HG13 | 42:DU:65:GLN:N | 2.23 | 0.53 |
| 44:DX:23:ARG:O | 44:DX:27:ASN:N | 2.41 | 0.53 |
| 1:AA:320:A:H2' | 1:AA:321:A:C8 | 2.44 | 0.53 |
| 1:AA:429:U:H3' | 3:AD:8:LEU:HD23 | 1.91 | 0.53 |
| 1:AA:462:G:H3' | 1:AA:463:U:C6 | 2.44 | 0.53 |
| 1:AA:632:U:H3' | 1:AA:633:G:H5' | 1.90 | 0.53 |
| 1:AA:709:U:H2' | 1:AA:710:G:C8 | 2.43 | 0.53 |
| 1:AA:784:A:H2' | 1:AA:785:G:C8 | 2.44 | 0.53 |
| 20:AB:101:THR:HA | 20:AB:178:LEU:HD21 | 1.91 | 0.53 |
| 1:AA:546:A:OP2 | 3:AD:67:LEU:HB3 | 2.09 | 0.53 |
| 5:AF:53:LYS:H | 5:AF:53:LYS:HZ2 | 1.57 | 0.53 |
| 6:AG:29:LEU:HD23 | 6:AG:29:LEU:O | 2.09 | 0.53 |
| 7:AH:31:LEU:O | 7:AH:35:ILE:HG13 | 2.09 | 0.53 |
| 9:AJ:76:ILE:HD13 | 9:AJ:79:PRO:HB3 | 1.91 | 0.53 |
| 16:AQ:29:LYS:HG3 | 16:AQ:34:GLY:HA2 | 1.90 | 0.53 |
| 23:BB:1198:U:H2' | 23:BB:1199:U:H6 | 1.74 | 0.53 |
| 23:BB:1229:C:H2' | 23:BB:1230:A:C8 | 2.44 | 0.53 |
| 23:BB:1792:G:O2' | 23:BB:1793:C:H5' | 2.09 | 0.53 |
| 23:BB:2415:G:H2' | 23:BB:2416:C:H6 | 1.74 | 0.53 |
| 23:BB:2600:A:O2' | 23:BB:2601:C:H5' | 2.09 | 0.53 |
| 23:BB:2648:G:H2' | 23:BB:2649:C:C6 | 2.43 | 0.53 |
| 23:BB:2803:G:H2' | 23:BB:2804:U:H6 | 1.72 | 0.53 |
| 23:BB:948:C:H2' | 23:BB:949:G:C8 | 2.44 | 0.53 |
| 22:BA:89:U:O2 | 23:BB:958:U:H2' | 2.08 | 0.53 |
| 25:BC:115:ILE:HA | 25:BC:124:LYS:NZ | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BC:209:ALA:HA | 25:BC:212:TRP:NE1 | 2.24 | 0.53 |
| 26:BD:90:PHE:N | 26:BD:94:GLN:OE1 | 2.42 | 0.53 |
| 27:BE:2:GLU:HA | 27:BE:13:THR:OG1 | 2.09 | 0.53 |
| 29:BG:106:LEU:O | 29:BG:108:PHE:N | 2.41 | 0.53 |
| 33:BL:142:ILE:HG22 | 33:BL:143:GLU:N | 2.24 | 0.53 |
| 36:BO:7:ARG:HA | 36:BO:10:ARG:NH2 | 2.24 | 0.53 |
| 39:BR:3:ALA:O | 39:BR:13:ARG:HA | 2.09 | 0.53 |
| 41:BT:32:LEU:O | 41:BT:83:ALA:HB2 | 2.09 | 0.53 |
| 46:BZ:66:THR:O | 46:BZ:69:ALA:HB3 | 2.08 | 0.53 |
| 1:CA:1245:C:H2' | 1:CA:1246:A:C8 | 2.43 | 0.53 |
| 1:CA:312:C:H2' | 1:CA:313:A:C8 | 2.44 | 0.53 |
| 1:CA:505:G:H2' | 1:CA:506:G:C8 | 2.44 | 0.53 |
| 1:CA:539:A:H2' | 1:CA:540:G:H8 | 1.72 | 0.53 |
| 1:CA:91:U:H2' | 1:CA:92:U:H6 | 1.72 | 0.53 |
| 2:CC:190:THR:HG22 | 2:CC:191:THR:N | 2.24 | 0.53 |
| 2:CC:57:GLU:O | 2:CC:63:ILE:HA | 2.09 | 0.53 |
| 16:CQ:24:ILE:O | 16:CQ:40:THR:HA | 2.09 | 0.53 |
| 16:CQ:7:LEU:O | 16:CQ:60:ILE:HD13 | 2.09 | 0.53 |
| 18:CS:39:ILE:HB | 18:CS:65:MET:O | 2.09 | 0.53 |
| 21:CU:36:PHE:HA | 21:CU:39:LYS:HE2 | 1.91 | 0.53 |
| 23:DB:1193:G:H2' | 23:DB:1194:A:H5'' | 1.90 | 0.53 |
| 23:DB:1949:G:H2' | 23:DB:1950:G:H8 | 1.69 | 0.53 |
| 23:DB:2021:C:P | 47:D0:8:THR:HG21 | 2.49 | 0.53 |
| 23:DB:346:A:H2' | 23:DB:347:A:O4' | 2.09 | 0.53 |
| 23:DB:584:C:OP1 | 38:DQ:5:ARG:HB3 | 2.07 | 0.53 |
| 23:DB:674:G:H1' | 27:DE:69:ARG:NE | 2.24 | 0.53 |
| 23:DB:705:A:N6 | 23:DB:726:G:O2' | 2.41 | 0.53 |
| 23:DB:947:A:O2' | 23:DB:984:A:H2 | 1.92 | 0.53 |
| 25:DC:12:ARG:HA | 25:DC:15:VAL:HG23 | 1.90 | 0.53 |
| 23:DB:2774:C:OP1 | 26:DD:169:ARG:HG3 | 2.08 | 0.53 |
| 27:DE:5:LEU:HD22 | 27:DE:122:GLU:HG3 | 1.91 | 0.53 |
| 27:DE:128:ALA:H | 27:DE:133:LEU:CD1 | 2.22 | 0.53 |
| 27:DE:46:GLN:HB3 | 27:DE:86:ALA:HA | 1.91 | 0.53 |
| 28:DF:28:PRO:HG3 | 28:DF:159:ALA:HB2 | 1.90 | 0.53 |
| 28:DF:12:VAL:O | 28:DF:16:MET:HG2 | 2.09 | 0.53 |
| 31:DJ:123:LYS:HG2 | 31:DJ:132:HIS:NE2 | 2.23 | 0.53 |
| 37:DP:6:GLN:O | 37:DP:9:GLN:HG2 | 2.09 | 0.53 |
| 40:DS:17:VAL:HG11 | 40:DS:103:ILE:HG12 | 1.91 | 0.53 |
| 24:DV:72:VAL:HG21 | 24:DV:91:PHE:CB | 2.34 | 0.53 |
| 1:AA:434:U:H3' | 1:AA:435:A:H8 | 1.72 | 0.52 |
| 1:AA:806:C:H2' | 1:AA:807:A:H8 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:8:A:H61 | 3:AD:53:GLN:HE22 | 1.56 | 0.52 |
| 1:AA:930:C:H2' | 1:AA:931:C:O4' | 2.08 | 0.52 |
| 3:AD:53:GLN:HB3 | 3:AD:202:LEU:HB2 | 1.91 | 0.52 |
| 1:AA:9:G:OP2 | 4:AE:125:LYS:HD3 | 2.09 | 0.52 |
| 6:AG:15:PRO:HG2 | 6:AG:43:TYR:OH | 2.10 | 0.52 |
| 8:AI:44:ARG:O | 8:AI:47:VAL:HG22 | 2.08 | 0.52 |
| 23:BB:1145:C:O2' | 23:BB:1146:C:H5' | 2.08 | 0.52 |
| 23:BB:123:G:H2' | 23:BB:124:G:C8 | 2.44 | 0.52 |
| 23:BB:1746:A:H2' | 23:BB:1747:U:C6 | 2.45 | 0.52 |
| 23:BB:189:G:H2' | 23:BB:205:G:H22 | 1.72 | 0.52 |
| 23:BB:2386:A:H2' | 23:BB:2387:U:C6 | 2.44 | 0.52 |
| 23:BB:2389:G:H5'' | 23:BB:2390:U:H5' | 1.91 | 0.52 |
| 23:BB:2814:A:H2' | 23:BB:2815:C:H6 | 1.74 | 0.52 |
| 23:BB:553:G:O2' | 23:BB:554:U:H5' | 2.10 | 0.52 |
| 27:BE:106:LYS:HE2 | 27:BE:200:LEU:HB3 | 1.91 | 0.52 |
| 23:BB:674:G:O3' | 27:BE:60:TRP:CZ2 | 2.62 | 0.52 |
| 28:BF:11:VAL:HG12 | 28:BF:12:VAL:N | 2.15 | 0.52 |
| 52:BI:2:LYS:NZ | 52:BI:2:LYS:HB3 | 2.24 | 0.52 |
| 52:BI:81:LYS:HG3 | 52:BI:82:ALA:N | 2.23 | 0.52 |
| 32:BK:101:GLY:HA2 | 37:BP:65:ASN:HB2 | 1.90 | 0.52 |
| 34:BM:126:ILE:HD12 | 34:BM:126:ILE:N | 2.24 | 0.52 |
| 46:BZ:5:CYS:SG | 46:BZ:8:THR:HG23 | 2.49 | 0.52 |
| 1:CA:1018:G:H2' | 1:CA:1019:A:C8 | 2.45 | 0.52 |
| 1:CA:55:A:OP2 | 1:CA:352:C:N4 | 2.41 | 0.52 |
| 20:CB:27:LYS:HB3 | 20:CB:28:PRO:HD3 | 1.91 | 0.52 |
| 2:CC:166:TRP:HA | 2:CC:166:TRP:CE3 | 2.44 | 0.52 |
| 1:CA:546:A:OP2 | 3:CD:67:LEU:HB3 | 2.09 | 0.52 |
| 8:CI:27:ILE:HG21 | 8:CI:34:LEU:HD13 | 1.91 | 0.52 |
| 19:CT:49:ALA:HA | 19:CT:52:GLU:HB3 | 1.89 | 0.52 |
| 23:DB:1771:C:O2' | 23:DB:1772:A:H5' | 2.09 | 0.52 |
| 23:DB:1947:C:H2' | 23:DB:1948:G:C8 | 2.44 | 0.52 |
| 23:DB:2106:U:H2' | 23:DB:2107:G:C8 | 2.44 | 0.52 |
| 23:DB:2471:A:O2' | 23:DB:2472:G:O5' | 2.27 | 0.52 |
| 23:DB:418:C:H2' | 23:DB:419:U:C6 | 2.44 | 0.52 |
| 23:DB:581:C:H2' | 23:DB:582:A:H8 | 1.73 | 0.52 |
| 23:DB:832:U:H2' | 23:DB:833:A:C8 | 2.44 | 0.52 |
| 23:DB:851:C:H2' | 23:DB:852:U:H6 | 1.74 | 0.52 |
| 23:DB:909:A:H2' | 23:DB:912:C:H5 | 1.72 | 0.52 |
| 23:DB:969:G:OP1 | 45:DY:17:PRO:HG3 | 2.08 | 0.52 |
| 25:DC:20:ASN:OD1 | 25:DC:22:GLU:HG2 | 2.08 | 0.52 |
| 23:DB:2597:G:H5' | 25:DC:240:GLY:HA3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DF:133:GLU:HA | 28:DF:150:GLY:HA2 | 1.90 | 0.52 |
| 52:DI:57:VAL:HG23 | 52:DI:71:LYS:NZ | 2.24 | 0.52 |
| 31:DJ:25:LEU:HB2 | 31:DJ:62:VAL:HG22 | 1.90 | 0.52 |
| 35:DN:108:ALA:O | 35:DN:110:MET:HE3 | 2.09 | 0.52 |
| 35:DN:8:ARG:HG2 | 35:DN:10:LEU:HD22 | 1.91 | 0.52 |
| 37:DP:6:GLN:O | 37:DP:10:GLU:HG2 | 2.10 | 0.52 |
| 37:DP:3:ILE:CD1 | 37:DP:7:LEU:HD11 | 2.38 | 0.52 |
| 42:DU:81:ARG:HB2 | 42:DU:96:LYS:HG3 | 1.91 | 0.52 |
| 46:DZ:69:ALA:HA | 46:DZ:72:ARG:NH2 | 2.24 | 0.52 |
| 1:AA:169:C:O2' | 1:AA:170:U:H5' | 2.09 | 0.52 |
| 1:AA:269:C:H2' | 1:AA:270:A:H8 | 1.73 | 0.52 |
| 1:AA:490:C:H2' | 1:AA:491:G:H8 | 1.73 | 0.52 |
| 1:AA:782:A:H2' | 1:AA:783:C:O4' | 2.09 | 0.52 |
| 2:AC:156:LEU:HD11 | 2:AC:165:GLU:HB2 | 1.91 | 0.52 |
| 12:AM:17:ALA:CB | 12:AM:44:ILE:HD11 | 2.39 | 0.52 |
| 11:AL:7:VAL:HG22 | 16:AQ:33:TYR:CD1 | 2.44 | 0.52 |
| 35:BN:99:LYS:O | 47:B0:42:ILE:HG12 | 2.08 | 0.52 |
| 23:BB:1170:C:H2' | 23:BB:1171:G:C8 | 2.45 | 0.52 |
| 23:BB:1369:G:O2' | 23:BB:1370:C:H5' | 2.09 | 0.52 |
| 23:BB:1387:A:H2' | 23:BB:1388:G:H8 | 1.74 | 0.52 |
| 23:BB:1511:G:H2' | 23:BB:1512:C:H6 | 1.74 | 0.52 |
| 23:BB:1733:G:H2' | 23:BB:1734:G:C8 | 2.43 | 0.52 |
| 23:BB:196:A:H2' | 23:BB:196:A:N3 | 2.23 | 0.52 |
| 23:BB:247:G:H4' | 23:BB:386:G:C5 | 2.44 | 0.52 |
| 23:BB:37:C:O2' | 27:BE:45:ALA:HA | 2.10 | 0.52 |
| 30:BH:110:VAL:HB | 30:BH:132:PHE:CZ | 2.44 | 0.52 |
| 32:BK:71:ARG:CG | 32:BK:105:ARG:HH21 | 2.22 | 0.52 |
| 33:BL:135:ILE:HG12 | 33:BL:140:GLY:HA3 | 1.91 | 0.52 |
| 38:BQ:59:LEU:O | 38:BQ:62:ALA:HB3 | 2.08 | 0.52 |
| 24:BV:63:ILE:HD12 | 24:BV:63:ILE:N | 2.25 | 0.52 |
| 23:BB:77:G:H5' | 44:BX:52:ARG:HG2 | 1.91 | 0.52 |
| 1:CA:1124:G:H4' | 9:CJ:40:ILE:HG12 | 1.91 | 0.52 |
| 1:CA:1324:A:H2' | 1:CA:1325:C:O4' | 2.10 | 0.52 |
| 1:CA:1423:G:H2' | 1:CA:1424:U:H6 | 1.73 | 0.52 |
| 1:CA:1521:C:H2' | 1:CA:1522:U:C6 | 2.44 | 0.52 |
| 1:CA:370:C:H2' | 1:CA:371:A:C8 | 2.45 | 0.52 |
| 1:CA:390:U:H2' | 1:CA:391:G:H8 | 1.74 | 0.52 |
| 1:CA:455:G:O2' | 1:CA:456:A:H5' | 2.08 | 0.52 |
| 1:CA:657:U:O2' | 1:CA:658:C:H5' | 2.09 | 0.52 |
| 20:CB:65:LYS:HG2 | 20:CB:89:PHE:HE1 | 1.74 | 0.52 |
| 2:CC:155:ARG:NH2 | 2:CC:192:TYR:HB2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CD:117:VAL:O | 3:CD:130:ASN:HA | 2.10 | 0.52 |
| 6:CG:104:VAL:O | 6:CG:108:ARG:HG3 | 2.09 | 0.52 |
| 13:CN:50:LEU:HG | 13:CN:51:PRO:HD3 | 1.92 | 0.52 |
| 16:CQ:75:VAL:HG23 | 16:CQ:76:ARG:N | 2.25 | 0.52 |
| 47:D0:52:LYS:NZ | 47:D0:56:LYS:H | 2.06 | 0.52 |
| 48:D1:3:GLY:C | 48:D1:5:ARG:H | 2.11 | 0.52 |
| 22:DA:54:G:H21 | 28:DF:25:MET:HE3 | 1.75 | 0.52 |
| 23:DB:931:U:H3 | 23:DB:1166:G:H21 | 1.56 | 0.52 |
| 23:DB:1332:G:HO2' | 23:DB:1609:A:H2 | 1.56 | 0.52 |
| 23:DB:163:C:O4' | 23:DB:163:C:O2 | 2.25 | 0.52 |
| 23:DB:2028:U:H2' | 23:DB:2029:G:C8 | 2.44 | 0.52 |
| 23:DB:2092:U:H4' | 23:DB:2093:G:H5'' | 1.90 | 0.52 |
| 23:DB:2882:A:C3' | 23:DB:2883:A:H5'' | 2.39 | 0.52 |
| 23:DB:2886:A:H3' | 23:DB:2887:A:C8 | 2.42 | 0.52 |
| 23:DB:989:G:OP2 | 45:DY:13:ILE:HD11 | 2.10 | 0.52 |
| 26:DD:46:ARG:NH1 | 26:DD:85:ALA:HA | 2.24 | 0.52 |
| 26:DD:5:VAL:H | 26:DD:32:ASN:ND2 | 1.94 | 0.52 |
| 26:DD:7:LYS:O | 26:DD:9:VAL:HG12 | 2.08 | 0.52 |
| 28:DF:131:VAL:O | 28:DF:132:ARG:HB2 | 2.09 | 0.52 |
| 29:DG:19:ASN:HB2 | 29:DG:22:VAL:HB | 1.90 | 0.52 |
| 29:DG:6:ALA:HB3 | 29:DG:68:ARG:NE | 2.24 | 0.52 |
| 30:DH:133:GLN:HB3 | 30:DH:139:PHE:CB | 2.39 | 0.52 |
| 31:DJ:125:TYR:HH | 31:DJ:132:HIS:CE1 | 2.26 | 0.52 |
| 31:DJ:25:LEU:HD22 | 31:DJ:26:GLY:N | 2.18 | 0.52 |
| 23:DB:993:G:H1' | 39:DR:91:GLN:NE2 | 2.25 | 0.52 |
| 41:DT:29:THR:HA | 41:DT:86:THR:CA | 2.35 | 0.52 |
| 41:DT:28:ASN:CA | 41:DT:91:GLN:HE22 | 2.20 | 0.52 |
| 42:DU:82:VAL:CG1 | 42:DU:93:ARG:HB3 | 2.39 | 0.52 |
| 24:DV:16:ALA:HA | 24:DV:19:ARG:HE | 1.73 | 0.52 |
| 1:AA:1320:C:C5 | 18:AS:36:ARG:HA | 2.45 | 0.52 |
| 1:AA:79:G:H8 | 1:AA:79:G:OP2 | 1.93 | 0.52 |
| 1:AA:927:G:O2' | 1:AA:928:G:H5' | 2.09 | 0.52 |
| 8:AI:55:ASP:HB2 | 8:AI:59:LYS:HG3 | 1.92 | 0.52 |
| 51:B4:10:LEU:HD13 | 51:B4:33:HIS:HA | 1.90 | 0.52 |
| 23:BB:1000:A:H2' | 23:BB:1001:A:H8 | 1.71 | 0.52 |
| 23:BB:126:A:O2' | 23:BB:127:A:H5' | 2.09 | 0.52 |
| 23:BB:1386:C:OP2 | 23:BB:1396:U:H5 | 1.93 | 0.52 |
| 23:BB:1571:A:H2' | 23:BB:1572:A:C8 | 2.44 | 0.52 |
| 23:BB:1846:G:H2' | 23:BB:1847:A:O4' | 2.10 | 0.52 |
| 23:BB:1131:G:N2 | 23:BB:2024:G:H21 | 2.07 | 0.52 |
| 23:BB:2352:A:C6 | 43:BW:30:VAL:HG11 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:2411:A:H2' | 23:BB:2412:A:C8 | 2.44 | 0.52 |
| 23:BB:527:C:H5' | 56:BB:3416:HOH:O | 2.09 | 0.52 |
| 23:BB:936:A:H2' | 23:BB:937:C:H6 | 1.73 | 0.52 |
| 26:BD:16:THR:HB | 26:BD:18:ASP:OD1 | 2.09 | 0.52 |
| 30:BH:132:PHE:N | 30:BH:142:VAL:HG23 | 2.24 | 0.52 |
| 31:BJ:55:ILE:CB | 31:BJ:123:LYS:HB2 | 2.37 | 0.52 |
| 23:BB:1287:A:P | 35:BN:104:ALA:HB3 | 2.49 | 0.52 |
| 35:BN:59:SER:O | 35:BN:63:ARG:HB2 | 2.08 | 0.52 |
| 38:BQ:104:ALA:O | 38:BQ:105:PHE:HB3 | 2.08 | 0.52 |
| 38:BQ:68:ALA:HA | 38:BQ:71:ASN:HB3 | 1.91 | 0.52 |
| 39:BR:14:VAL:HG21 | 39:BR:98:ILE:HG12 | 1.91 | 0.52 |
| 39:BR:16:GLU:H | 39:BR:101:ILE:CG1 | 2.22 | 0.52 |
| 41:BT:12:ARG:HG2 | 44:BX:29:ARG:HH12 | 1.74 | 0.52 |
| 1:CA:1302:C:H4' | 1:CA:1303:C:OP2 | 2.09 | 0.52 |
| 1:CA:1379:G:O2' | 1:CA:1380:U:H5' | 2.09 | 0.52 |
| 1:CA:814:A:H5' | 1:CA:1511:G:H4' | 1.90 | 0.52 |
| 1:CA:165:G:O2' | 1:CA:166:U:H5' | 2.09 | 0.52 |
| 1:CA:443:C:H2' | 1:CA:444:G:C8 | 2.44 | 0.52 |
| 1:CA:45:G:H2' | 1:CA:46:G:H8 | 1.74 | 0.52 |
| 1:CA:900:A:H2' | 1:CA:901:A:C8 | 2.44 | 0.52 |
| 2:CC:35:ASP:HB3 | 2:CC:39:ARG:HH12 | 1.75 | 0.52 |
| 3:CD:157:ALA:O | 3:CD:160:LEU:HD22 | 2.09 | 0.52 |
| 6:CG:15:PRO:HG2 | 6:CG:43:TYR:OH | 2.09 | 0.52 |
| 8:CI:32:ARG:NH1 | 8:CI:37:TYR:HA | 2.24 | 0.52 |
| 9:CJ:28:THR:O | 9:CJ:31:ARG:HG2 | 2.10 | 0.52 |
| 23:DB:2015:A:N3 | 47:D0:2:VAL:HG22 | 2.23 | 0.52 |
| 47:D0:5:ASN:O | 47:D0:7:PRO:HD3 | 2.09 | 0.52 |
| 23:DB:1790:C:H2' | 23:DB:1791:A:C8 | 2.44 | 0.52 |
| 23:DB:1923:U:H2' | 23:DB:1924:C:H6 | 1.74 | 0.52 |
| 23:DB:196:A:N3 | 23:DB:196:A:H2' | 2.24 | 0.52 |
| 23:DB:2572:A:OP2 | 26:DD:151:THR:HB | 2.09 | 0.52 |
| 23:DB:2659:G:N2 | 23:DB:2661:G:H5'' | 2.23 | 0.52 |
| 23:DB:2662:A:H2' | 23:DB:2663:G:O4' | 2.09 | 0.52 |
| 23:DB:500:G:N2 | 23:DB:502:A:H3' | 2.24 | 0.52 |
| 23:DB:528:A:C2 | 23:DB:2043:C:H4' | 2.44 | 0.52 |
| 23:DB:75:G:H4' | 44:DX:48:ARG:HH22 | 1.75 | 0.52 |
| 23:DB:812:C:H5'' | 23:DB:1250:G:O2' | 2.09 | 0.52 |
| 23:DB:912:C:O2' | 23:DB:913:U:H5' | 2.09 | 0.52 |
| 25:DC:159:THR:O | 25:DC:194:VAL:HG12 | 2.09 | 0.52 |
| 26:DD:114:LYS:HB2 | 26:DD:116:LYS:HE3 | 1.91 | 0.52 |
| 29:DG:88:LEU:O | 29:DG:88:LEU:HD12 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DG:7:PRO:O | 29:DG:8:VAL:HB | 2.09 | 0.52 |
| 52:DI:75:ALA:O | 52:DI:79:LEU:HG | 2.10 | 0.52 |
| 32:DK:20:MET:C | 32:DK:41:ILE:HG13 | 2.29 | 0.52 |
| 36:DO:25:ARG:HD2 | 36:DO:93:ASP:HB2 | 1.90 | 0.52 |
| 36:DO:30:ARG:HG3 | 36:DO:30:ARG:HH11 | 1.74 | 0.52 |
| 38:DQ:71:ASN:ND2 | 38:DQ:109:VAL:HG11 | 2.24 | 0.52 |
| 38:DQ:59:LEU:O | 38:DQ:62:ALA:HB3 | 2.09 | 0.52 |
| 38:DQ:71:ASN:ND2 | 38:DQ:73:ILE:HG22 | 2.24 | 0.52 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:H6 | 1.73 | 0.52 |
| 1:AA:399:G:H2' | 1:AA:400:C:C6 | 2.44 | 0.52 |
| 1:AA:552:U:O2' | 1:AA:553:A:H5' | 2.10 | 0.52 |
| 1:AA:586:C:O2' | 1:AA:878:A:H4' | 2.10 | 0.52 |
| 3:AD:55:ARG:HG3 | 3:AD:55:ARG:NH1 | 2.25 | 0.52 |
| 10:AK:126:ARG:HA | 10:AK:126:ARG:NE | 2.24 | 0.52 |
| 11:AL:43:LYS:NZ | 11:AL:44:PRO:HD3 | 2.24 | 0.52 |
| 12:AM:44:ILE:HA | 12:AM:47:LEU:HD23 | 1.90 | 0.52 |
| 13:AN:5:MET:HB3 | 13:AN:62:ARG:HH12 | 1.74 | 0.52 |
| 17:AR:60:ARG:O | 17:AR:64:LEU:HD13 | 2.09 | 0.52 |
| 10:AK:124:LYS:HA | 21:AU:34:ARG:HG2 | 1.91 | 0.52 |
| 49:B2:19:ARG:HH21 | 49:B2:19:ARG:HG2 | 1.73 | 0.52 |
| 49:B2:30:VAL:HA | 49:B2:33:ARG:HH21 | 1.73 | 0.52 |
| 51:B4:7:VAL:HG13 | 51:B4:8:LYS:H | 1.74 | 0.52 |
| 23:BB:1050:A:H2' | 23:BB:1051:G:C8 | 2.42 | 0.52 |
| 23:BB:1060:U:O2 | 23:BB:1088:A:C8 | 2.63 | 0.52 |
| 23:BB:1097:U:C2' | 23:BB:1098:A:H5' | 2.38 | 0.52 |
| 23:BB:1117:C:H2' | 23:BB:1118:C:H6 | 1.74 | 0.52 |
| 23:BB:1196:C:H2' | 23:BB:1197:G:C8 | 2.44 | 0.52 |
| 23:BB:1442:U:H2' | 23:BB:1443:U:H6 | 1.73 | 0.52 |
| 23:BB:308:G:H2' | 23:BB:309:A:O4' | 2.09 | 0.52 |
| 25:BC:91:ALA:CB | 25:BC:105:ALA:HB2 | 2.37 | 0.52 |
| 25:BC:93:VAL:HG12 | 25:BC:101:ARG:O | 2.09 | 0.52 |
| 27:BE:5:LEU:HD22 | 27:BE:122:GLU:HG3 | 1.90 | 0.52 |
| 28:BF:177:ARG:NH1 | 28:BF:177:ARG:HA | 2.24 | 0.52 |
| 29:BG:93:TYR:C | 29:BG:94:ARG:HG3 | 2.29 | 0.52 |
| 30:BH:73:ASN:N | 30:BH:73:ASN:ND2 | 2.57 | 0.52 |
| 23:BB:2547:A:H4' | 32:BK:29:HIS:CE1 | 2.45 | 0.52 |
| 33:BL:109:LYS:O | 33:BL:111:ILE:HG12 | 2.09 | 0.52 |
| 35:BN:103:ARG:CG | 35:BN:104:ALA:H | 2.22 | 0.52 |
| 36:BO:52:SER:OG | 36:BO:54:VAL:HG12 | 2.10 | 0.52 |
| 38:BQ:78:PHE:CE2 | 38:BQ:82:LEU:HD11 | 2.44 | 0.52 |
| 44:BX:56:LEU:O | 44:BX:58:ASN:N | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BZ:68:LEU:HB3 | 46:BZ:78:TYR:HE1 | 1.75 | 0.52 |
| 1:CA:1207:G:O2' | 1:CA:1208:C:H5' | 2.09 | 0.52 |
| 1:CA:1386:G:H2' | 1:CA:1387:G:C8 | 2.45 | 0.52 |
| 1:CA:1434:A:H2' | 1:CA:1435:G:C8 | 2.44 | 0.52 |
| 1:CA:160:A:H2' | 1:CA:161:A:O4' | 2.09 | 0.52 |
| 1:CA:252:U:H2' | 1:CA:253:A:H8 | 1.74 | 0.52 |
| 1:CA:562:U:H2' | 1:CA:562:U:OP2 | 2.09 | 0.52 |
| 20:CB:186:VAL:HB | 20:CB:190:SER:HB2 | 1.90 | 0.52 |
| 4:CE:15:ILE:HD12 | 4:CE:35:LEU:HG | 1.90 | 0.52 |
| 5:CF:74:LEU:HG | 5:CF:78:PHE:CE1 | 2.45 | 0.52 |
| 6:CG:126:ALA:HA | 6:CG:134:VAL:HG13 | 1.90 | 0.52 |
| 10:CK:74:LYS:C | 10:CK:76:TYR:H | 2.12 | 0.52 |
| 13:CN:97:LYS:HZ2 | 13:CN:97:LYS:HB3 | 1.74 | 0.52 |
| 16:CQ:3:LYS:HE2 | 16:CQ:3:LYS:HA | 1.91 | 0.52 |
| 18:CS:12:LEU:O | 18:CS:15:LEU:HB2 | 2.10 | 0.52 |
| 23:DB:1021:A:H61 | 23:DB:1142:A:H61 | 1.58 | 0.52 |
| 23:DB:1196:C:H2' | 23:DB:1197:G:C8 | 2.44 | 0.52 |
| 23:DB:718:A:H3' | 23:DB:719:C:C6 | 2.42 | 0.52 |
| 23:DB:729:G:C8 | 25:DC:206:LYS:HE3 | 2.44 | 0.52 |
| 31:DJ:42:ALA:O | 31:DJ:44:TYR:N | 2.43 | 0.52 |
| 34:DM:97:GLN:HB2 | 34:DM:98:PRO:CD | 2.39 | 0.52 |
| 37:DP:31:VAL:HG12 | 37:DP:38:ARG:O | 2.09 | 0.52 |
| 24:DV:1:MET:O | 24:DV:62:THR:HG23 | 2.09 | 0.52 |
| 44:DX:3:ALA:O | 44:DX:6:LEU:HB2 | 2.09 | 0.52 |
| 1:AA:996:A:H2 | 1:AA:1045:C:HO2' | 1.55 | 0.52 |
| 1:AA:1300:G:H1' | 1:AA:1301:U:H5 | 1.73 | 0.52 |
| 1:AA:1461:G:H2' | 1:AA:1462:C:C6 | 2.44 | 0.52 |
| 1:AA:151:A:H5' | 1:AA:152:A:OP2 | 2.09 | 0.52 |
| 1:AA:215:C:H2' | 1:AA:216:U:C6 | 2.45 | 0.52 |
| 1:AA:312:C:H2' | 1:AA:313:A:H8 | 1.74 | 0.52 |
| 1:AA:314:C:O2' | 1:AA:315:A:H5' | 2.09 | 0.52 |
| 1:AA:608:A:H3' | 56:AA:2292:HOH:O | 2.09 | 0.52 |
| 2:AC:34:SER:O | 2:AC:38:VAL:HG22 | 2.10 | 0.52 |
| 3:AD:117:VAL:O | 3:AD:130:ASN:HA | 2.10 | 0.52 |
| 8:AI:35:GLU:HG3 | 8:AI:44:ARG:HD3 | 1.92 | 0.52 |
| 10:AK:81:LEU:HD23 | 10:AK:81:LEU:N | 2.24 | 0.52 |
| 12:AM:10:ASP:CA | 12:AM:44:ILE:HD13 | 2.39 | 0.52 |
| 21:AU:3:ILE:HD13 | 21:AU:19:LYS:HA | 1.91 | 0.52 |
| 22:BA:39:A:O2' | 22:BA:40:U:H5' | 2.10 | 0.52 |
| 23:BB:1453:A:OP1 | 23:BB:1453:A:H4' | 2.09 | 0.52 |
| 23:BB:2365:G:H4' | 43:BW:59:PHE:CE1 | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:394:C:H2' | 23:BB:395:U:O4' | 2.10 | 0.52 |
| 23:BB:499:U:H5' | 42:BU:44:HIS:CE1 | 2.44 | 0.52 |
| 23:BB:704:G:H1' | 23:BB:727:A:H61 | 1.74 | 0.52 |
| 29:BG:154:GLU:C | 29:BG:156:TYR:H | 2.13 | 0.52 |
| 32:BK:109:SER:C | 32:BK:111:LYS:H | 2.12 | 0.52 |
| 33:BL:78:ARG:HG2 | 33:BL:113:ALA:CB | 2.39 | 0.52 |
| 33:BL:61:LEU:N | 33:BL:61:LEU:HD12 | 2.25 | 0.52 |
| 23:BB:812:C:H4' | 38:BQ:12:ARG:HH12 | 1.75 | 0.52 |
| 38:BQ:59:LEU:HD13 | 38:BQ:60:TRP:N | 2.25 | 0.52 |
| 24:BV:14:LYS:HE3 | 24:BV:18:ARG:NH2 | 2.25 | 0.52 |
| 46:BZ:68:LEU:HB3 | 46:BZ:78:TYR:CE1 | 2.44 | 0.52 |
| 1:CA:1004:A:H5' | 1:CA:1024:G:H22 | 1.74 | 0.52 |
| 1:CA:1384:C:H2' | 1:CA:1385:G:C8 | 2.44 | 0.52 |
| 1:CA:5:U:H4' | 1:CA:6:G:H5' | 1.91 | 0.52 |
| 20:CB:112:ARG:HA | 20:CB:115:ASP:OD2 | 2.09 | 0.52 |
| 3:CD:75:TYR:HE1 | 3:CD:200:VAL:HA | 1.74 | 0.52 |
| 6:CG:61:PHE:O | 6:CG:65:LEU:HD13 | 2.10 | 0.52 |
| 8:CI:44:ARG:O | 8:CI:47:VAL:HG22 | 2.09 | 0.52 |
| 9:CJ:12:ALA:HB3 | 9:CJ:18:ILE:HB | 1.91 | 0.52 |
| 23:DB:1130:U:O2 | 23:DB:2025:C:H5'' | 2.10 | 0.52 |
| 23:DB:1442:U:H2' | 23:DB:1443:U:H6 | 1.73 | 0.52 |
| 23:DB:1642:G:O2' | 23:DB:1643:G:H5' | 2.10 | 0.52 |
| 23:DB:1828:G:O6 | 25:DC:220:ARG:HD2 | 2.10 | 0.52 |
| 23:DB:1847:A:H4' | 23:DB:1848:A:H8 | 1.74 | 0.52 |
| 23:DB:1854:A:N6 | 23:DB:1888:G:H1' | 2.24 | 0.52 |
| 23:DB:2543:G:H8 | 23:DB:2543:G:H5' | 1.74 | 0.52 |
| 23:DB:2592:G:H2' | 23:DB:2593:U:O4' | 2.10 | 0.52 |
| 23:DB:2813:A:H2' | 23:DB:2814:A:H8 | 1.74 | 0.52 |
| 23:DB:283:G:H2' | 23:DB:284:U:O4' | 2.10 | 0.52 |
| 23:DB:405:U:H4' | 23:DB:405:U:OP2 | 2.10 | 0.52 |
| 23:DB:753:A:H2' | 23:DB:754:U:H6 | 1.72 | 0.52 |
| 25:DC:6:LYS:HB3 | 25:DC:8:THR:HG22 | 1.92 | 0.52 |
| 26:DD:154:LYS:H | 26:DD:154:LYS:HD3 | 1.74 | 0.52 |
| 26:DD:13:ARG:HD3 | 26:DD:15:PHE:CE1 | 2.45 | 0.52 |
| 26:DD:90:PHE:N | 26:DD:94:GLN:OE1 | 2.42 | 0.52 |
| 28:DF:72:SER:CA | 28:DF:80:GLN:H | 2.20 | 0.52 |
| 23:DB:2529:G:H4' | 29:DG:174:LYS:HD2 | 1.90 | 0.52 |
| 32:DK:105:ARG:HD2 | 32:DK:122:VAL:HG11 | 1.91 | 0.52 |
| 1:AA:1121:U:H2' | 1:AA:1122:U:O4' | 2.09 | 0.52 |
| 1:AA:1121:U:O2' | 1:AA:1122:U:H5' | 2.10 | 0.52 |
| 1:AA:1127:G:O2' | 1:AA:1128:C:H5' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1521:C:H2' | 1:AA:1522:U:C6 | 2.45 | 0.52 |
| 1:AA:252:U:H2' | 1:AA:253:A:C8 | 2.45 | 0.52 |
| 1:AA:411:A:C4 | 1:AA:413:G:H1' | 2.45 | 0.52 |
| 1:AA:560:A:N1 | 1:AA:566:G:H5' | 2.24 | 0.52 |
| 1:AA:957:U:O2 | 1:AA:959:A:H8 | 1.92 | 0.52 |
| 2:AC:35:ASP:HB3 | 2:AC:39:ARG:HH12 | 1.75 | 0.52 |
| 2:AC:88:LYS:O | 2:AC:88:LYS:HE3 | 2.09 | 0.52 |
| 3:AD:157:ALA:O | 3:AD:160:LEU:HD22 | 2.10 | 0.52 |
| 21:AU:40:PRO:HA | 21:AU:44:ARG:HD2 | 1.91 | 0.52 |
| 48:B1:6:GLU:HB2 | 48:B1:52:LYS:HZ3 | 1.75 | 0.52 |
| 23:BB:1043:C:O2' | 23:BB:1044:C:H5' | 2.10 | 0.52 |
| 23:BB:1397:U:H5'' | 23:BB:1398:C:H5 | 1.74 | 0.52 |
| 23:BB:2083:G:H2' | 23:BB:2084:C:H6 | 1.74 | 0.52 |
| 23:BB:2098:U:H2' | 23:BB:2099:U:H6 | 1.75 | 0.52 |
| 23:BB:2487:G:H2' | 23:BB:2488:G:C8 | 2.45 | 0.52 |
| 23:BB:228:C:O2 | 23:BB:418:C:H4' | 2.09 | 0.52 |
| 23:BB:705:A:N6 | 23:BB:726:G:O2' | 2.42 | 0.52 |
| 26:BD:180:VAL:HG22 | 26:BD:187:LEU:CD1 | 2.40 | 0.52 |
| 26:BD:8:LYS:HB2 | 26:BD:201:LEU:HD11 | 1.91 | 0.52 |
| 27:BE:182:ALA:O | 27:BE:183:PHE:HB2 | 2.09 | 0.52 |
| 28:BF:133:GLU:HA | 28:BF:150:GLY:HA2 | 1.90 | 0.52 |
| 28:BF:62:GLN:HE22 | 28:BF:90:LEU:HA | 1.75 | 0.52 |
| 30:BH:27:ARG:HG2 | 30:BH:27:ARG:HH21 | 1.75 | 0.52 |
| 32:BK:17:ARG:HB3 | 32:BK:45:GLU:CG | 2.38 | 0.52 |
| 34:BM:94:ALA:O | 34:BM:96:ILE:HG23 | 2.09 | 0.52 |
| 23:BB:815:C:OP2 | 39:BR:85:LYS:HE2 | 2.10 | 0.52 |
| 41:BT:59:ASN:O | 41:BT:84:TYR:HB2 | 2.08 | 0.52 |
| 1:CA:1273:C:H2' | 1:CA:1274:A:O4' | 2.09 | 0.52 |
| 1:CA:301:G:H2' | 1:CA:302:G:H8 | 1.75 | 0.52 |
| 7:CH:55:LYS:NZ | 7:CH:55:LYS:HA | 2.25 | 0.52 |
| 8:CI:46:VAL:HG23 | 8:CI:47:VAL:H | 1.74 | 0.52 |
| 10:CK:95:THR:HG23 | 10:CK:96:ILE:N | 2.25 | 0.52 |
| 14:CO:35:ILE:CD1 | 14:CO:58:MET:HG3 | 2.39 | 0.52 |
| 15:CP:25:ARG:HD3 | 15:CP:25:ARG:N | 2.21 | 0.52 |
| 15:CP:59:HIS:O | 15:CP:63:GLN:HG3 | 2.08 | 0.52 |
| 49:D2:30:VAL:HA | 49:D2:33:ARG:HH21 | 1.75 | 0.52 |
| 23:DB:100:U:OP1 | 23:DB:100:U:H3' | 2.09 | 0.52 |
| 23:DB:138:U:H5'' | 23:DB:139:U:OP1 | 2.09 | 0.52 |
| 23:DB:1453:A:OP1 | 23:DB:1453:A:H4' | 2.10 | 0.52 |
| 23:DB:1607:C:H4' | 23:DB:1608:A:O5' | 2.09 | 0.52 |
| 23:DB:2144:G:C2 | 23:DB:2146:C:H5' | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2298:A:H2' | 23:DB:2299:U:O4' | 2.09 | 0.52 |
| 23:DB:2657:A:H2' | 23:DB:2658:C:O4' | 2.10 | 0.52 |
| 23:DB:693:A:H2' | 23:DB:694:U:C6 | 2.44 | 0.52 |
| 26:DD:116:LYS:HB3 | 26:DD:118:PHE:CZ | 2.44 | 0.52 |
| 28:DF:3:LEU:HD11 | 28:DF:172:PHE:CG | 2.45 | 0.52 |
| 35:DN:106:ASP:C | 35:DN:108:ALA:H | 2.12 | 0.52 |
| 35:DN:28:LEU:HD12 | 35:DN:48:VAL:HG21 | 1.91 | 0.52 |
| 35:DN:49:GLU:HA | 35:DN:94:TYR:HD2 | 1.74 | 0.52 |
| 32:DK:101:GLY:HA2 | 37:DP:65:ASN:HB2 | 1.92 | 0.52 |
| 23:DB:812:C:H4' | 38:DQ:12:ARG:NH2 | 2.23 | 0.52 |
| 41:DT:81:LYS:HG3 | 41:DT:82:LYS:N | 2.24 | 0.52 |
| 24:DV:9:ARG:CZ | 24:DV:20:LEU:HD11 | 2.40 | 0.52 |
| 43:DW:17:ALA:HA | 43:DW:35:ILE:CG2 | 2.38 | 0.52 |
| 43:DW:59:PHE:CE2 | 43:DW:61:LYS:HG3 | 2.45 | 0.52 |
| 1:AA:1029:U:O3' | 1:AA:1030:U:H3' | 2.10 | 0.52 |
| 1:AA:1326:U:H2' | 1:AA:1327:C:C6 | 2.44 | 0.52 |
| 1:AA:398:U:H2' | 1:AA:399:G:C8 | 2.45 | 0.52 |
| 2:AC:178:ARG:HG2 | 2:AC:206:ILE:HA | 1.90 | 0.52 |
| 3:AD:94:GLU:HG3 | 3:AD:99:ASN:HD21 | 1.75 | 0.52 |
| 12:AM:22:TYR:CD1 | 12:AM:65:GLU:HA | 2.45 | 0.52 |
| 18:AS:12:LEU:O | 18:AS:15:LEU:HB2 | 2.09 | 0.52 |
| 19:AT:66:ILE:HG23 | 19:AT:70:LYS:HB3 | 1.92 | 0.52 |
| 21:AU:24:LYS:HZ3 | 21:AU:25:ALA:N | 1.99 | 0.52 |
| 23:BB:1487:U:H2' | 23:BB:1488:C:H6 | 1.74 | 0.52 |
| 23:BB:1576:U:O2' | 23:BB:1577:C:H5' | 2.09 | 0.52 |
| 23:BB:1607:C:H4' | 23:BB:1608:A:O5' | 2.10 | 0.52 |
| 23:BB:2276:G:OP2 | 34:BM:85:GLY:N | 2.40 | 0.52 |
| 23:BB:2598:A:OP1 | 25:BC:233:GLY:HA3 | 2.10 | 0.52 |
| 23:BB:2814:A:H2' | 23:BB:2815:C:C6 | 2.45 | 0.52 |
| 23:BB:93:G:H2' | 23:BB:94:A:O4' | 2.10 | 0.52 |
| 28:BF:62:GLN:HG3 | 28:BF:91:ARG:HH11 | 1.75 | 0.52 |
| 29:BG:152:ARG:HH11 | 29:BG:162:ARG:HA | 1.74 | 0.52 |
| 31:BJ:15:TRP:HB3 | 31:BJ:137:PRO:HG3 | 1.92 | 0.52 |
| 31:BJ:71:ASP:HA | 31:BJ:88:THR:OG1 | 2.10 | 0.52 |
| 32:BK:4:GLU:OE2 | 32:BK:23:LYS:HD2 | 2.10 | 0.52 |
| 34:BM:31:PHE:O | 34:BM:131:VAL:HG23 | 2.09 | 0.52 |
| 37:BP:20:ARG:NE | 37:BP:91:VAL:HG21 | 2.21 | 0.52 |
| 41:BT:29:THR:HA | 41:BT:86:THR:CA | 2.34 | 0.52 |
| 24:BV:57:TYR:HA | 24:BV:74:ALA:HB3 | 1.91 | 0.52 |
| 43:BW:49:ASN:O | 43:BW:50:VAL:HG13 | 2.09 | 0.52 |
| 46:BZ:69:ALA:HA | 46:BZ:72:ARG:NH2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:469:C:H2' | 1:CA:470:C:H6 | 1.75 | 0.52 |
| 1:CA:818:G:C3' | 1:CA:819:A:H5'' | 2.40 | 0.52 |
| 3:CD:187:ARG:NH1 | 3:CD:191:SER:HB3 | 2.25 | 0.52 |
| 4:CE:113:VAL:HG23 | 4:CE:114:LEU:N | 2.25 | 0.52 |
| 8:CI:46:VAL:HG23 | 8:CI:47:VAL:N | 2.25 | 0.52 |
| 9:CJ:76:ILE:HD13 | 9:CJ:79:PRO:HB3 | 1.91 | 0.52 |
| 9:CJ:93:ALA:HB3 | 9:CJ:96:VAL:HG22 | 1.91 | 0.52 |
| 11:CL:41:PRO:HB3 | 11:CL:49:ARG:NH1 | 2.24 | 0.52 |
| 13:CN:16:ALA:HA | 13:CN:20:PHE:HB2 | 1.92 | 0.52 |
| 23:DB:161:A:C3' | 23:DB:162:U:H5'' | 2.37 | 0.52 |
| 23:DB:1826:G:H2' | 23:DB:1827:U:H6 | 1.75 | 0.52 |
| 23:DB:2083:G:H2' | 23:DB:2084:C:C6 | 2.45 | 0.52 |
| 23:DB:2329:U:H2' | 23:DB:2330:G:C8 | 2.44 | 0.52 |
| 23:DB:2617:U:C2' | 23:DB:2618:G:H5' | 2.39 | 0.52 |
| 23:DB:296:U:H2' | 23:DB:297:G:C8 | 2.44 | 0.52 |
| 23:DB:587:C:N3 | 33:DL:33:ARG:NH2 | 2.57 | 0.52 |
| 23:DB:946:C:H2' | 23:DB:947:A:C8 | 2.44 | 0.52 |
| 29:DG:152:ARG:HH11 | 29:DG:162:ARG:HA | 1.75 | 0.52 |
| 29:DG:154:GLU:C | 29:DG:156:TYR:H | 2.13 | 0.52 |
| 30:DH:5:LEU:HD13 | 30:DH:13:GLY:HA2 | 1.92 | 0.52 |
| 33:DL:73:ILE:O | 33:DL:105:ILE:HG23 | 2.09 | 0.52 |
| 33:DL:92:LEU:HD21 | 33:DL:123:ARG:NH1 | 2.25 | 0.52 |
| 35:DN:63:ARG:O | 35:DN:66:ALA:HB3 | 2.09 | 0.52 |
| 37:DP:50:ARG:HB3 | 37:DP:56:SER:HB3 | 1.92 | 0.52 |
| 41:DT:59:ASN:O | 41:DT:84:TYR:HB2 | 2.10 | 0.52 |
| 1:AA:1207:G:O2' | 1:AA:1208:C:H5' | 2.10 | 0.52 |
| 20:AB:134:LEU:HA | 20:AB:137:THR:HG23 | 1.90 | 0.52 |
| 6:AG:135:LYS:HE2 | 6:AG:136:LYS:N | 2.24 | 0.52 |
| 11:AL:49:ARG:HH12 | 11:AL:88:ASP:CB | 2.23 | 0.52 |
| 13:AN:50:LEU:CD2 | 13:AN:51:PRO:HD3 | 2.40 | 0.52 |
| 18:AS:63:ASP:O | 18:AS:66:VAL:HG22 | 2.10 | 0.52 |
| 21:AU:11:PHE:HA | 2:CC:70:ALA:O | 2.09 | 0.52 |
| 23:BB:1080:A:H1' | 52:BI:127:SER:HA | 1.90 | 0.52 |
| 23:BB:1199:U:H2' | 23:BB:1200:C:C6 | 2.45 | 0.52 |
| 23:BB:1454:C:H5' | 35:BN:63:ARG:NE | 2.22 | 0.52 |
| 23:BB:1774:C:O2 | 23:BB:1774:C:H2' | 2.10 | 0.52 |
| 23:BB:2757:A:H2' | 23:BB:2757:A:N3 | 2.23 | 0.52 |
| 23:BB:2836:U:H2' | 23:BB:2837:A:C8 | 2.45 | 0.52 |
| 23:BB:286:U:H2' | 23:BB:287:G:C8 | 2.44 | 0.52 |
| 23:BB:781:A:OP1 | 25:BC:216:ARG:NH2 | 2.42 | 0.52 |
| 26:BD:51:THR:HG21 | 26:BD:76:GLY:HA3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BD:34:VAL:HG12 | 26:BD:94:GLN:H | 1.74 | 0.52 |
| 52:BI:17:ALA:O | 52:BI:18:ASN:CB | 2.58 | 0.52 |
| 52:BI:23:VAL:HG23 | 52:BI:24:GLY:N | 2.25 | 0.52 |
| 52:BI:48:ILE:HG22 | 52:BI:49:GLU:HG2 | 1.91 | 0.52 |
| 33:BL:124:GLY:N | 33:BL:143:GLU:HG3 | 2.25 | 0.52 |
| 35:BN:28:LEU:HD12 | 35:BN:48:VAL:HG21 | 1.91 | 0.52 |
| 38:BQ:78:PHE:O | 38:BQ:82:LEU:HG | 2.10 | 0.52 |
| 41:BT:27:SER:O | 41:BT:28:ASN:HB3 | 2.10 | 0.52 |
| 24:BV:16:ALA:HA | 24:BV:19:ARG:HE | 1.74 | 0.52 |
| 43:BW:23:LYS:NZ | 43:BW:24:ARG:HG3 | 2.25 | 0.52 |
| 46:BZ:39:TRP:HB2 | 46:BZ:46:PHE:CE2 | 2.44 | 0.52 |
| 1:CA:1427:C:H2' | 1:CA:1428:A:H8 | 1.74 | 0.52 |
| 1:CA:436:C:O2' | 1:CA:437:U:H5' | 2.10 | 0.52 |
| 1:CA:803:G:H2' | 1:CA:804:U:O4' | 2.09 | 0.52 |
| 1:CA:806:C:H2' | 1:CA:807:A:H8 | 1.74 | 0.52 |
| 20:CB:31:PHE:HB2 | 20:CB:41:ASN:HA | 1.91 | 0.52 |
| 2:CC:35:ASP:HB3 | 2:CC:39:ARG:NH1 | 2.25 | 0.52 |
| 3:CD:33:ILE:O | 3:CD:35:GLN:HG3 | 2.10 | 0.52 |
| 5:CF:37:HIS:O | 5:CF:97:THR:HG23 | 2.10 | 0.52 |
| 6:CG:21:LEU:HG | 6:CG:22:LEU:H | 1.74 | 0.52 |
| 8:CI:44:ARG:HE | 8:CI:48:ARG:HH22 | 1.57 | 0.52 |
| 10:CK:28:ASN:HD21 | 10:CK:47:GLY:H | 1.56 | 0.52 |
| 12:CM:111:PRO:O | 12:CM:113:LYS:HG3 | 2.10 | 0.52 |
| 9:CJ:52:LEU:HB2 | 13:CN:80:ARG:HE | 1.74 | 0.52 |
| 16:CQ:29:LYS:HG3 | 16:CQ:34:GLY:HA2 | 1.91 | 0.52 |
| 17:CR:58:ILE:O | 17:CR:62:ARG:HG3 | 2.10 | 0.52 |
| 21:CU:40:PRO:HA | 21:CU:44:ARG:HD2 | 1.92 | 0.52 |
| 23:DB:1219:U:H2' | 23:DB:1220:G:H8 | 1.73 | 0.52 |
| 23:DB:1395:A:H4' | 23:DB:1397:U:C5 | 2.45 | 0.52 |
| 23:DB:1886:U:H2' | 23:DB:1887:C:C6 | 2.45 | 0.52 |
| 23:DB:1979:U:O2' | 23:DB:1980:G:H5' | 2.10 | 0.52 |
| 23:DB:257:C:H2' | 23:DB:258:G:O4' | 2.09 | 0.52 |
| 23:DB:338:G:N2 | 23:DB:339:U:H1' | 2.24 | 0.52 |
| 23:DB:582:A:H2' | 23:DB:583:G:H8 | 1.74 | 0.52 |
| 25:DC:183:VAL:HG22 | 25:DC:184:GLU:H | 1.75 | 0.52 |
| 28:DF:104:THR:HB | 28:DF:105:ILE:HD12 | 1.92 | 0.52 |
| 29:DG:84:LYS:H | 29:DG:85:LYS:HD2 | 1.75 | 0.52 |
| 30:DH:72:ILE:HG23 | 30:DH:108:VAL:HG11 | 1.92 | 0.52 |
| 52:DI:126:ARG:HB3 | 52:DI:126:ARG:NH1 | 2.24 | 0.52 |
| 52:DI:63:ASP:O | 52:DI:64:ARG:HB2 | 2.09 | 0.52 |
| 31:DJ:81:ILE:HG23 | 31:DJ:82:GLY:N | 2.21 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2548:U:H1' | 32:DK:23:LYS:NZ | 2.24 | 0.52 |
| 33:DL:73:ILE:HD12 | 33:DL:106:GLU:HB2 | 1.90 | 0.52 |
| 36:DO:24:THR:O | 36:DO:90:VAL:HB | 2.10 | 0.52 |
| 38:DQ:71:ASN:HD21 | 38:DQ:109:VAL:HG11 | 1.75 | 0.52 |
| 40:DS:24:ILE:HG23 | 40:DS:32:ALA:HB1 | 1.91 | 0.52 |
| 46:DZ:63:GLY:HA3 | 46:DZ:66:THR:OG1 | 2.10 | 0.52 |
| 1:AA:1168:U:H4' | 1:AA:1169:A:OP2 | 2.10 | 0.52 |
| 1:AA:1238:A:H2 | 1:AA:1241:G:N3 | 2.07 | 0.52 |
| 1:AA:1245:C:H2' | 1:AA:1246:A:C8 | 2.45 | 0.52 |
| 1:AA:165:G:O2' | 1:AA:166:U:H5' | 2.10 | 0.52 |
| 1:AA:17:U:O2' | 1:AA:18:C:H5' | 2.10 | 0.52 |
| 1:AA:398:U:H2' | 1:AA:399:G:H8 | 1.73 | 0.52 |
| 1:AA:455:G:O2' | 1:AA:456:A:H5' | 2.10 | 0.52 |
| 2:AC:120:THR:HG22 | 2:AC:188:ALA:HB2 | 1.92 | 0.52 |
| 2:AC:166:TRP:HA | 2:AC:166:TRP:CE3 | 2.45 | 0.52 |
| 5:AF:52:ASN:HA | 5:AF:53:LYS:HZ3 | 1.75 | 0.52 |
| 1:AA:36:C:H4' | 11:AL:118:VAL:O | 2.09 | 0.52 |
| 14:AO:35:ILE:CD1 | 14:AO:58:MET:HG3 | 2.38 | 0.52 |
| 21:AU:40:PRO:O | 21:AU:44:ARG:HB2 | 2.10 | 0.52 |
| 23:BB:1107:G:H2' | 23:BB:1108:U:H6 | 1.74 | 0.52 |
| 23:BB:1210:G:C5' | 23:BB:1212:G:H5'' | 2.39 | 0.52 |
| 23:BB:1849:G:H2' | 23:BB:1850:G:H8 | 1.75 | 0.52 |
| 1:AA:1483:A:H1' | 23:BB:1948:G:H1' | 1.90 | 0.52 |
| 23:BB:433:C:H2' | 23:BB:434:U:C6 | 2.45 | 0.52 |
| 23:BB:644:A:H2' | 23:BB:644:A:N3 | 2.24 | 0.52 |
| 25:BC:211:ARG:C | 25:BC:213:ARG:H | 2.12 | 0.52 |
| 26:BD:149:ASN:C | 26:BD:152:PRO:HD2 | 2.29 | 0.52 |
| 28:BF:43:ILE:HG23 | 28:BF:44:ALA:N | 2.13 | 0.52 |
| 29:BG:6:ALA:HB3 | 29:BG:68:ARG:NE | 2.24 | 0.52 |
| 30:BH:31:VAL:O | 30:BH:32:PRO:C | 2.47 | 0.52 |
| 34:BM:21:ALA:HB2 | 34:BM:100:LYS:HG2 | 1.90 | 0.52 |
| 34:BM:126:ILE:HD12 | 34:BM:126:ILE:H | 1.75 | 0.52 |
| 24:BV:65:VAL:C | 24:BV:67:GLY:H | 2.12 | 0.52 |
| 1:CA:1020:G:H2' | 1:CA:1021:A:H5' | 1.91 | 0.52 |
| 1:CA:1166:G:H2' | 1:CA:1168:U:OP2 | 2.09 | 0.52 |
| 1:CA:1436:U:H2' | 1:CA:1437:A:H8 | 1.75 | 0.52 |
| 1:CA:151:A:H5' | 1:CA:152:A:OP2 | 2.09 | 0.52 |
| 1:CA:636:U:H2' | 1:CA:637:C:C6 | 2.45 | 0.52 |
| 2:CC:165:GLU:HG3 | 2:CC:166:TRP:H | 1.75 | 0.52 |
| 2:CC:19:SER:HB2 | 2:CC:39:ARG:HH22 | 1.74 | 0.52 |
| 12:CM:86:ARG:CG | 12:CM:96:VAL:HG11 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:CS:44:ILE:O | 18:CS:44:ILE:HG23 | 2.10 | 0.52 |
| 19:CT:68:LYS:HA | 19:CT:68:LYS:HZ3 | 1.75 | 0.52 |
| 22:DA:30:C:O2 | 22:DA:30:C:H2' | 2.09 | 0.52 |
| 22:DA:54:G:H21 | 28:DF:25:MET:CE | 2.22 | 0.52 |
| 23:DB:1221:C:O2' | 23:DB:1222:U:H5' | 2.10 | 0.52 |
| 23:DB:1387:A:H2' | 23:DB:1388:G:H8 | 1.73 | 0.52 |
| 23:DB:1688:U:H2' | 23:DB:1698:A:N6 | 2.25 | 0.52 |
| 23:DB:1720:U:O2' | 23:DB:1721:G:H5' | 2.10 | 0.52 |
| 23:DB:182:A:H2' | 23:DB:183:C:H6 | 1.74 | 0.52 |
| 23:DB:1863:G:H2' | 23:DB:1864:U:O4' | 2.09 | 0.52 |
| 23:DB:2577:A:H5'' | 23:DB:2578:G:H5' | 1.90 | 0.52 |
| 23:DB:438:G:H2' | 23:DB:439:A:C8 | 2.45 | 0.52 |
| 23:DB:519:U:H2' | 23:DB:520:G:H8 | 1.74 | 0.52 |
| 26:DD:16:THR:HB | 26:DD:18:ASP:OD1 | 2.10 | 0.52 |
| 26:DD:180:VAL:HG22 | 26:DD:187:LEU:CD1 | 2.40 | 0.52 |
| 29:DG:93:TYR:C | 29:DG:94:ARG:HG3 | 2.29 | 0.52 |
| 23:DB:1099:G:H5'' | 52:DI:2:LYS:HB2 | 1.92 | 0.52 |
| 52:DI:32:VAL:HG22 | 52:DI:60:VAL:CG2 | 2.40 | 0.52 |
| 33:DL:61:LEU:HD12 | 33:DL:61:LEU:N | 2.25 | 0.52 |
| 23:DB:857:G:O2' | 43:DW:19:ARG:HD2 | 2.10 | 0.52 |
| 43:DW:36:ILE:O | 43:DW:39:GLN:HB3 | 2.09 | 0.52 |
| 46:DZ:21:ALA:HB3 | 46:DZ:23:ASN:HD21 | 1.73 | 0.52 |
| 1:AA:376:G:H2' | 1:AA:377:G:C8 | 2.45 | 0.52 |
| 1:AA:469:C:H2' | 1:AA:470:C:H6 | 1.75 | 0.52 |
| 1:AA:547:A:H4' | 1:AA:548:G:O5' | 2.10 | 0.52 |
| 20:AB:204:ASP:O | 20:AB:208:ALA:HB3 | 2.09 | 0.52 |
| 3:AD:199:ILE:HD12 | 3:AD:200:VAL:N | 2.25 | 0.52 |
| 3:AD:33:ILE:HG13 | 3:AD:34:GLU:N | 2.25 | 0.52 |
| 7:AH:17:GLN:NE2 | 7:AH:62:LEU:HB3 | 2.25 | 0.52 |
| 1:AA:707:U:H4' | 10:AK:21:HIS:CD2 | 2.45 | 0.52 |
| 13:AN:50:LEU:H | 13:AN:51:PRO:CD | 2.23 | 0.52 |
| 14:AO:52:ARG:HD2 | 23:BB:715:A:H61 | 1.75 | 0.52 |
| 17:AR:63:TYR:N | 17:AR:63:TYR:CD2 | 2.77 | 0.52 |
| 48:B1:25:ASN:OD1 | 48:B1:27:ARG:HB2 | 2.09 | 0.52 |
| 23:BB:1060:U:P | 52:BI:74:PRO:HA | 2.49 | 0.52 |
| 23:BB:1373:A:H5'' | 23:BB:2213:U:O4 | 2.10 | 0.52 |
| 23:BB:2636:C:O5' | 26:BD:81:GLU:HB2 | 2.09 | 0.52 |
| 23:BB:265:A:O2' | 23:BB:266:G:H4' | 2.10 | 0.52 |
| 23:BB:839:U:H2' | 23:BB:840:C:C6 | 2.45 | 0.52 |
| 23:BB:920:A:H2' | 23:BB:921:C:C6 | 2.45 | 0.52 |
| 26:BD:154:LYS:H | 26:BD:154:LYS:HD3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:BD:69:ALA:CA | 26:BD:73:VAL:HB | 2.40 | 0.52 |
| 27:BE:149:ILE:HG23 | 27:BE:188:MET:CA | 2.40 | 0.52 |
| 27:BE:32:VAL:HG23 | 27:BE:33:VAL:N | 2.25 | 0.52 |
| 28:BF:29:ARG:H | 28:BF:29:ARG:CD | 2.23 | 0.52 |
| 31:BJ:84:ILE:HG23 | 31:BJ:84:ILE:O | 2.09 | 0.52 |
| 33:BL:110:VAL:HG23 | 33:BL:126:ARG:O | 2.09 | 0.52 |
| 35:BN:96:ARG:HG2 | 35:BN:96:ARG:HH21 | 1.74 | 0.52 |
| 38:BQ:60:TRP:C | 38:BQ:64:ILE:HG12 | 2.31 | 0.52 |
| 38:BQ:71:ASN:ND2 | 38:BQ:73:ILE:HG22 | 2.25 | 0.52 |
| 39:BR:39:LEU:HA | 39:BR:49:ILE:HG12 | 1.92 | 0.52 |
| 40:BS:71:VAL:HG22 | 40:BS:71:VAL:O | 2.10 | 0.52 |
| 23:BB:142:A:C2 | 41:BT:2:ILE:HG22 | 2.44 | 0.52 |
| 42:BU:48:VAL:O | 42:BU:50:ALA:N | 2.43 | 0.52 |
| 46:BZ:17:ASN:HB2 | 46:BZ:25:THR:OG1 | 2.08 | 0.52 |
| 1:CA:1092:A:H5'' | 6:CG:3:ARG:NH1 | 2.25 | 0.52 |
| 1:CA:169:C:O2' | 1:CA:170:U:H5' | 2.09 | 0.52 |
| 1:CA:45:G:H2' | 1:CA:46:G:C8 | 2.45 | 0.52 |
| 1:CA:505:G:H4' | 1:CA:534:U:C4 | 2.45 | 0.52 |
| 20:CB:18:GLN:O | 20:CB:37:VAL:HG23 | 2.09 | 0.52 |
| 6:CG:13:PRO:O | 6:CG:14:ASP:O | 2.27 | 0.52 |
| 8:CI:61:ASP:C | 8:CI:62:LEU:HD13 | 2.30 | 0.52 |
| 18:CS:43:MET:O | 18:CS:46:LEU:HB2 | 2.09 | 0.52 |
| 18:CS:49:ALA:O | 18:CS:56:HIS:HD2 | 1.93 | 0.52 |
| 48:D1:8:ILE:HD11 | 48:D1:52:LYS:HG3 | 1.90 | 0.52 |
| 22:DA:14:U:H4' | 22:DA:70:C:O2 | 2.09 | 0.52 |
| 23:DB:1100:C:H2' | 23:DB:1101:U:C6 | 2.42 | 0.52 |
| 23:DB:1259:G:H2' | 23:DB:1260:A:C8 | 2.45 | 0.52 |
| 23:DB:1373:A:H5'' | 23:DB:2213:U:O4 | 2.10 | 0.52 |
| 23:DB:1482:G:H2' | 23:DB:1483:G:H8 | 1.75 | 0.52 |
| 23:DB:1571:A:H2' | 23:DB:1572:A:C8 | 2.45 | 0.52 |
| 23:DB:964:C:O2' | 23:DB:2273:A:H1' | 2.09 | 0.52 |
| 23:DB:2805:C:O2' | 23:DB:2806:C:H5' | 2.10 | 0.52 |
| 23:DB:41:C:H2' | 23:DB:42:A:H8 | 1.74 | 0.52 |
| 23:DB:925:A:O2' | 23:DB:926:G:H5' | 2.10 | 0.52 |
| 26:DD:164:GLN:HG3 | 26:DD:165:MET:N | 2.23 | 0.52 |
| 23:DB:2751:G:OP2 | 29:DG:2:ARG:HD2 | 2.10 | 0.52 |
| 52:DI:45:THR:HA | 52:DI:48:ILE:CG2 | 2.40 | 0.52 |
| 32:DK:34:GLY:O | 32:DK:36:GLY:N | 2.43 | 0.52 |
| 40:DS:17:VAL:C | 40:DS:19:LEU:N | 2.64 | 0.52 |
| 41:DT:11:LEU:CD2 | 41:DT:46:ALA:HB1 | 2.40 | 0.52 |
| 43:DW:32:ALA:C | 43:DW:34:SER:H | 2.12 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:2336:A:H61 | 43:DW:40:ARG:HG3 | 1.74 | 0.52 |
| 1:AA:1101:A:H4' | 1:AA:1102:A:O5' | 2.10 | 0.51 |
| 1:AA:1120:C:H2' | 1:AA:1121:U:C6 | 2.46 | 0.51 |
| 1:AA:1151:A:O2' | 1:AA:1152:A:H8 | 1.92 | 0.51 |
| 1:AA:160:A:H2' | 1:AA:161:A:O4' | 2.10 | 0.51 |
| 1:AA:730:G:O2' | 1:AA:766:A:H5' | 2.09 | 0.51 |
| 3:AD:185:PRO:HB2 | 3:AD:190:LEU:HD12 | 1.91 | 0.51 |
| 6:AG:129:ASN:HA | 6:AG:134:VAL:HG21 | 1.92 | 0.51 |
| 6:AG:42:VAL:O | 6:AG:46:LEU:HB2 | 2.10 | 0.51 |
| 6:AG:99:ALA:O | 6:AG:103:ILE:HG13 | 2.10 | 0.51 |
| 8:AI:71:ILE:N | 8:AI:71:ILE:HD12 | 2.25 | 0.51 |
| 11:AL:106:VAL:CG2 | 11:AL:116:TYR:HB3 | 2.40 | 0.51 |
| 13:AN:26:LEU:HA | 13:AN:29:ILE:HB | 1.93 | 0.51 |
| 17:AR:23:LYS:HG3 | 17:AR:24:ASP:N | 2.26 | 0.51 |
| 47:B0:43:THR:HG21 | 47:B0:47:TYR:HB2 | 1.91 | 0.51 |
| 48:B1:6:GLU:H | 48:B1:6:GLU:CD | 2.13 | 0.51 |
| 22:BA:70:C:O2' | 22:BA:71:C:H5' | 2.10 | 0.51 |
| 23:BB:136:G:H2' | 23:BB:137:U:C5 | 2.44 | 0.51 |
| 23:BB:2436:G:O2' | 23:BB:2437:G:H5' | 2.11 | 0.51 |
| 23:BB:2543:G:H2' | 23:BB:2544:G:C8 | 2.45 | 0.51 |
| 23:BB:299:A:N6 | 23:BB:322:A:O2' | 2.42 | 0.51 |
| 23:BB:41:C:H2' | 23:BB:42:A:H8 | 1.75 | 0.51 |
| 23:BB:504:A:H2' | 23:BB:504:A:N3 | 2.24 | 0.51 |
| 23:BB:642:U:HO2' | 23:BB:643:A:H8 | 1.58 | 0.51 |
| 23:BB:947:A:H2' | 23:BB:948:C:H6 | 1.74 | 0.51 |
| 26:BD:25:THR:HG21 | 26:BD:193:VAL:CG2 | 2.39 | 0.51 |
| 23:BB:2653:U:O2' | 29:BG:109:SER:HB2 | 2.10 | 0.51 |
| 30:BH:25:TYR:CG | 30:BH:30:LEU:HG | 2.45 | 0.51 |
| 30:BH:31:VAL:CB | 30:BH:32:PRO:HD3 | 2.33 | 0.51 |
| 52:BI:100:ILE:O | 52:BI:139:VAL:HA | 2.10 | 0.51 |
| 32:BK:12:ASP:OD2 | 32:BK:85:VAL:HG13 | 2.09 | 0.51 |
| 33:BL:73:ILE:O | 33:BL:105:ILE:HG23 | 2.10 | 0.51 |
| 33:BL:81:ASP:HA | 33:BL:84:LYS:HD2 | 1.91 | 0.51 |
| 35:BN:83:LEU:HA | 35:BN:86:ARG:HB2 | 1.92 | 0.51 |
| 38:BQ:26:ALA:C | 38:BQ:28:SER:H | 2.13 | 0.51 |
| 39:BR:19:THR:CG2 | 39:BR:97:LYS:HD2 | 2.40 | 0.51 |
| 39:BR:16:GLU:CA | 39:BR:98:ILE:HG22 | 2.37 | 0.51 |
| 1:CA:1347:G:H22 | 1:CA:1373:G:H2' | 1.72 | 0.51 |
| 1:CA:1461:G:H2' | 1:CA:1462:C:C6 | 2.43 | 0.51 |
| 1:CA:1524:C:H2' | 1:CA:1525:G:C8 | 2.45 | 0.51 |
| 1:CA:205:A:H2' | 1:CA:206:C:C6 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:CF:70:VAL:HA | 5:CF:73:GLU:HG3 | 1.91 | 0.51 |
| 7:CH:17:GLN:OE1 | 7:CH:69:ALA:HB1 | 2.10 | 0.51 |
| 4:CE:156:ARG:HB2 | 7:CH:43:GLY:HA3 | 1.91 | 0.51 |
| 13:CN:68:ARG:HH11 | 13:CN:71:GLY:H | 1.57 | 0.51 |
| 14:CO:80:LEU:O | 14:CO:84:LEU:HD13 | 2.10 | 0.51 |
| 18:CS:61:VAL:HA | 18:CS:65:MET:SD | 2.49 | 0.51 |
| 21:CU:40:PRO:O | 21:CU:44:ARG:HB2 | 2.10 | 0.51 |
| 49:D2:43:THR:O | 49:D2:44:VAL:C | 2.47 | 0.51 |
| 23:DB:141:G:N3 | 23:DB:141:G:H3' | 2.24 | 0.51 |
| 23:DB:165:A:H2' | 23:DB:166:U:C6 | 2.45 | 0.51 |
| 23:DB:2151:U:O2' | 23:DB:2152:G:H5' | 2.10 | 0.51 |
| 23:DB:245:G:H2' | 23:DB:246:C:H6 | 1.75 | 0.51 |
| 23:DB:2570:G:H2' | 23:DB:2571:U:O4' | 2.10 | 0.51 |
| 23:DB:2809:A:H2' | 23:DB:2810:A:C8 | 2.45 | 0.51 |
| 23:DB:2868:A:H2' | 23:DB:2869:G:C8 | 2.45 | 0.51 |
| 23:DB:2786:U:H5'' | 26:DD:70:LYS:HG3 | 1.92 | 0.51 |
| 27:DE:161:ALA:CA | 27:DE:164:LEU:HB2 | 2.35 | 0.51 |
| 52:DI:54:ILE:C | 52:DI:54:ILE:HD13 | 2.29 | 0.51 |
| 35:DN:2:ARG:C | 35:DN:2:ARG:HE | 2.14 | 0.51 |
| 38:DQ:90:ASP:O | 38:DQ:94:LEU:HB2 | 2.09 | 0.51 |
| 39:DR:60:LYS:N | 39:DR:100:GLY:HA3 | 2.23 | 0.51 |
| 41:DT:57:VAL:HG12 | 41:DT:86:THR:OG1 | 2.09 | 0.51 |
| 24:DV:70:ILE:HD13 | 24:DV:70:ILE:N | 2.23 | 0.51 |
| 24:DV:77:VAL:HA | 24:DV:89:ILE:HG22 | 1.90 | 0.51 |
| 1:AA:1220:G:H2' | 1:AA:1221:G:H8 | 1.74 | 0.51 |
| 1:AA:1478:U:H2' | 1:AA:1479:C:C6 | 2.45 | 0.51 |
| 1:AA:1530:G:H2' | 1:AA:1531:A:H8 | 1.75 | 0.51 |
| 1:AA:238:A:C2' | 1:AA:239:U:H5'' | 2.36 | 0.51 |
| 1:AA:458:U:H2' | 1:AA:459:A:H8 | 1.75 | 0.51 |
| 1:AA:724:G:O2' | 1:AA:725:G:H5' | 2.10 | 0.51 |
| 4:AE:35:LEU:HD22 | 4:AE:133:ILE:HA | 1.92 | 0.51 |
| 4:AE:113:VAL:HG11 | 4:AE:136:VAL:HG23 | 1.90 | 0.51 |
| 5:AF:73:GLU:O | 5:AF:77:THR:HG23 | 2.10 | 0.51 |
| 7:AH:100:ILE:HG13 | 7:AH:128:VAL:O | 2.10 | 0.51 |
| 10:AK:74:LYS:C | 10:AK:76:TYR:H | 2.14 | 0.51 |
| 15:AP:72:ALA:HA | 15:AP:75:ILE:HD12 | 1.92 | 0.51 |
| 18:AS:29:PRO:HA | 18:AS:47:THR:O | 2.11 | 0.51 |
| 1:AA:1315:U:H5 | 18:AS:5:LYS:HZ1 | 1.57 | 0.51 |
| 19:AT:49:ALA:C | 19:AT:52:GLU:HB3 | 2.31 | 0.51 |
| 48:B1:29:LYS:N | 48:B1:30:PRO:HD3 | 2.26 | 0.51 |
| 23:BB:1495:A:H2' | 23:BB:1496:A:C8 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2662:A:H2' | 23:BB:2663:G:O4' | 2.11 | 0.51 |
| 23:BB:279:A:H61 | 23:BB:361:G:H1' | 1.75 | 0.51 |
| 23:BB:7:G:H4' | 31:BJ:15:TRP:CZ2 | 2.46 | 0.51 |
| 23:BB:861:A:H2' | 23:BB:862:G:O4' | 2.10 | 0.51 |
| 25:BC:18:VAL:O | 25:BC:18:VAL:HG13 | 2.09 | 0.51 |
| 25:BC:6:LYS:HB3 | 25:BC:8:THR:HG22 | 1.92 | 0.51 |
| 30:BH:83:LYS:O | 30:BH:91:PHE:N | 2.43 | 0.51 |
| 34:BM:73:ILE:HG13 | 34:BM:93:VAL:HB | 1.92 | 0.51 |
| 40:BS:57:ASN:O | 40:BS:61:ASN:HB2 | 2.10 | 0.51 |
| 24:BV:80:HIS:HA | 24:BV:87:GLN:OE1 | 2.10 | 0.51 |
| 46:BZ:6:GLN:NE2 | 46:BZ:50:ARG:N | 2.57 | 0.51 |
| 1:CA:1097:C:H2' | 1:CA:1098:C:H6 | 1.76 | 0.51 |
| 1:CA:1150:A:O2' | 1:CA:1151:A:H5' | 2.10 | 0.51 |
| 1:CA:1349:A:OP1 | 8:CI:121:ARG:HB2 | 2.11 | 0.51 |
| 1:CA:1459:G:H2' | 1:CA:1460:C:H6 | 1.75 | 0.51 |
| 1:CA:1521:C:H2' | 1:CA:1522:U:H6 | 1.75 | 0.51 |
| 1:CA:224:U:H2' | 1:CA:225:C:C6 | 2.45 | 0.51 |
| 1:CA:501:C:H1' | 1:CA:549:C:H1' | 1.91 | 0.51 |
| 1:CA:584:G:O2' | 1:CA:585:G:H5' | 2.10 | 0.51 |
| 1:CA:83:C:HO2' | 1:CA:84:U:H3' | 1.73 | 0.51 |
| 2:CC:13:ILE:HD13 | 2:CC:13:ILE:N | 2.24 | 0.51 |
| 13:CN:64:ARG:HB2 | 13:CN:77:GLY:O | 2.11 | 0.51 |
| 17:CR:63:TYR:CD2 | 17:CR:63:TYR:N | 2.78 | 0.51 |
| 21:CU:39:LYS:O | 21:CU:43:GLU:HB3 | 2.10 | 0.51 |
| 51:D4:8:LYS:O | 51:D4:25:VAL:HG21 | 2.10 | 0.51 |
| 23:DB:1021:A:H62 | 23:DB:1141:U:H3 | 1.57 | 0.51 |
| 23:DB:1260:A:H2' | 23:DB:1261:C:H6 | 1.75 | 0.51 |
| 23:DB:1454:C:C5 | 35:DN:64:ARG:HG2 | 2.45 | 0.51 |
| 23:DB:2674:G:H2' | 23:DB:2675:A:C8 | 2.46 | 0.51 |
| 23:DB:299:A:H2' | 23:DB:300:A:C8 | 2.46 | 0.51 |
| 23:DB:504:A:H2' | 23:DB:504:A:N3 | 2.24 | 0.51 |
| 23:DB:980:A:C6 | 23:DB:981:A:N1 | 2.79 | 0.51 |
| 28:DF:62:GLN:HE22 | 28:DF:90:LEU:HA | 1.75 | 0.51 |
| 30:DH:135:HIS:CG | 30:DH:136:SER:H | 2.29 | 0.51 |
| 23:DB:1063:G:H4' | 52:DI:135:MET:HG2 | 1.91 | 0.51 |
| 34:DM:134:THR:HG22 | 34:DM:136:MET:H | 1.74 | 0.51 |
| 38:DQ:94:LEU:CD2 | 39:DR:11:GLN:HB2 | 2.40 | 0.51 |
| 39:DR:49:ILE:HB | 39:DR:53:PHE:O | 2.10 | 0.51 |
| 43:DW:45:HIS:HB3 | 43:DW:52:CYS:HB2 | 1.92 | 0.51 |
| 46:DZ:40:VAL:HG22 | 46:DZ:45:ARG:O | 2.10 | 0.51 |
| 1:AA:1229:A:H2' | 1:AA:1230:C:C6 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:254:G:H4' | 16:AQ:19:SER:OG | 2.10 | 0.51 |
| 2:AC:35:ASP:HB3 | 2:AC:39:ARG:NH1 | 2.26 | 0.51 |
| 4:AE:10:LEU:HA | 4:AE:39:GLY:O | 2.10 | 0.51 |
| 5:AF:5:GLU:HA | 5:AF:63:ASN:HA | 1.92 | 0.51 |
| 11:AL:82:ARG:HH11 | 11:AL:82:ARG:HG2 | 1.75 | 0.51 |
| 49:B2:43:THR:O | 49:B2:44:VAL:C | 2.48 | 0.51 |
| 51:B4:3:VAL:HB | 51:B4:37:GLN:HE22 | 1.75 | 0.51 |
| 23:BB:1203:U:H3' | 23:BB:1204:A:H5'' | 1.92 | 0.51 |
| 23:BB:1430:G:H2' | 23:BB:1431:A:O4' | 2.10 | 0.51 |
| 23:BB:165:A:H2' | 23:BB:166:U:C6 | 2.44 | 0.51 |
| 23:BB:1794:A:O2' | 23:BB:1795:C:H5' | 2.10 | 0.51 |
| 23:BB:2395:C:H2' | 23:BB:2396:G:O4' | 2.10 | 0.51 |
| 23:BB:62:U:C2' | 23:BB:63:A:H5' | 2.39 | 0.51 |
| 23:BB:60:G:C6 | 23:BB:74:A:N6 | 2.78 | 0.51 |
| 27:BE:98:LYS:NZ | 27:BE:99:LYS:HG2 | 2.24 | 0.51 |
| 28:BF:104:THR:HB | 28:BF:105:ILE:HD12 | 1.92 | 0.51 |
| 28:BF:103:ILE:HD11 | 28:BF:174:PHE:CG | 2.46 | 0.51 |
| 28:BF:103:ILE:HD11 | 28:BF:174:PHE:HA | 1.92 | 0.51 |
| 30:BH:26:ALA:C | 30:BH:28:ASN:H | 2.14 | 0.51 |
| 52:BI:125:THR:O | 52:BI:129:GLU:HG3 | 2.10 | 0.51 |
| 33:BL:3:LEU:O | 33:BL:5:THR:N | 2.43 | 0.51 |
| 34:BM:97:GLN:HB2 | 34:BM:98:PRO:CD | 2.40 | 0.51 |
| 36:BO:111:ARG:HD2 | 36:BO:117:PHE:C | 2.31 | 0.51 |
| 1:CA:1006:G:H2' | 1:CA:1007:U:C6 | 2.45 | 0.51 |
| 1:CA:279:A:C5' | 1:CA:280:C:H3' | 2.40 | 0.51 |
| 1:CA:60:A:H4' | 1:CA:61:G:O5' | 2.10 | 0.51 |
| 1:CA:81:A:O2' | 1:CA:82:G:H5' | 2.09 | 0.51 |
| 1:CA:844:G:H2' | 1:CA:846:G:C8 | 2.45 | 0.51 |
| 1:CA:98:A:H2' | 1:CA:99:C:C6 | 2.45 | 0.51 |
| 3:CD:185:PRO:HB2 | 3:CD:190:LEU:HD12 | 1.92 | 0.51 |
| 4:CE:55:VAL:N | 4:CE:56:PRO:HD2 | 2.25 | 0.51 |
| 8:CI:35:GLU:HG3 | 8:CI:44:ARG:HD3 | 1.91 | 0.51 |
| 10:CK:126:ARG:NE | 10:CK:126:ARG:HA | 2.24 | 0.51 |
| 12:CM:36:ALA:HB1 | 12:CM:54:THR:HB | 1.92 | 0.51 |
| 1:CA:1320:C:C5 | 18:CS:36:ARG:HA | 2.46 | 0.51 |
| 23:DB:154:U:H2' | 23:DB:155:A:H8 | 1.74 | 0.51 |
| 23:DB:199:A:O2' | 23:DB:200:U:H5' | 2.10 | 0.51 |
| 23:DB:2336:A:N6 | 43:DW:40:ARG:HG3 | 2.25 | 0.51 |
| 23:DB:2411:A:H2' | 23:DB:2412:A:C8 | 2.45 | 0.51 |
| 23:DB:2728:U:H2' | 23:DB:2729:G:C8 | 2.45 | 0.51 |
| 23:DB:2880:C:O4' | 35:DN:91:ALA:HB3 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:526:A:N6 | 23:DB:2626:C:H4' | 2.26 | 0.51 |
| 23:DB:545:U:H4' | 23:DB:550:C:C2 | 2.45 | 0.51 |
| 23:DB:644:A:H2' | 23:DB:644:A:N3 | 2.24 | 0.51 |
| 23:DB:664:G:H2' | 23:DB:665:U:C6 | 2.45 | 0.51 |
| 23:DB:720:U:H2' | 23:DB:721:A:H8 | 1.75 | 0.51 |
| 25:DC:53:ILE:HG23 | 25:DC:53:ILE:O | 2.10 | 0.51 |
| 27:DE:153:LEU:HG | 27:DE:154:ASP:N | 2.25 | 0.51 |
| 27:DE:58:LYS:HD3 | 27:DE:58:LYS:N | 2.16 | 0.51 |
| 31:DJ:106:LYS:HE3 | 31:DJ:106:LYS:HA | 1.93 | 0.51 |
| 33:DL:142:ILE:HG22 | 33:DL:143:GLU:N | 2.24 | 0.51 |
| 23:DB:495:G:H1' | 40:DS:57:ASN:ND2 | 2.25 | 0.51 |
| 42:DU:48:VAL:O | 42:DU:48:VAL:HG13 | 2.10 | 0.51 |
| 43:DW:37:VAL:CG1 | 43:DW:38:ARG:HH11 | 2.22 | 0.51 |
| 46:DZ:68:LEU:HB3 | 46:DZ:78:TYR:CE1 | 2.46 | 0.51 |
| 1:AA:104:G:O2' | 1:AA:105:G:H5' | 2.11 | 0.51 |
| 1:AA:1136:C:H3' | 1:AA:1136:C:OP1 | 2.10 | 0.51 |
| 1:AA:1297:G:H1' | 1:AA:1298:U:C5 | 2.43 | 0.51 |
| 1:AA:1430:A:H2' | 1:AA:1431:A:O4' | 2.10 | 0.51 |
| 1:AA:1471:U:O2' | 1:AA:1472:U:H5' | 2.10 | 0.51 |
| 1:AA:522:C:H2' | 1:AA:523:A:O4' | 2.10 | 0.51 |
| 1:AA:501:C:H1' | 1:AA:549:C:H1' | 1.91 | 0.51 |
| 1:AA:636:U:H2' | 1:AA:637:C:C6 | 2.45 | 0.51 |
| 2:AC:50:SER:HB2 | 2:AC:70:ALA:HB3 | 1.91 | 0.51 |
| 7:AH:4:ASP:OD1 | 7:AH:7:ALA:HB2 | 2.11 | 0.51 |
| 10:AK:110:THR:HA | 21:AU:3:ILE:O | 2.10 | 0.51 |
| 18:AS:10:ILE:HG22 | 18:AS:37:SER:HB3 | 1.91 | 0.51 |
| 19:AT:49:ALA:O | 19:AT:52:GLU:HB3 | 2.11 | 0.51 |
| 48:B1:8:ILE:HD11 | 48:B1:52:LYS:HG3 | 1.92 | 0.51 |
| 51:B4:27:CYS:SG | 51:B4:29:ALA:HB3 | 2.51 | 0.51 |
| 22:BA:74:U:H2' | 22:BA:75:G:H8 | 1.73 | 0.51 |
| 23:BB:107:G:H2' | 23:BB:108:G:H8 | 1.76 | 0.51 |
| 23:BB:1511:G:H2' | 23:BB:1512:C:C6 | 2.45 | 0.51 |
| 23:BB:1793:C:H2' | 23:BB:1794:A:C8 | 2.46 | 0.51 |
| 23:BB:1973:G:H2' | 23:BB:1974:C:C6 | 2.45 | 0.51 |
| 23:BB:2085:U:O2' | 23:BB:2086:U:H5' | 2.11 | 0.51 |
| 23:BB:2538:C:O2' | 23:BB:2539:C:H5' | 2.11 | 0.51 |
| 23:BB:2556:C:H2' | 23:BB:2557:G:O4' | 2.11 | 0.51 |
| 23:BB:2740:A:H2' | 23:BB:2741:A:C8 | 2.46 | 0.51 |
| 23:BB:438:G:H2' | 23:BB:439:A:C8 | 2.46 | 0.51 |
| 23:BB:596:U:H2' | 23:BB:597:G:H8 | 1.75 | 0.51 |
| 23:BB:674:G:H5'' | 27:BE:71:GLY:N | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:744:U:H2' | 23:BB:745:G:O4' | 2.11 | 0.51 |
| 25:BC:245:THR:C | 25:BC:247:TRP:H | 2.14 | 0.51 |
| 23:BB:2772:C:H4' | 26:BD:171:THR:CG2 | 2.41 | 0.51 |
| 27:BE:112:LEU:C | 27:BE:114:ARG:H | 2.13 | 0.51 |
| 27:BE:29:HIS:O | 27:BE:33:VAL:HG23 | 2.10 | 0.51 |
| 35:BN:81:ASN:O | 35:BN:85:PRO:HD2 | 2.10 | 0.51 |
| 37:BP:50:ARG:HB3 | 37:BP:56:SER:HB3 | 1.93 | 0.51 |
| 38:BQ:56:PHE:O | 38:BQ:59:LEU:HB3 | 2.10 | 0.51 |
| 39:BR:16:GLU:HA | 39:BR:98:ILE:O | 2.09 | 0.51 |
| 40:BS:66:ILE:HG12 | 40:BS:67:ASP:N | 2.24 | 0.51 |
| 23:BB:329:G:N2 | 42:BU:16:LYS:HE3 | 2.25 | 0.51 |
| 24:BV:77:VAL:HA | 24:BV:89:ILE:HG22 | 1.92 | 0.51 |
| 2:CC:34:SER:O | 2:CC:38:VAL:HG22 | 2.10 | 0.51 |
| 4:CE:113:VAL:HG11 | 4:CE:136:VAL:HG23 | 1.92 | 0.51 |
| 6:CG:131:GLY:O | 6:CG:134:VAL:HG22 | 2.11 | 0.51 |
| 6:CG:135:LYS:HE2 | 6:CG:136:LYS:N | 2.25 | 0.51 |
| 7:CH:11:THR:HA | 7:CH:14:ARG:NH1 | 2.25 | 0.51 |
| 11:CL:49:ARG:HH12 | 11:CL:88:ASP:CB | 2.24 | 0.51 |
| 15:CP:20:VAL:HG23 | 15:CP:35:ARG:HA | 1.92 | 0.51 |
| 5:CF:100:SER:HA | 17:CR:23:LYS:HE2 | 1.91 | 0.51 |
| 19:CT:85:LEU:HD23 | 19:CT:86:ALA:N | 2.23 | 0.51 |
| 49:D2:31:LEU:HD22 | 49:D2:42:LEU:HD12 | 1.92 | 0.51 |
| 23:DB:117:G:H5' | 23:DB:126:A:C8 | 2.29 | 0.51 |
| 23:DB:1820:U:H4' | 23:DB:1821:A:OP2 | 2.11 | 0.51 |
| 23:DB:2352:A:N1 | 43:DW:30:VAL:HG11 | 2.25 | 0.51 |
| 23:DB:281:C:H2' | 23:DB:282:A:C8 | 2.44 | 0.51 |
| 23:DB:693:A:OP1 | 25:DC:38:LYS:HG2 | 2.11 | 0.51 |
| 23:DB:836:G:H2' | 23:DB:837:C:H6 | 1.70 | 0.51 |
| 23:DB:839:U:H2' | 23:DB:840:C:H6 | 1.76 | 0.51 |
| 23:DB:948:C:H2' | 23:DB:949:G:C8 | 2.45 | 0.51 |
| 23:DB:975:A:H1' | 23:DB:990:A:C2 | 2.45 | 0.51 |
| 25:DC:211:ARG:C | 25:DC:213:ARG:H | 2.13 | 0.51 |
| 26:DD:9:VAL:O | 26:DD:9:VAL:HG13 | 2.11 | 0.51 |
| 23:DB:1256:G:H21 | 27:DE:77:ILE:HG22 | 1.74 | 0.51 |
| 33:DL:42:SER:C | 33:DL:44:GLY:H | 2.13 | 0.51 |
| 37:DP:103:THR:HG22 | 37:DP:104:GLY:N | 2.25 | 0.51 |
| 39:DR:80:ARG:O | 39:DR:81:LYS:HD3 | 2.11 | 0.51 |
| 24:DV:57:TYR:HA | 24:DV:74:ALA:HB3 | 1.92 | 0.51 |
| 43:DW:70:VAL:O | 43:DW:70:VAL:HG22 | 2.11 | 0.51 |
| 23:DB:188:G:OP1 | 46:DZ:14:THR:HG23 | 2.10 | 0.51 |
| 46:DZ:33:LEU:O | 46:DZ:34:HIS:CG | 2.64 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:762:U:H2' | 1:AA:763:G:C8 | 2.45 | 0.51 |
| 1:AA:79:G:H2' | 1:AA:80:A:N7 | 2.25 | 0.51 |
| 20:AB:119:GLN:O | 20:AB:125:PHE:HB3 | 2.10 | 0.51 |
| 5:AF:38:ARG:HH21 | 5:AF:63:ASN:HD21 | 1.53 | 0.51 |
| 9:AJ:30:LYS:NZ | 9:AJ:36:VAL:HB | 2.25 | 0.51 |
| 15:AP:25:ARG:CD | 15:AP:25:ARG:H | 2.23 | 0.51 |
| 5:AF:100:SER:HA | 17:AR:23:LYS:HE2 | 1.91 | 0.51 |
| 18:AS:11:ASP:OD1 | 18:AS:34:SER:HA | 2.10 | 0.51 |
| 19:AT:43:LYS:HE2 | 19:AT:44:ALA:N | 2.22 | 0.51 |
| 21:AU:39:LYS:O | 21:AU:43:GLU:HB3 | 2.09 | 0.51 |
| 23:BB:1580:A:H2' | 23:BB:1581:G:O4' | 2.11 | 0.51 |
| 23:BB:2188:U:H2' | 23:BB:2189:U:H6 | 1.73 | 0.51 |
| 23:BB:241:A:OP1 | 23:BB:241:A:H8 | 1.93 | 0.51 |
| 23:BB:2674:G:H2' | 23:BB:2675:A:C8 | 2.45 | 0.51 |
| 23:BB:2869:G:H2' | 23:BB:2870:C:O4' | 2.10 | 0.51 |
| 23:BB:297:G:H5'' | 42:BU:84:PHE:HB3 | 1.93 | 0.51 |
| 23:BB:492:A:H2' | 23:BB:493:G:O4' | 2.10 | 0.51 |
| 23:BB:544:C:H2' | 23:BB:545:U:C5 | 2.45 | 0.51 |
| 23:BB:81:G:H2' | 23:BB:82:U:O4' | 2.09 | 0.51 |
| 26:BD:51:THR:HG22 | 26:BD:52:THR:N | 2.24 | 0.51 |
| 27:BE:117:ARG:NH1 | 33:BL:2:ARG:HB2 | 2.25 | 0.51 |
| 27:BE:1:MET:O | 27:BE:13:THR:HA | 2.09 | 0.51 |
| 23:BB:2745:C:O3' | 29:BG:141:GLY:HA3 | 2.10 | 0.51 |
| 30:BH:49:ALA:HB3 | 30:BH:50:ARG:CZ | 2.41 | 0.51 |
| 39:BR:39:LEU:N | 39:BR:39:LEU:HD23 | 2.26 | 0.51 |
| 40:BS:73:LYS:HE3 | 40:BS:74:ILE:N | 2.25 | 0.51 |
| 41:BT:39:THR:O | 41:BT:39:THR:HG23 | 2.10 | 0.51 |
| 43:BW:45:HIS:HB3 | 43:BW:52:CYS:HB2 | 1.93 | 0.51 |
| 44:BX:13:GLU:HA | 44:BX:16:THR:OG1 | 2.11 | 0.51 |
| 45:BY:50:VAL:HA | 45:BY:52:PHE:CE1 | 2.45 | 0.51 |
| 46:BZ:5:CYS:SG | 46:BZ:7:VAL:HG12 | 2.50 | 0.51 |
| 46:BZ:7:VAL:HG21 | 46:BZ:59:ILE:CD1 | 2.40 | 0.51 |
| 1:CA:1361:G:C2' | 1:CA:1362:A:H5'' | 2.36 | 0.51 |
| 1:CA:137:U:H2' | 1:CA:138:G:C8 | 2.45 | 0.51 |
| 1:CA:1477:U:H2' | 1:CA:1478:U:H6 | 1.75 | 0.51 |
| 1:CA:452:A:H2' | 1:CA:453:G:O4' | 2.09 | 0.51 |
| 20:CB:212:TYR:O | 20:CB:216:VAL:HG22 | 2.11 | 0.51 |
| 20:CB:95:TRP:HH2 | 20:CB:100:LEU:HB2 | 1.75 | 0.51 |
| 12:CM:76:ILE:HG23 | 12:CM:79:LEU:HD12 | 1.93 | 0.51 |
| 23:DB:1117:C:H2' | 23:DB:1118:C:C6 | 2.46 | 0.51 |
| 23:DB:2634:A:H2' | 23:DB:2635:A:C8 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:38:A:N3 | 27:DE:43:THR:HB | 2.25 | 0.51 |
| 23:DB:455:C:N3 | 23:DB:472:A:H2' | 2.26 | 0.51 |
| 23:DB:4:U:H2' | 23:DB:5:A:C8 | 2.45 | 0.51 |
| 23:DB:642:U:HO2' | 23:DB:643:A:H8 | 1.57 | 0.51 |
| 23:DB:58:G:N3 | 23:DB:73:A:H2 | 2.08 | 0.51 |
| 23:DB:1565:C:H5'' | 25:DC:17:LYS:HE2 | 1.92 | 0.51 |
| 25:DC:141:HIS:NE2 | 25:DC:194:VAL:HB | 2.26 | 0.51 |
| 27:DE:1:MET:HB2 | 27:DE:16:GLU:HB2 | 1.91 | 0.51 |
| 28:DF:62:GLN:HG3 | 28:DF:91:ARG:NH1 | 2.25 | 0.51 |
| 27:DE:29:HIS:NE2 | 33:DL:8:PRO:HG3 | 2.24 | 0.51 |
| 44:DX:18:LEU:O | 44:DX:22:LEU:HB3 | 2.10 | 0.51 |
| 23:DB:200:U:O2' | 46:DZ:22:LEU:HD12 | 2.10 | 0.51 |
| 1:AA:968:A:C8 | 1:AA:1062:U:H4' | 2.44 | 0.51 |
| 1:AA:1512:U:H2' | 1:AA:1513:A:H8 | 1.75 | 0.51 |
| 1:AA:218:U:H2' | 1:AA:219:U:H6 | 1.74 | 0.51 |
| 1:AA:531:U:H3 | 1:AA:1208:C:H5'' | 1.76 | 0.51 |
| 7:AH:11:THR:HA | 7:AH:14:ARG:NH1 | 2.25 | 0.51 |
| 12:AM:14:ALA:HB2 | 12:AM:42:VAL:HG23 | 1.92 | 0.51 |
| 23:BB:1022:G:N2 | 23:BB:1142:A:C2 | 2.76 | 0.51 |
| 23:BB:1203:U:H3' | 23:BB:1204:A:C5' | 2.40 | 0.51 |
| 23:BB:1247:A:O2' | 23:BB:1248:G:H5' | 2.11 | 0.51 |
| 23:BB:1541:C:H2' | 23:BB:1542:U:O4' | 2.11 | 0.51 |
| 23:BB:1921:G:H2' | 23:BB:1922:G:H8 | 1.76 | 0.51 |
| 23:BB:1965:C:H5'' | 23:BB:1966:A:H2' | 1.92 | 0.51 |
| 23:BB:2098:U:H2' | 23:BB:2099:U:C6 | 2.45 | 0.51 |
| 23:BB:2075:U:H2' | 23:BB:2238:G:N2 | 2.26 | 0.51 |
| 23:BB:2246:G:H2' | 23:BB:2247:A:C8 | 2.46 | 0.51 |
| 23:BB:2700:A:H2' | 23:BB:2701:U:C6 | 2.46 | 0.51 |
| 23:BB:2882:A:H3' | 23:BB:2883:A:H5'' | 1.92 | 0.51 |
| 23:BB:526:A:N6 | 23:BB:2626:C:H4' | 2.26 | 0.51 |
| 25:BC:130:PRO:HG2 | 25:BC:133:ASN:ND2 | 2.25 | 0.51 |
| 25:BC:93:VAL:HG13 | 25:BC:94:LEU:H | 1.75 | 0.51 |
| 26:BD:141:ARG:O | 26:BD:142:VAL:HG13 | 2.10 | 0.51 |
| 27:BE:150:THR:HG21 | 27:BE:153:LEU:HA | 1.92 | 0.51 |
| 22:BA:42:C:C6 | 28:BF:65:LEU:HD13 | 2.46 | 0.51 |
| 32:BK:60:ALA:HB2 | 32:BK:86:LEU:HA | 1.93 | 0.51 |
| 32:BK:79:PHE:CD1 | 32:BK:79:PHE:N | 2.78 | 0.51 |
| 35:BN:106:ASP:C | 35:BN:108:ALA:H | 2.13 | 0.51 |
| 38:BQ:24:TYR:CG | 38:BQ:25:GLY:N | 2.78 | 0.51 |
| 43:BW:18:LYS:HG3 | 43:BW:19:ARG:H | 1.76 | 0.51 |
| 46:BZ:63:GLY:O | 46:BZ:67:VAL:HG23 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1464:U:H2' | 1:CA:1465:A:C8 | 2.45 | 0.51 |
| 1:CA:394:G:H2' | 1:CA:395:C:H6 | 1.74 | 0.51 |
| 1:CA:398:U:H2' | 1:CA:399:G:H8 | 1.76 | 0.51 |
| 1:CA:420:U:H2' | 1:CA:422:C:C5 | 2.46 | 0.51 |
| 1:CA:448:A:H2' | 1:CA:449:G:C8 | 2.46 | 0.51 |
| 1:CA:919:A:O2' | 1:CA:920:U:H5' | 2.11 | 0.51 |
| 3:CD:199:ILE:HD12 | 3:CD:200:VAL:N | 2.26 | 0.51 |
| 7:CH:51:GLU:HB3 | 7:CH:57:GLU:HB3 | 1.91 | 0.51 |
| 11:CL:14:LYS:HG2 | 11:CL:15:VAL:N | 2.26 | 0.51 |
| 49:D2:19:ARG:HG2 | 49:D2:19:ARG:HH21 | 1.74 | 0.51 |
| 22:DA:109:A:H2' | 22:DA:110:C:O4' | 2.10 | 0.51 |
| 22:DA:54:G:O2' | 22:DA:55:U:H5' | 2.10 | 0.51 |
| 23:DB:1041:G:C2 | 23:DB:1042:G:N7 | 2.79 | 0.51 |
| 23:DB:2015:A:H2' | 23:DB:2016:U:O4' | 2.10 | 0.51 |
| 23:DB:2093:G:O5' | 30:DH:24:GLY:HA3 | 2.10 | 0.51 |
| 23:DB:2471:A:O2' | 23:DB:2472:G:C8 | 2.59 | 0.51 |
| 23:DB:544:C:H2' | 23:DB:545:U:C5 | 2.45 | 0.51 |
| 23:DB:664:G:H2' | 23:DB:665:U:H6 | 1.76 | 0.51 |
| 23:DB:813:U:H2' | 23:DB:814:C:H6 | 1.76 | 0.51 |
| 23:DB:877:A:H2' | 23:DB:900:A:N6 | 2.26 | 0.51 |
| 27:DE:182:ALA:O | 27:DE:183:PHE:HB2 | 2.11 | 0.51 |
| 28:DF:134:GLN:HB3 | 28:DF:149:ARG:HB3 | 1.93 | 0.51 |
| 28:DF:47:LYS:HA | 28:DF:50:ASP:OD1 | 2.10 | 0.51 |
| 29:DG:10:VAL:CG1 | 29:DG:16:VAL:HG21 | 2.40 | 0.51 |
| 30:DH:65:ALA:HA | 30:DH:68:ARG:CG | 2.40 | 0.51 |
| 52:DI:85:ILE:CD1 | 52:DI:137:LEU:HD21 | 2.40 | 0.51 |
| 32:DK:19:VAL:C | 32:DK:41:ILE:HD11 | 2.31 | 0.51 |
| 33:DL:81:ASP:HA | 33:DL:84:LYS:HD2 | 1.92 | 0.51 |
| 35:DN:38:LEU:CB | 35:DN:39:PRO:HD3 | 2.38 | 0.51 |
| 36:DO:66:GLY:HA2 | 36:DO:102:ARG:NE | 2.26 | 0.51 |
| 37:DP:20:ARG:NE | 37:DP:91:VAL:HG21 | 2.22 | 0.51 |
| 40:DS:24:ILE:HD11 | 40:DS:36:LEU:CD1 | 2.31 | 0.51 |
| 43:DW:30:VAL:HA | 43:DW:60:ALA:O | 2.10 | 0.51 |
| 1:AA:1008:U:H5'' | 13:AN:23:ARG:HH22 | 1.75 | 0.51 |
| 1:AA:1219:A:H2' | 1:AA:1220:G:C8 | 2.46 | 0.51 |
| 1:AA:176:C:H3' | 1:AA:177:G:H21 | 1.76 | 0.51 |
| 1:AA:188:C:H2' | 1:AA:189:A:O4' | 2.10 | 0.51 |
| 1:AA:285:C:H2' | 1:AA:286:C:C6 | 2.45 | 0.51 |
| 1:AA:797:C:O2' | 1:AA:798:U:H5' | 2.10 | 0.51 |
| 20:AB:69:VAL:HB | 20:AB:162:VAL:CG2 | 2.40 | 0.51 |
| 3:AD:187:ARG:NH1 | 3:AD:191:SER:HB3 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AE:15:ILE:HD12 | 4:AE:35:LEU:HG | 1.92 | 0.51 |
| 6:AG:61:PHE:O | 6:AG:65:LEU:HD13 | 2.11 | 0.51 |
| 9:AJ:12:ALA:HB3 | 9:AJ:18:ILE:HB | 1.92 | 0.51 |
| 14:AO:52:ARG:HG3 | 14:AO:56:LEU:HD13 | 1.92 | 0.51 |
| 18:AS:49:ALA:O | 18:AS:56:HIS:HD2 | 1.93 | 0.51 |
| 21:AU:13:VAL:O | 21:AU:13:VAL:HG13 | 2.10 | 0.51 |
| 23:BB:1193:G:H2' | 23:BB:1194:A:H5'' | 1.93 | 0.51 |
| 23:BB:1256:G:H21 | 27:BE:77:ILE:HG22 | 1.75 | 0.51 |
| 23:BB:1688:U:H2' | 23:BB:1698:A:N6 | 2.26 | 0.51 |
| 23:BB:1949:G:H2' | 23:BB:1950:G:H8 | 1.75 | 0.51 |
| 23:BB:2065:C:H1' | 23:BB:2449:U:O2 | 2.11 | 0.51 |
| 23:BB:2449:U:H4' | 23:BB:2450:A:OP1 | 2.11 | 0.51 |
| 23:BB:2634:A:H2' | 23:BB:2635:A:C8 | 2.46 | 0.51 |
| 23:BB:315:G:H2' | 23:BB:316:C:C6 | 2.46 | 0.51 |
| 23:BB:794:A:H2' | 23:BB:795:C:H6 | 1.76 | 0.51 |
| 23:BB:836:G:H2' | 23:BB:837:C:H6 | 1.72 | 0.51 |
| 25:BC:245:THR:OG1 | 25:BC:249:VAL:HG23 | 2.10 | 0.51 |
| 25:BC:53:ILE:O | 25:BC:53:ILE:HG23 | 2.11 | 0.51 |
| 27:BE:128:ALA:H | 27:BE:133:LEU:CD1 | 2.24 | 0.51 |
| 30:BH:103:VAL:HG12 | 30:BH:106:ALA:HB3 | 1.91 | 0.51 |
| 30:BH:83:LYS:HD2 | 30:BH:91:PHE:CD1 | 2.45 | 0.51 |
| 52:BI:29:GLN:HA | 52:BI:29:GLN:HE21 | 1.75 | 0.51 |
| 31:BJ:36:LEU:O | 31:BJ:51:GLY:HA3 | 2.10 | 0.51 |
| 31:BJ:44:TYR:CD2 | 38:BQ:59:LEU:HD21 | 2.45 | 0.51 |
| 31:BJ:42:ALA:O | 31:BJ:44:TYR:N | 2.43 | 0.51 |
| 37:BP:98:TYR:C | 37:BP:100:ARG:H | 2.13 | 0.51 |
| 38:BQ:80:ASN:ND2 | 38:BQ:81:GLY:H | 2.09 | 0.51 |
| 41:BT:12:ARG:HE | 44:BX:29:ARG:NH1 | 2.09 | 0.51 |
| 1:CA:285:C:H2' | 1:CA:286:C:C6 | 2.45 | 0.51 |
| 1:CA:369:G:O2' | 1:CA:370:C:H5' | 2.10 | 0.51 |
| 1:CA:462:G:H3' | 1:CA:463:U:C6 | 2.45 | 0.51 |
| 1:CA:730:G:O2' | 1:CA:766:A:H5' | 2.09 | 0.51 |
| 20:CB:130:LYS:O | 20:CB:134:LEU:HB2 | 2.10 | 0.51 |
| 20:CB:205:ALA:HB3 | 20:CB:208:ALA:CB | 2.39 | 0.51 |
| 3:CD:53:GLN:HB3 | 3:CD:202:LEU:HB2 | 1.93 | 0.51 |
| 6:CG:110:ARG:HD3 | 6:CG:118:ARG:HA | 1.92 | 0.51 |
| 6:CG:20:GLU:O | 6:CG:23:ALA:HB3 | 2.11 | 0.51 |
| 6:CG:99:ALA:O | 6:CG:103:ILE:HG13 | 2.10 | 0.51 |
| 7:CH:115:ALA:O | 7:CH:120:LEU:HD23 | 2.11 | 0.51 |
| 9:CJ:41:PRO:HA | 9:CJ:72:ARG:HD3 | 1.93 | 0.51 |
| 11:CL:113:ARG:HE | 11:CL:120:ARG:HA | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CL:43:LYS:NZ | 11:CL:44:PRO:HD3 | 2.25 | 0.51 |
| 23:DB:1000:A:H2' | 23:DB:1001:A:H8 | 1.74 | 0.51 |
| 23:DB:973:A:O4' | 23:DB:1188:U:C6 | 2.64 | 0.51 |
| 23:DB:1219:U:H2' | 23:DB:1220:G:C8 | 2.46 | 0.51 |
| 23:DB:2078:C:O2' | 23:DB:2079:U:H5' | 2.11 | 0.51 |
| 23:DB:2398:U:H2' | 23:DB:2399:G:C8 | 2.45 | 0.51 |
| 23:DB:289:G:H2' | 23:DB:290:U:H6 | 1.76 | 0.51 |
| 23:DB:757:G:H2' | 23:DB:758:C:H5' | 1.92 | 0.51 |
| 25:DC:245:THR:C | 25:DC:247:TRP:H | 2.14 | 0.51 |
| 25:DC:43:ASN:HB2 | 25:DC:49:THR:CG2 | 2.40 | 0.51 |
| 28:DF:102:LEU:HA | 28:DF:106:ALA:HB3 | 1.91 | 0.51 |
| 30:DH:1:MET:HE3 | 30:DH:26:ALA:HB3 | 1.93 | 0.51 |
| 52:DI:78:LEU:HD13 | 52:DI:108:ILE:HG23 | 1.92 | 0.51 |
| 31:DJ:71:ASP:HA | 31:DJ:88:THR:OG1 | 2.11 | 0.51 |
| 31:DJ:89:PHE:CE1 | 31:DJ:93:ILE:HD13 | 2.45 | 0.51 |
| 36:DO:110:ALA:HA | 36:DO:113:ALA:HB3 | 1.92 | 0.51 |
| 37:DP:56:SER:HB2 | 37:DP:75:THR:HB | 1.93 | 0.51 |
| 23:DB:1163:G:H4' | 39:DR:92:TRP:CD1 | 2.45 | 0.51 |
| 24:DV:44:HIS:CE1 | 24:DV:85:LYS:HB2 | 2.46 | 0.51 |
| 46:DZ:2:SER:O | 46:DZ:4:VAL:HG13 | 2.11 | 0.51 |
| 1:AA:1427:C:H2' | 1:AA:1428:A:H8 | 1.75 | 0.51 |
| 1:AA:610:U:O2 | 1:AA:610:U:O4' | 2.29 | 0.51 |
| 2:AC:78:LYS:C | 2:AC:80:GLY:H | 2.14 | 0.51 |
| 14:AO:42:PHE:CE1 | 14:AO:55:LEU:HD22 | 2.46 | 0.51 |
| 14:AO:63:ARG:HH12 | 14:AO:87:ARG:HH22 | 1.57 | 0.51 |
| 49:B2:39:ARG:HH11 | 49:B2:39:ARG:HG3 | 1.76 | 0.51 |
| 23:BB:1150:C:H2' | 23:BB:1151:A:H8 | 1.76 | 0.51 |
| 23:BB:1642:G:O2' | 23:BB:1643:G:H5' | 2.11 | 0.51 |
| 23:BB:1858:A:H2' | 23:BB:1859:U:O4' | 2.11 | 0.51 |
| 23:BB:1880:U:H2' | 23:BB:1881:C:C6 | 2.45 | 0.51 |
| 23:BB:199:A:O2' | 23:BB:200:U:H5' | 2.11 | 0.51 |
| 23:BB:2233:U:H2' | 23:BB:2234:G:C8 | 2.46 | 0.51 |
| 23:BB:2258:C:H5' | 23:BB:2259:U:C5 | 2.39 | 0.51 |
| 23:BB:964:C:O2' | 23:BB:2273:A:H1' | 2.11 | 0.51 |
| 23:BB:2379:G:H2' | 23:BB:2380:C:C6 | 2.46 | 0.51 |
| 23:BB:2398:U:H2' | 23:BB:2399:G:C8 | 2.46 | 0.51 |
| 23:BB:596:U:H2' | 23:BB:597:G:C8 | 2.45 | 0.51 |
| 23:BB:69:C:H2' | 23:BB:70:G:C8 | 2.46 | 0.51 |
| 25:BC:14:HIS:O | 25:BC:16:VAL:HG23 | 2.10 | 0.51 |
| 25:BC:173:LEU:HD13 | 25:BC:173:LEU:N | 2.25 | 0.51 |
| 26:BD:117:GLY:O | 26:BD:119:ALA:N | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BE:153:LEU:HG | 27:BE:154:ASP:H | 1.76 | 0.51 |
| 29:BG:7:PRO:O | 29:BG:8:VAL:HB | 2.10 | 0.51 |
| 29:BG:91:VAL:O | 29:BG:93:TYR:N | 2.44 | 0.51 |
| 32:BK:18:ARG:O | 32:BK:45:GLU:HB2 | 2.11 | 0.51 |
| 33:BL:2:ARG:HG2 | 33:BL:2:ARG:O | 2.11 | 0.51 |
| 35:BN:8:ARG:HG2 | 35:BN:10:LEU:HD22 | 1.93 | 0.51 |
| 37:BP:112:ARG:HB2 | 37:BP:112:ARG:NH1 | 2.26 | 0.51 |
| 39:BR:6:GLN:HE22 | 39:BR:9:GLY:CA | 2.23 | 0.51 |
| 41:BT:12:ARG:CD | 44:BX:29:ARG:HH12 | 2.23 | 0.51 |
| 1:CA:1118:U:H1' | 1:CA:1179:A:C4 | 2.46 | 0.51 |
| 1:CA:272:C:H2' | 1:CA:273:U:H6 | 1.74 | 0.51 |
| 1:CA:389:A:H2' | 1:CA:389:A:N3 | 2.24 | 0.51 |
| 1:CA:58:C:O2' | 1:CA:59:A:H5' | 2.11 | 0.51 |
| 1:CA:738:C:H2' | 1:CA:739:C:H6 | 1.75 | 0.51 |
| 3:CD:31:CYS:SG | 3:CD:33:ILE:HB | 2.51 | 0.51 |
| 3:CD:18:LEU:HG | 3:CD:63:ILE:HG12 | 1.92 | 0.51 |
| 4:CE:10:LEU:HA | 4:CE:39:GLY:O | 2.11 | 0.51 |
| 13:CN:61:ASN:HB3 | 13:CN:72:PHE:CE2 | 2.46 | 0.51 |
| 14:CO:52:ARG:HG3 | 14:CO:56:LEU:HD13 | 1.93 | 0.51 |
| 21:CU:43:GLU:HA | 21:CU:46:ARG:NE | 2.26 | 0.51 |
| 23:DB:1046:A:H3' | 23:DB:1047:G:C5' | 2.41 | 0.51 |
| 23:DB:1319:C:O2' | 23:DB:1320:C:H5' | 2.11 | 0.51 |
| 23:DB:1726:C:H2' | 23:DB:1727:C:C6 | 2.46 | 0.51 |
| 23:DB:1857:G:O2' | 23:DB:1858:A:H8 | 1.92 | 0.51 |
| 23:DB:2070:A:H2' | 23:DB:2071:A:C8 | 2.46 | 0.51 |
| 23:DB:2514:U:H2' | 23:DB:2515:C:C6 | 2.46 | 0.51 |
| 23:DB:2634:A:H2' | 23:DB:2635:A:H8 | 1.76 | 0.51 |
| 23:DB:464:U:H2' | 23:DB:465:G:O4' | 2.11 | 0.51 |
| 23:DB:855:G:H21 | 43:DW:23:LYS:CG | 2.15 | 0.51 |
| 25:DC:115:ILE:HA | 25:DC:124:LYS:NZ | 2.26 | 0.51 |
| 26:DD:34:VAL:HG12 | 26:DD:94:GLN:H | 1.75 | 0.51 |
| 22:DA:42:C:C6 | 28:DF:65:LEU:HD13 | 2.46 | 0.51 |
| 32:DK:115:ILE:HG23 | 32:DK:116:ILE:N | 2.26 | 0.51 |
| 32:DK:47:ILE:CG1 | 32:DK:48:PRO:HD2 | 2.36 | 0.51 |
| 35:DN:115:LEU:O | 35:DN:117:ASP:N | 2.44 | 0.51 |
| 36:DO:36:TYR:HA | 36:DO:52:SER:HB3 | 1.92 | 0.51 |
| 37:DP:20:ARG:HB3 | 37:DP:23:ASP:CG | 2.32 | 0.51 |
| 26:DD:10:GLY:HA2 | 37:DP:4:ILE:HD11 | 1.91 | 0.51 |
| 38:DQ:59:LEU:HD13 | 38:DQ:60:TRP:N | 2.26 | 0.51 |
| 39:DR:49:ILE:HD12 | 39:DR:49:ILE:O | 2.11 | 0.51 |
| 42:DU:11:ILE:O | 42:DU:11:ILE:HD13 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DW:23:LYS:NZ | 43:DW:24:ARG:HG3 | 2.26 | 0.51 |
| 1:AA:1302:C:H4' | 1:AA:1303:C:OP2 | 2.10 | 0.51 |
| 1:AA:620:C:C2 | 3:AD:131:ILE:HG21 | 2.46 | 0.51 |
| 1:AA:663:A:O2' | 1:AA:664:G:H5' | 2.11 | 0.51 |
| 20:AB:95:TRP:HH2 | 20:AB:100:LEU:HB2 | 1.76 | 0.51 |
| 20:AB:119:GLN:C | 20:AB:125:PHE:HB3 | 2.31 | 0.51 |
| 3:AD:72:ARG:HD3 | 3:AD:203:TYR:CZ | 2.45 | 0.51 |
| 6:AG:126:ALA:HA | 6:AG:134:VAL:HG13 | 1.92 | 0.51 |
| 7:AH:27:PRO:HA | 7:AH:56:PRO:O | 2.11 | 0.51 |
| 10:AK:28:ASN:HD21 | 10:AK:47:GLY:H | 1.59 | 0.51 |
| 12:AM:3:ILE:HD12 | 12:AM:9:PRO:HD2 | 1.93 | 0.51 |
| 23:BB:1120:G:O2' | 23:BB:1121:C:H5' | 2.11 | 0.51 |
| 23:BB:1335:C:H2' | 23:BB:1336:A:C8 | 2.46 | 0.51 |
| 23:BB:1863:G:H2' | 23:BB:1864:U:O4' | 2.10 | 0.51 |
| 23:BB:2597:G:H5' | 25:BC:240:GLY:HA3 | 1.93 | 0.51 |
| 23:BB:2630:G:H2' | 23:BB:2631:G:H8 | 1.76 | 0.51 |
| 23:BB:263:G:H2' | 23:BB:264:C:O4' | 2.11 | 0.51 |
| 25:BC:128:THR:CA | 25:BC:190:THR:HG22 | 2.35 | 0.51 |
| 26:BD:8:LYS:HG2 | 26:BD:197:THR:H | 1.76 | 0.51 |
| 28:BF:122:ASP:OD2 | 28:BF:126:ASN:HB2 | 2.10 | 0.51 |
| 28:BF:91:ARG:HD3 | 28:BF:91:ARG:N | 2.26 | 0.51 |
| 52:BI:33:ASN:HD21 | 52:BI:64:ARG:NH1 | 2.03 | 0.51 |
| 32:BK:26:GLY:O | 32:BK:30:ARG:HD2 | 2.10 | 0.51 |
| 36:BO:56:LYS:O | 36:BO:57:ALA:C | 2.49 | 0.51 |
| 1:AA:1432:G:C5' | 37:BP:105:LYS:HG2 | 2.31 | 0.51 |
| 39:BR:49:ILE:O | 39:BR:49:ILE:HD12 | 2.11 | 0.51 |
| 43:BW:17:ALA:HB1 | 43:BW:37:VAL:H | 1.76 | 0.51 |
| 43:BW:48:ALA:HB3 | 43:BW:81:ILE:HG13 | 1.93 | 0.51 |
| 45:BY:20:LYS:HA | 45:BY:23:LEU:HB2 | 1.93 | 0.51 |
| 1:CA:1136:C:OP1 | 1:CA:1136:C:H3' | 2.10 | 0.51 |
| 1:CA:176:C:H3' | 1:CA:177:G:H21 | 1.76 | 0.51 |
| 1:CA:254:G:O2' | 1:CA:255:G:H5' | 2.11 | 0.51 |
| 1:CA:565:U:H3' | 1:CA:566:G:H2' | 1.92 | 0.51 |
| 1:CA:791:G:C6 | 1:CA:792:A:N7 | 2.79 | 0.51 |
| 20:CB:16:GLY:HA2 | 20:CB:40:ILE:HG13 | 1.93 | 0.51 |
| 2:CC:171:ARG:NH1 | 2:CC:171:ARG:HB2 | 2.25 | 0.51 |
| 8:CI:55:ASP:HB2 | 8:CI:59:LYS:HG3 | 1.93 | 0.51 |
| 15:CP:39:PHE:CG | 15:CP:40:ASN:N | 2.78 | 0.51 |
| 15:CP:46:LYS:C | 15:CP:48:GLU:H | 2.12 | 0.51 |
| 16:CQ:30:HIS:HB3 | 16:CQ:33:TYR:HB2 | 1.93 | 0.51 |
| 22:DA:51:G:OP1 | 36:DO:63:LYS:HE3 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1242:U:H2' | 23:DB:1243:C:C6 | 2.46 | 0.51 |
| 23:DB:1584:U:H5'' | 23:DB:1585:C:C5 | 2.46 | 0.51 |
| 23:DB:1827:U:C2' | 23:DB:1828:G:H5' | 2.41 | 0.51 |
| 23:DB:2258:C:H5' | 23:DB:2259:U:C5 | 2.40 | 0.51 |
| 23:DB:2283:C:H5'' | 23:DB:2389:G:O2' | 2.11 | 0.51 |
| 23:DB:2394:C:H2' | 23:DB:2395:C:C6 | 2.46 | 0.51 |
| 23:DB:2408:U:O2' | 23:DB:2409:G:H5' | 2.11 | 0.51 |
| 23:DB:2460:U:O5' | 23:DB:2460:U:H6 | 1.93 | 0.51 |
| 25:DC:136:VAL:HG12 | 25:DC:137:GLY:N | 2.26 | 0.51 |
| 26:DD:151:THR:HB | 26:DD:152:PRO:HD3 | 1.93 | 0.51 |
| 27:DE:98:LYS:NZ | 27:DE:99:LYS:HG2 | 2.26 | 0.51 |
| 29:DG:123:GLU:O | 29:DG:125:PRO:HD3 | 2.11 | 0.51 |
| 30:DH:103:VAL:HG22 | 30:DH:108:VAL:O | 2.11 | 0.51 |
| 30:DH:94:ILE:HG22 | 30:DH:122:LEU:CB | 2.40 | 0.51 |
| 23:DB:1098:A:C3' | 52:DI:4:VAL:N | 2.73 | 0.51 |
| 52:DI:85:ILE:HD12 | 52:DI:87:SER:O | 2.10 | 0.51 |
| 32:DK:105:ARG:HD2 | 32:DK:105:ARG:H | 1.76 | 0.51 |
| 32:DK:43:ILE:CG2 | 32:DK:46:ALA:HB2 | 2.41 | 0.51 |
| 36:DO:58:ILE:O | 36:DO:62:LEU:HB2 | 2.11 | 0.51 |
| 39:DR:7:SER:HB2 | 39:DR:22:LEU:CB | 2.40 | 0.51 |
| 40:DS:23:LEU:HD21 | 47:D0:21:LEU:HB3 | 1.92 | 0.51 |
| 41:DT:38:ALA:HB3 | 41:DT:81:LYS:HZ3 | 1.74 | 0.51 |
| 44:DX:26:PHE:HD1 | 44:DX:27:ASN:ND2 | 2.07 | 0.51 |
| 1:AA:1225:A:H5' | 1:AA:1226:C:OP2 | 2.11 | 0.51 |
| 1:AA:1352:C:H2' | 1:AA:1353:G:C8 | 2.46 | 0.51 |
| 1:AA:1448:C:H2' | 1:AA:1449:C:H6 | 1.76 | 0.51 |
| 1:AA:512:U:H2' | 1:AA:513:C:H6 | 1.75 | 0.51 |
| 1:AA:772:U:H2' | 1:AA:773:G:C8 | 2.46 | 0.51 |
| 1:AA:807:A:H2' | 1:AA:808:C:C6 | 2.45 | 0.51 |
| 20:AB:143:LEU:HB3 | 20:AB:147:LEU:HD12 | 1.93 | 0.51 |
| 5:AF:21:MET:HB3 | 5:AF:25:TYR:CZ | 2.46 | 0.51 |
| 8:AI:120:ALA:O | 8:AI:121:ARG:HG2 | 2.11 | 0.51 |
| 11:AL:113:ARG:HE | 11:AL:120:ARG:HA | 1.75 | 0.51 |
| 13:AN:2:LYS:O | 13:AN:6:LYS:HG3 | 2.11 | 0.51 |
| 13:AN:50:LEU:HD23 | 13:AN:51:PRO:HD3 | 1.93 | 0.51 |
| 51:B4:15:LYS:O | 51:B4:16:ILE:HB | 2.11 | 0.51 |
| 22:BA:60:C:H2' | 22:BA:61:G:H8 | 1.76 | 0.51 |
| 23:BB:1149:G:H2' | 23:BB:1150:C:H6 | 1.75 | 0.51 |
| 23:BB:1324:G:C6 | 23:BB:1331:G:C6 | 2.98 | 0.51 |
| 23:BB:2101:A:H3' | 23:BB:2102:G:H5'' | 1.92 | 0.51 |
| 23:BB:2405:G:H1' | 23:BB:2412:A:H61 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2529:G:H4' | 29:BG:174:LYS:HB2 | 1.91 | 0.51 |
| 23:BB:4:U:H2' | 23:BB:5:A:H8 | 1.76 | 0.51 |
| 25:BC:35:LYS:HG2 | 25:BC:36:ASN:N | 2.23 | 0.51 |
| 26:BD:116:LYS:HD2 | 26:BD:123:LYS:HE2 | 1.93 | 0.51 |
| 23:BB:674:G:H4' | 27:BE:69:ARG:HB3 | 1.92 | 0.51 |
| 28:BF:91:ARG:O | 28:BF:92:GLY:C | 2.49 | 0.51 |
| 32:BK:120:PRO:HA | 37:BP:65:ASN:ND2 | 2.25 | 0.51 |
| 32:BK:79:PHE:HD2 | 37:BP:69:VAL:HG12 | 1.75 | 0.51 |
| 35:BN:55:ALA:HA | 35:BN:80:PHE:CE1 | 2.46 | 0.51 |
| 36:BO:111:ARG:HG2 | 36:BO:117:PHE:CZ | 2.46 | 0.51 |
| 36:BO:84:GLU:C | 36:BO:86:GLY:H | 2.15 | 0.51 |
| 39:BR:22:LEU:HD12 | 39:BR:25:LEU:HD23 | 1.91 | 0.51 |
| 39:BR:4:VAL:O | 39:BR:38:VAL:HA | 2.11 | 0.51 |
| 41:BT:10:VAL:HG21 | 41:BT:42:GLU:HG3 | 1.92 | 0.51 |
| 24:BV:16:ALA:CA | 24:BV:19:ARG:HH21 | 2.25 | 0.51 |
| 46:BZ:2:SER:O | 46:BZ:4:VAL:HG13 | 2.10 | 0.51 |
| 1:CA:1238:A:H5' | 1:CA:1336:C:N4 | 2.26 | 0.51 |
| 1:CA:1471:U:O2' | 1:CA:1472:U:H5' | 2.10 | 0.51 |
| 1:CA:1515:G:O2' | 1:CA:1516:G:H5' | 2.11 | 0.51 |
| 1:CA:612:C:H2' | 1:CA:613:C:C6 | 2.46 | 0.51 |
| 1:CA:734:G:H2' | 1:CA:735:C:C6 | 2.45 | 0.51 |
| 1:CA:79:G:H2' | 1:CA:80:A:H8 | 1.75 | 0.51 |
| 20:CB:69:VAL:HB | 20:CB:162:VAL:CG2 | 2.40 | 0.51 |
| 8:CI:25:GLY:HA3 | 8:CI:57:VAL:HA | 1.92 | 0.51 |
| 23:DB:1098:A:C4 | 52:DI:3:LYS:O | 2.63 | 0.51 |
| 23:DB:1245:G:OP1 | 33:DL:13:LYS:HE3 | 2.11 | 0.51 |
| 23:DB:1742:U:H2' | 23:DB:1743:G:C8 | 2.45 | 0.51 |
| 23:DB:1792:G:P | 25:DC:204:LEU:HD12 | 2.51 | 0.51 |
| 23:DB:2269:G:H4' | 43:DW:19:ARG:NH1 | 2.20 | 0.51 |
| 23:DB:460:A:H4' | 41:DT:72:GLN:HB2 | 1.92 | 0.51 |
| 25:DC:142:ASN:CG | 25:DC:142:ASN:O | 2.49 | 0.51 |
| 25:DC:91:ALA:CB | 25:DC:105:ALA:HB2 | 2.40 | 0.51 |
| 26:DD:10:GLY:O | 26:DD:11:MET:HB2 | 2.11 | 0.51 |
| 28:DF:62:GLN:HB2 | 28:DF:91:ARG:HH11 | 1.75 | 0.51 |
| 31:DJ:25:LEU:O | 31:DJ:27:ARG:N | 2.43 | 0.51 |
| 31:DJ:44:TYR:O | 31:DJ:45:THR:HB | 2.10 | 0.51 |
| 31:DJ:64:VAL:HG22 | 31:DJ:68:LYS:HD3 | 1.93 | 0.51 |
| 33:DL:124:GLY:N | 33:DL:143:GLU:HG3 | 2.24 | 0.51 |
| 33:DL:110:VAL:HG23 | 33:DL:126:ARG:O | 2.11 | 0.51 |
| 33:DL:135:ILE:HG12 | 33:DL:140:GLY:CA | 2.40 | 0.51 |
| 33:DL:18:ARG:C | 33:DL:19:LEU:HD12 | 2.31 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DL:2:ARG:O | 33:DL:2:ARG:HG2 | 2.10 | 0.51 |
| 1:AA:1283:U:H2' | 1:AA:1284:C:C6 | 2.46 | 0.50 |
| 1:AA:1361:G:C2' | 1:AA:1362:A:H5'' | 2.39 | 0.50 |
| 1:AA:1417:G:N2 | 1:AA:1482:G:H2' | 2.25 | 0.50 |
| 1:AA:1500:A:H2' | 1:AA:1501:C:H5' | 1.93 | 0.50 |
| 1:AA:584:G:O2' | 1:AA:585:G:H5' | 2.11 | 0.50 |
| 1:AA:658:C:H2' | 1:AA:659:U:C6 | 2.45 | 0.50 |
| 20:AB:212:TYR:O | 20:AB:216:VAL:HG22 | 2.10 | 0.50 |
| 20:AB:23:ASN:HD22 | 20:AB:24:PRO:CD | 2.23 | 0.50 |
| 4:AE:132:PRO:O | 4:AE:136:VAL:HG12 | 2.11 | 0.50 |
| 5:AF:51:ILE:HD11 | 5:AF:86:ARG:HG3 | 1.93 | 0.50 |
| 6:AG:20:GLU:O | 6:AG:23:ALA:HB3 | 2.11 | 0.50 |
| 7:AH:47:ASP:CG | 7:AH:48:PHE:H | 2.15 | 0.50 |
| 7:AH:55:LYS:NZ | 7:AH:55:LYS:HA | 2.27 | 0.50 |
| 8:AI:25:GLY:HA3 | 8:AI:57:VAL:HA | 1.93 | 0.50 |
| 13:AN:16:ALA:HA | 13:AN:20:PHE:HB2 | 1.93 | 0.50 |
| 15:AP:43:ALA:HA | 15:AP:46:LYS:HE3 | 1.93 | 0.50 |
| 22:BA:7:G:O2' | 22:BA:8:C:H5' | 2.10 | 0.50 |
| 23:BB:1023:U:H2' | 23:BB:1024:G:H5' | 1.93 | 0.50 |
| 23:BB:1744:A:H2' | 23:BB:1745:A:C8 | 2.46 | 0.50 |
| 23:BB:184:C:H2' | 23:BB:185:G:C8 | 2.45 | 0.50 |
| 23:BB:1872:A:O5' | 23:BB:1872:A:H8 | 1.95 | 0.50 |
| 23:BB:2721:A:H2' | 23:BB:2722:G:H8 | 1.76 | 0.50 |
| 23:BB:307:G:N2 | 23:BB:309:A:H3' | 2.25 | 0.50 |
| 23:BB:79:C:HO2' | 23:BB:346:A:H1' | 1.75 | 0.50 |
| 23:BB:521:U:H2' | 23:BB:522:A:H8 | 1.74 | 0.50 |
| 23:BB:718:A:H5' | 23:BB:719:C:C5 | 2.46 | 0.50 |
| 23:BB:794:A:H2' | 23:BB:795:C:C6 | 2.46 | 0.50 |
| 26:BD:148:GLN:HG3 | 26:BD:152:PRO:CB | 2.41 | 0.50 |
| 29:BG:25:ILE:HD13 | 29:BG:74:MET:HE2 | 1.93 | 0.50 |
| 29:BG:8:VAL:HG11 | 29:BG:49:LEU:CB | 2.34 | 0.50 |
| 30:BH:130:VAL:O | 30:BH:142:VAL:HB | 2.11 | 0.50 |
| 52:BI:49:GLU:CG | 52:BI:54:ILE:HD11 | 2.41 | 0.50 |
| 39:BR:60:LYS:N | 39:BR:100:GLY:HA3 | 2.24 | 0.50 |
| 39:BR:62:GLU:O | 39:BR:96:VAL:HA | 2.10 | 0.50 |
| 40:BS:29:VAL:HG11 | 40:BS:55:ILE:CD1 | 2.37 | 0.50 |
| 1:CA:1229:A:H2' | 1:CA:1230:C:C6 | 2.46 | 0.50 |
| 1:CA:1283:U:H2' | 1:CA:1284:C:C6 | 2.45 | 0.50 |
| 1:CA:1484:C:H2' | 1:CA:1485:U:O4' | 2.11 | 0.50 |
| 1:CA:317:U:H2' | 1:CA:318:G:H8 | 1.75 | 0.50 |
| 1:CA:458:U:H2' | 1:CA:459:A:H8 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:493:A:H3' | 1:CA:494:G:C8 | 2.46 | 0.50 |
| 1:CA:784:A:H2' | 1:CA:785:G:H8 | 1.75 | 0.50 |
| 2:CC:178:ARG:HG2 | 2:CC:206:ILE:HA | 1.93 | 0.50 |
| 5:CF:69:GLU:OE1 | 5:CF:70:VAL:HG13 | 2.11 | 0.50 |
| 8:CI:71:ILE:HD12 | 8:CI:71:ILE:N | 2.24 | 0.50 |
| 9:CJ:44:THR:HG23 | 9:CJ:69:THR:O | 2.11 | 0.50 |
| 13:CN:50:LEU:HD23 | 13:CN:51:PRO:HD3 | 1.92 | 0.50 |
| 14:CO:42:PHE:CE1 | 14:CO:55:LEU:HD22 | 2.46 | 0.50 |
| 18:CS:20:LYS:O | 18:CS:23:GLU:HG3 | 2.11 | 0.50 |
| 18:CS:6:LYS:O | 18:CS:8:PRO:HD3 | 2.10 | 0.50 |
| 10:CK:111:ASP:HB2 | 21:CU:19:LYS:HE3 | 1.91 | 0.50 |
| 10:CK:110:THR:HA | 21:CU:3:ILE:O | 2.12 | 0.50 |
| 51:D4:10:LEU:HD22 | 51:D4:33:HIS:CD2 | 2.46 | 0.50 |
| 23:DB:1099:G:O2' | 23:DB:1100:C:H5' | 2.11 | 0.50 |
| 23:DB:1401:G:H2' | 23:DB:1402:U:C6 | 2.46 | 0.50 |
| 23:DB:1430:G:H2' | 23:DB:1431:A:O4' | 2.10 | 0.50 |
| 23:DB:1509:A:C8 | 23:DB:1509:A:H5'' | 2.46 | 0.50 |
| 23:DB:212:G:H2' | 23:DB:213:A:H8 | 1.76 | 0.50 |
| 23:DB:2838:G:H2' | 23:DB:2839:G:H8 | 1.76 | 0.50 |
| 23:DB:2885:G:H2' | 23:DB:2886:A:C4' | 2.41 | 0.50 |
| 23:DB:623:C:H2' | 23:DB:624:C:C6 | 2.46 | 0.50 |
| 23:DB:917:A:C2 | 23:DB:918:A:H1' | 2.46 | 0.50 |
| 23:DB:942:G:H2' | 23:DB:943:A:H8 | 1.76 | 0.50 |
| 25:DC:171:VAL:HG23 | 25:DC:185:ALA:HB2 | 1.92 | 0.50 |
| 25:DC:43:ASN:HD22 | 25:DC:44:ASN:H | 1.59 | 0.50 |
| 26:DD:8:LYS:HB2 | 26:DD:201:LEU:HD11 | 1.93 | 0.50 |
| 26:DD:35:THR:OG1 | 26:DD:49:GLN:HG2 | 2.11 | 0.50 |
| 27:DE:32:VAL:HG23 | 27:DE:33:VAL:N | 2.25 | 0.50 |
| 28:DF:86:CYS:O | 28:DF:88:VAL:HG23 | 2.12 | 0.50 |
| 29:DG:148:ARG:HD3 | 29:DG:152:ARG:NE | 2.26 | 0.50 |
| 30:DH:48:GLU:CB | 30:DH:51:ARG:HH21 | 2.15 | 0.50 |
| 32:DK:17:ARG:HB3 | 32:DK:45:GLU:CG | 2.40 | 0.50 |
| 32:DK:79:PHE:CD1 | 32:DK:79:PHE:N | 2.78 | 0.50 |
| 32:DK:8:LEU:H | 32:DK:8:LEU:HD12 | 1.76 | 0.50 |
| 34:DM:40:ARG:HB3 | 34:DM:95:LEU:HD12 | 1.92 | 0.50 |
| 38:DQ:94:LEU:HD12 | 39:DR:13:ARG:HB2 | 1.93 | 0.50 |
| 23:DB:815:C:OP2 | 39:DR:85:LYS:HE2 | 2.11 | 0.50 |
| 40:DS:84:ARG:HB3 | 40:DS:96:ILE:HG23 | 1.93 | 0.50 |
| 42:DU:11:ILE:HA | 42:DU:21:ARG:HG2 | 1.93 | 0.50 |
| 44:DX:17:GLU:HB3 | 44:DX:53:VAL:CG1 | 2.40 | 0.50 |
| 1:AA:1434:A:H2' | 1:AA:1435:G:C8 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:394:G:H2' | 1:AA:395:C:H6 | 1.75 | 0.50 |
| 1:AA:448:A:H2' | 1:AA:449:G:C8 | 2.46 | 0.50 |
| 1:AA:464:U:H2' | 1:AA:466:A:OP2 | 2.11 | 0.50 |
| 1:AA:575:G:H4' | 1:AA:576:C:O5' | 2.11 | 0.50 |
| 1:AA:627:G:H2' | 1:AA:628:G:C8 | 2.47 | 0.50 |
| 1:AA:708:C:O2' | 1:AA:709:U:H5' | 2.10 | 0.50 |
| 1:AA:586:C:H5" | 7:AH:81:GLY:HA2 | 1.93 | 0.50 |
| 8:AI:78:ILE:HG22 | 8:AI:82:ILE:HD11 | 1.93 | 0.50 |
| 9:AJ:8:ILE:HD12 | 9:AJ:8:ILE:N | 2.25 | 0.50 |
| 14:AO:55:LEU:O | 14:AO:59:VAL:HG23 | 2.11 | 0.50 |
| 23:BB:122:G:O2' | 23:BB:123:G:H5' | 2.11 | 0.50 |
| 23:BB:1458:U:C2' | 23:BB:1459:G:H5" | 2.41 | 0.50 |
| 23:BB:1799:G:C5 | 25:BC:175:LEU:HD13 | 2.46 | 0.50 |
| 23:BB:1857:G:H2' | 23:BB:1884:G:H22 | 1.75 | 0.50 |
| 23:BB:1998:A:OP2 | 26:BD:141:ARG:NH2 | 2.43 | 0.50 |
| 23:BB:2460:U:H6 | 23:BB:2460:U:O5' | 1.94 | 0.50 |
| 23:BB:257:C:H2' | 23:BB:258:G:O4' | 2.10 | 0.50 |
| 23:BB:2674:G:H4' | 32:BK:30:ARG:HG3 | 1.93 | 0.50 |
| 23:BB:693:A:H2' | 23:BB:694:U:C6 | 2.47 | 0.50 |
| 23:BB:968:C:H2' | 23:BB:969:G:C8 | 2.44 | 0.50 |
| 28:BF:71:LYS:O | 28:BF:72:SER:HB3 | 2.11 | 0.50 |
| 22:BA:43:C:O2' | 28:BF:91:ARG:HD2 | 2.11 | 0.50 |
| 29:BG:140:ILE:HA | 29:BG:143:VAL:CG2 | 2.41 | 0.50 |
| 32:BK:115:ILE:HG23 | 32:BK:116:ILE:N | 2.26 | 0.50 |
| 33:BL:131:ALA:O | 33:BL:134:ALA:HB3 | 2.12 | 0.50 |
| 33:BL:95:LEU:H | 33:BL:95:LEU:HD12 | 1.76 | 0.50 |
| 34:BM:42:THR:O | 34:BM:45:GLN:HB2 | 2.12 | 0.50 |
| 23:BB:200:U:O2' | 46:BZ:22:LEU:HD12 | 2.11 | 0.50 |
| 1:CA:1101:A:H4' | 1:CA:1102:A:O5' | 2.11 | 0.50 |
| 1:CA:1500:A:H2' | 1:CA:1501:C:H5' | 1.93 | 0.50 |
| 1:CA:547:A:H4' | 1:CA:548:G:O5' | 2.11 | 0.50 |
| 1:CA:586:C:O2' | 1:CA:878:A:H4' | 2.11 | 0.50 |
| 1:CA:807:A:H2' | 1:CA:808:C:C6 | 2.47 | 0.50 |
| 1:CA:974:A:H8 | 1:CA:974:A:OP1 | 1.93 | 0.50 |
| 20:CB:143:LEU:HB3 | 20:CB:147:LEU:HD12 | 1.94 | 0.50 |
| 20:CB:83:ALA:HA | 20:CB:88:GLN:NE2 | 2.26 | 0.50 |
| 2:CC:161:ILE:N | 2:CC:161:ILE:HD12 | 2.26 | 0.50 |
| 2:CC:96:VAL:HB | 2:CC:97:PRO:HD2 | 1.93 | 0.50 |
| 4:CE:35:LEU:HD22 | 4:CE:133:ILE:HA | 1.94 | 0.50 |
| 4:CE:87:VAL:HG23 | 4:CE:92:ARG:HA | 1.93 | 0.50 |
| 16:CQ:39:ARG:HG3 | 16:CQ:39:ARG:HH11 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1930:G:H2' | 23:DB:1968:G:N1 | 2.26 | 0.50 |
| 23:DB:230:G:H2' | 23:DB:231:A:H8 | 1.75 | 0.50 |
| 23:DB:2544:G:O2' | 23:DB:2545:G:H5' | 2.11 | 0.50 |
| 23:DB:2567:G:H2' | 23:DB:2568:U:C6 | 2.46 | 0.50 |
| 23:DB:2798:U:H5'' | 23:DB:2799:A:OP1 | 2.11 | 0.50 |
| 23:DB:2811:G:O2' | 23:DB:2812:G:H5' | 2.11 | 0.50 |
| 23:DB:2875:C:H2' | 23:DB:2876:G:C8 | 2.46 | 0.50 |
| 25:DC:128:THR:CA | 25:DC:190:THR:HG22 | 2.36 | 0.50 |
| 25:DC:209:ALA:HA | 25:DC:212:TRP:CE2 | 2.47 | 0.50 |
| 27:DE:1:MET:HB3 | 27:DE:14:VAL:O | 2.11 | 0.50 |
| 27:DE:48:THR:HG23 | 27:DE:51:GLU:OE2 | 2.10 | 0.50 |
| 30:DH:114:GLU:CB | 30:DH:133:GLN:HG3 | 2.40 | 0.50 |
| 31:DJ:57:LEU:CD2 | 31:DJ:128:ASN:HA | 2.40 | 0.50 |
| 32:DK:4:GLU:OE2 | 32:DK:23:LYS:HD2 | 2.11 | 0.50 |
| 23:DB:832:U:O2 | 33:DL:52:GLY:HA2 | 2.11 | 0.50 |
| 36:DO:111:ARG:HG2 | 36:DO:117:PHE:CZ | 2.47 | 0.50 |
| 37:DP:112:ARG:HB2 | 37:DP:112:ARG:NH1 | 2.27 | 0.50 |
| 42:DU:73:ASN:C | 42:DU:75:ALA:H | 2.15 | 0.50 |
| 42:DU:80:ASP:HB2 | 42:DU:95:PHE:HD2 | 1.75 | 0.50 |
| 45:DY:37:ARG:HG2 | 45:DY:43:ILE:CD1 | 2.42 | 0.50 |
| 1:AA:1006:G:H2' | 1:AA:1007:U:C6 | 2.46 | 0.50 |
| 1:AA:1097:C:H2' | 1:AA:1098:C:C6 | 2.46 | 0.50 |
| 1:AA:1150:A:H4' | 9:AJ:43:PRO:HB3 | 1.94 | 0.50 |
| 1:AA:1150:A:O2' | 1:AA:1151:A:H5' | 2.12 | 0.50 |
| 1:AA:1379:G:O2' | 1:AA:1380:U:H5' | 2.11 | 0.50 |
| 1:AA:1493:A:H1' | 54:AA:2059:HYG:N36 | 2.19 | 0.50 |
| 1:AA:1515:G:O2' | 1:AA:1516:G:H5' | 2.11 | 0.50 |
| 1:AA:1521:C:H2' | 1:AA:1522:U:H6 | 1.75 | 0.50 |
| 1:AA:239:U:H5' | 1:AA:239:U:H6 | 1.74 | 0.50 |
| 1:AA:734:G:H2' | 1:AA:735:C:H6 | 1.76 | 0.50 |
| 20:AB:116:LEU:HA | 20:AB:119:GLN:HG3 | 1.93 | 0.50 |
| 2:AC:57:GLU:O | 2:AC:63:ILE:HA | 2.10 | 0.50 |
| 12:AM:15:VAL:O | 12:AM:19:THR:HG23 | 2.11 | 0.50 |
| 15:AP:39:PHE:CG | 15:AP:40:ASN:N | 2.79 | 0.50 |
| 21:AU:20:ARG:HD2 | 21:AU:20:ARG:N | 2.27 | 0.50 |
| 23:BB:839:U:H1' | 23:BB:1191:G:H1' | 1.94 | 0.50 |
| 23:BB:1197:G:H2' | 23:BB:1198:U:H6 | 1.75 | 0.50 |
| 23:BB:137:U:H2' | 23:BB:138:U:O4' | 2.10 | 0.50 |
| 23:BB:1439:A:N7 | 23:BB:1440:U:N1 | 2.59 | 0.50 |
| 23:BB:163:C:O2 | 23:BB:163:C:O4' | 2.25 | 0.50 |
| 23:BB:1838:C:H4' | 23:BB:1839:G:H8 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:1881:C:H2' | 23:BB:1882:U:O4' | 2.10 | 0.50 |
| 23:BB:2137:U:H2' | 23:BB:2138:G:O4' | 2.11 | 0.50 |
| 23:BB:2189:U:O2' | 23:BB:2190:G:H5' | 2.12 | 0.50 |
| 23:BB:2298:A:H2' | 23:BB:2299:U:O4' | 2.12 | 0.50 |
| 23:BB:201:C:H1' | 23:BB:250:G:O6 | 2.11 | 0.50 |
| 23:BB:2657:A:H2' | 23:BB:2658:C:O4' | 2.10 | 0.50 |
| 23:BB:2684:U:H2' | 23:BB:2685:G:O4' | 2.11 | 0.50 |
| 23:BB:2747:G:H2' | 23:BB:2748:A:C8 | 2.46 | 0.50 |
| 23:BB:2867:G:N3 | 23:BB:2867:G:C2' | 2.74 | 0.50 |
| 23:BB:305:C:H2' | 23:BB:306:U:C6 | 2.45 | 0.50 |
| 23:BB:41:C:H2' | 23:BB:42:A:C8 | 2.45 | 0.50 |
| 23:BB:850:U:O2' | 45:BY:22:THR:HG22 | 2.11 | 0.50 |
| 25:BC:142:ASN:O | 25:BC:142:ASN:CG | 2.49 | 0.50 |
| 25:BC:161:VAL:O | 25:BC:162:GLN:HB2 | 2.11 | 0.50 |
| 25:BC:43:ASN:HD22 | 25:BC:44:ASN:H | 1.59 | 0.50 |
| 29:BG:26:LYS:HG2 | 29:BG:27:GLY:N | 2.25 | 0.50 |
| 30:BH:72:ILE:HG13 | 30:BH:75:LEU:HD21 | 1.92 | 0.50 |
| 52:BI:11:GLN:O | 52:BI:11:GLN:HG3 | 2.10 | 0.50 |
| 52:BI:23:VAL:HG23 | 52:BI:24:GLY:H | 1.76 | 0.50 |
| 31:BJ:57:LEU:CD2 | 31:BJ:128:ASN:HA | 2.41 | 0.50 |
| 42:BU:21:ARG:HG3 | 42:BU:21:ARG:HH11 | 1.76 | 0.50 |
| 24:BV:51:GLN:HB2 | 24:BV:57:TYR:OH | 2.10 | 0.50 |
| 43:BW:17:ALA:HA | 43:BW:35:ILE:CG2 | 2.40 | 0.50 |
| 45:BY:23:LEU:CD1 | 45:BY:28:LEU:HB2 | 2.41 | 0.50 |
| 1:CA:1017:U:H2' | 1:CA:1018:G:C8 | 2.45 | 0.50 |
| 1:CA:1258:G:O2' | 1:CA:1259:C:H5' | 2.10 | 0.50 |
| 1:CA:34:C:H2' | 1:CA:35:G:H8 | 1.76 | 0.50 |
| 1:CA:663:A:O3' | 17:CR:52:ARG:NH2 | 2.43 | 0.50 |
| 4:CE:80:LEU:HA | 4:CE:146:MET:HE1 | 1.93 | 0.50 |
| 4:CE:35:LEU:HD21 | 4:CE:136:VAL:HG11 | 1.93 | 0.50 |
| 7:CH:7:ALA:O | 7:CH:11:THR:HG23 | 2.11 | 0.50 |
| 10:CK:33:ILE:HG12 | 10:CK:69:CYS:SG | 2.51 | 0.50 |
| 1:CA:720:C:OP1 | 17:CR:40:PRO:HG3 | 2.11 | 0.50 |
| 48:D1:6:GLU:HB2 | 48:D1:52:LYS:HZ3 | 1.77 | 0.50 |
| 22:DA:60:C:H2' | 22:DA:61:G:H8 | 1.77 | 0.50 |
| 23:DB:1140:C:H2' | 23:DB:1141:U:H5' | 1.94 | 0.50 |
| 23:DB:1197:G:O2' | 23:DB:1198:U:H5' | 2.12 | 0.50 |
| 23:DB:1881:C:H2' | 23:DB:1882:U:O4' | 2.12 | 0.50 |
| 23:DB:2515:C:H2' | 23:DB:2516:A:H8 | 1.76 | 0.50 |
| 23:DB:2543:G:H2' | 23:DB:2544:G:C8 | 2.46 | 0.50 |
| 23:DB:358:U:H2' | 23:DB:359:G:C8 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:425:G:O2' | 23:DB:426:C:H5' | 2.12 | 0.50 |
| 23:DB:591:U:H1' | 50:D3:1:PRO:H2 | 1.76 | 0.50 |
| 23:DB:920:A:H2' | 23:DB:921:C:H6 | 1.76 | 0.50 |
| 30:DH:113:SER:N | 30:DH:132:PHE:CZ | 2.79 | 0.50 |
| 30:DH:48:GLU:HA | 30:DH:51:ARG:NE | 2.26 | 0.50 |
| 36:DO:56:LYS:O | 36:DO:57:ALA:C | 2.49 | 0.50 |
| 41:DT:4:GLU:OE1 | 41:DT:5:GLU:HG2 | 2.11 | 0.50 |
| 42:DU:94:PHE:HA | 42:DU:101:THR:HA | 1.93 | 0.50 |
| 24:DV:16:ALA:CA | 24:DV:19:ARG:HH21 | 2.24 | 0.50 |
| 43:DW:27:GLY:O | 43:DW:63:ASP:HA | 2.11 | 0.50 |
| 43:DW:9:THR:HG23 | 43:DW:10:ARG:CD | 2.34 | 0.50 |
| 44:DX:13:GLU:HA | 44:DX:16:THR:OG1 | 2.11 | 0.50 |
| 1:AA:1291:U:H2' | 1:AA:1292:G:C8 | 2.46 | 0.50 |
| 1:AA:1389:C:H2' | 1:AA:1390:U:C6 | 2.47 | 0.50 |
| 1:AA:531:U:H3 | 1:AA:1208:C:C5' | 2.24 | 0.50 |
| 1:AA:974:A:H8 | 1:AA:974:A:OP1 | 1.95 | 0.50 |
| 1:AA:1074:G:C4' | 20:AB:102:ASN:HB2 | 2.42 | 0.50 |
| 20:AB:46:VAL:O | 20:AB:49:PHE:HB2 | 2.12 | 0.50 |
| 20:AB:68:PHE:HE1 | 20:AB:88:GLN:HB3 | 1.77 | 0.50 |
| 3:AD:48:SER:O | 3:AD:52:VAL:HG23 | 2.11 | 0.50 |
| 5:AF:51:ILE:O | 5:AF:51:ILE:HG23 | 2.11 | 0.50 |
| 6:AG:74:VAL:HG12 | 6:AG:87:PRO:HB3 | 1.93 | 0.50 |
| 7:AH:17:GLN:OE1 | 7:AH:69:ALA:HB1 | 2.11 | 0.50 |
| 8:AI:32:ARG:NH1 | 8:AI:37:TYR:HA | 2.27 | 0.50 |
| 10:AK:106:ILE:HG13 | 10:AK:107:THR:N | 2.22 | 0.50 |
| 11:AL:42:LYS:HB3 | 11:AL:44:PRO:HD2 | 1.93 | 0.50 |
| 14:AO:16:ARG:HH11 | 14:AO:16:ARG:HA | 1.75 | 0.50 |
| 15:AP:12:LYS:HD2 | 15:AP:13:LYS:HG3 | 1.93 | 0.50 |
| 1:AA:720:C:OP1 | 17:AR:40:PRO:HG3 | 2.12 | 0.50 |
| 22:BA:109:A:H2' | 22:BA:110:C:O4' | 2.11 | 0.50 |
| 23:BB:175:G:O2' | 23:BB:176:A:H5' | 2.11 | 0.50 |
| 23:BB:1820:U:H4' | 23:BB:1821:A:OP2 | 2.12 | 0.50 |
| 23:BB:1886:U:H2' | 23:BB:1887:C:C6 | 2.46 | 0.50 |
| 23:BB:2450:A:O2' | 23:BB:2451:A:H5' | 2.11 | 0.50 |
| 23:BB:2811:G:O2' | 23:BB:2812:G:H5' | 2.10 | 0.50 |
| 23:BB:2849:U:N3 | 23:BB:2867:G:C8 | 2.79 | 0.50 |
| 23:BB:58:G:N3 | 23:BB:73:A:H2 | 2.09 | 0.50 |
| 25:BC:136:VAL:HG12 | 25:BC:137:GLY:N | 2.26 | 0.50 |
| 25:BC:221:GLY:O | 25:BC:224:MET:HG3 | 2.11 | 0.50 |
| 29:BG:102:ILE:HG13 | 29:BG:116:LEU:HD11 | 1.94 | 0.50 |
| 31:BJ:64:VAL:O | 31:BJ:68:LYS:HD2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BL:57:LEU:C | 33:BL:59:ARG:H | 2.14 | 0.50 |
| 36:BO:110:ALA:HA | 36:BO:113:ALA:HB3 | 1.93 | 0.50 |
| 38:BQ:90:ASP:O | 38:BQ:94:LEU:HB2 | 2.10 | 0.50 |
| 40:BS:24:ILE:CD1 | 40:BS:36:LEU:HD21 | 2.41 | 0.50 |
| 42:BU:78:LYS:CD | 42:BU:79:ALA:H | 2.24 | 0.50 |
| 43:BW:23:LYS:CG | 43:BW:24:ARG:N | 2.75 | 0.50 |
| 43:BW:46:ALA:HB2 | 43:BW:78:PHE:HD1 | 1.76 | 0.50 |
| 1:CA:1029:U:O3' | 1:CA:1030:U:H3' | 2.11 | 0.50 |
| 1:CA:1124:G:H5'' | 9:CJ:37:ARG:O | 2.12 | 0.50 |
| 1:CA:1125:U:HO2' | 1:CA:1126:U:H2' | 1.75 | 0.50 |
| 1:CA:1150:A:H4' | 9:CJ:43:PRO:HB3 | 1.93 | 0.50 |
| 1:CA:1151:A:O2' | 1:CA:1152:A:H8 | 1.94 | 0.50 |
| 1:CA:1220:G:H2' | 1:CA:1221:G:H8 | 1.76 | 0.50 |
| 1:CA:560:A:H4' | 1:CA:561:U:H5'' | 1.92 | 0.50 |
| 1:CA:957:U:O2 | 1:CA:959:A:H8 | 1.94 | 0.50 |
| 2:CC:106:ARG:HH11 | 2:CC:106:ARG:HG2 | 1.77 | 0.50 |
| 6:CG:29:LEU:O | 6:CG:29:LEU:HD23 | 2.11 | 0.50 |
| 6:CG:42:VAL:O | 6:CG:46:LEU:HB2 | 2.11 | 0.50 |
| 8:CI:52:GLU:O | 8:CI:53:LEU:HD13 | 2.11 | 0.50 |
| 1:CA:779:C:H5'' | 10:CK:123:PRO:HB3 | 1.93 | 0.50 |
| 1:CA:538:G:OP2 | 11:CL:111:GLN:HB2 | 2.11 | 0.50 |
| 11:CL:33:CYS:H | 11:CL:54:VAL:HG13 | 1.75 | 0.50 |
| 17:CR:23:LYS:HG3 | 17:CR:24:ASP:N | 2.26 | 0.50 |
| 18:CS:39:ILE:HG21 | 18:CS:61:VAL:HG13 | 1.93 | 0.50 |
| 50:D3:16:THR:C | 50:D3:18:LYS:H | 2.14 | 0.50 |
| 23:DB:2421:G:N7 | 50:D3:30:HIS:NE2 | 2.58 | 0.50 |
| 22:DA:7:G:O2' | 22:DA:8:C:H5' | 2.11 | 0.50 |
| 23:DB:1060:U:O2 | 23:DB:1088:A:C8 | 2.64 | 0.50 |
| 23:DB:1511:G:H2' | 23:DB:1512:C:H6 | 1.75 | 0.50 |
| 23:DB:1796:U:O2' | 23:DB:1797:G:H5' | 2.11 | 0.50 |
| 23:DB:1858:A:H2' | 23:DB:1859:U:O4' | 2.11 | 0.50 |
| 23:DB:2072:C:O2' | 23:DB:2073:C:H5' | 2.11 | 0.50 |
| 23:DB:2849:U:H4' | 23:DB:2850:A:H5' | 1.93 | 0.50 |
| 23:DB:2872:A:H1' | 23:DB:2873:A:C8 | 2.46 | 0.50 |
| 23:DB:588:U:H2' | 23:DB:589:U:C6 | 2.46 | 0.50 |
| 25:DC:173:LEU:N | 25:DC:173:LEU:HD13 | 2.25 | 0.50 |
| 25:DC:246:PRO:HB2 | 25:DC:247:TRP:CZ3 | 2.46 | 0.50 |
| 27:DE:170:ARG:NH2 | 27:DE:176:ASP:HB2 | 2.26 | 0.50 |
| 28:DF:91:ARG:O | 28:DF:92:GLY:C | 2.49 | 0.50 |
| 52:DI:2:LYS:C | 52:DI:3:LYS:HD2 | 2.32 | 0.50 |
| 32:DK:10:VAL:HG21 | 32:DK:16:ALA:HA | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DL:47:ARG:HH21 | 33:DL:47:ARG:HB3 | 1.76 | 0.50 |
| 1:AA:1243:C:O2' | 1:AA:1244:G:H5' | 2.11 | 0.50 |
| 1:AA:137:U:H2' | 1:AA:138:G:H8 | 1.75 | 0.50 |
| 1:AA:1500:A:C2' | 1:AA:1501:C:H5' | 2.41 | 0.50 |
| 1:AA:193:C:H2' | 1:AA:194:C:H6 | 1.75 | 0.50 |
| 1:AA:600:A:OP2 | 7:AH:87:ARG:HG2 | 2.11 | 0.50 |
| 1:AA:602:A:O2' | 1:AA:603:U:H5' | 2.11 | 0.50 |
| 1:AA:634:C:H2' | 1:AA:635:A:H8 | 1.76 | 0.50 |
| 3:AD:7:LYS:HB2 | 3:AD:21:LYS:HE2 | 1.94 | 0.50 |
| 5:AF:18:VAL:HG21 | 5:AF:58:HIS:CE1 | 2.46 | 0.50 |
| 10:AK:83:VAL:HG22 | 10:AK:106:ILE:HD11 | 1.93 | 0.50 |
| 10:AK:95:THR:HG23 | 10:AK:96:ILE:N | 2.27 | 0.50 |
| 12:AM:106:ARG:HD3 | 12:AM:111:PRO:HA | 1.94 | 0.50 |
| 12:AM:36:ALA:HB1 | 12:AM:54:THR:HB | 1.92 | 0.50 |
| 50:B3:16:THR:C | 50:B3:18:LYS:H | 2.15 | 0.50 |
| 22:BA:76:G:H1 | 22:BA:101:A:N6 | 2.10 | 0.50 |
| 23:BB:1083:U:H2' | 23:BB:1085:A:OP2 | 2.11 | 0.50 |
| 23:BB:1150:C:O2' | 23:BB:1151:A:H5' | 2.11 | 0.50 |
| 23:BB:1199:U:H2' | 23:BB:1200:C:H6 | 1.76 | 0.50 |
| 23:BB:130:C:O2' | 23:BB:131:A:H5' | 2.11 | 0.50 |
| 23:BB:1374:G:H2' | 23:BB:1375:U:C6 | 2.47 | 0.50 |
| 23:BB:406:G:O2' | 23:BB:407:G:H5' | 2.12 | 0.50 |
| 23:BB:455:C:N3 | 23:BB:473:G:H5' | 2.26 | 0.50 |
| 23:BB:519:U:H2' | 23:BB:520:G:H8 | 1.77 | 0.50 |
| 23:BB:581:C:H2' | 23:BB:582:A:H8 | 1.77 | 0.50 |
| 23:BB:931:U:H3 | 23:BB:1166:G:H21 | 1.60 | 0.50 |
| 27:BE:48:THR:C | 27:BE:50:ALA:H | 2.13 | 0.50 |
| 28:BF:107:VAL:N | 28:BF:108:PRO:CD | 2.75 | 0.50 |
| 28:BF:1:ALA:O | 28:BF:4:HIS:HB3 | 2.11 | 0.50 |
| 31:BJ:48:VAL:HG12 | 31:BJ:50:THR:HG23 | 1.94 | 0.50 |
| 32:BK:105:ARG:H | 32:BK:105:ARG:CD | 2.24 | 0.50 |
| 34:BM:90:GLU:HA | 34:BM:90:GLU:OE1 | 2.12 | 0.50 |
| 37:BP:25:VAL:HA | 37:BP:85:VAL:C | 2.32 | 0.50 |
| 42:BU:81:ARG:HB2 | 42:BU:96:LYS:HG2 | 1.92 | 0.50 |
| 24:BV:89:ILE:HD12 | 24:BV:89:ILE:O | 2.12 | 0.50 |
| 1:CA:1219:A:H2' | 1:CA:1220:G:C8 | 2.46 | 0.50 |
| 20:CB:127:LYS:HD2 | 20:CB:128:LEU:HD13 | 1.94 | 0.50 |
| 3:CD:96:ARG:NH1 | 3:CD:133:SER:HA | 2.25 | 0.50 |
| 5:CF:73:GLU:O | 5:CF:77:THR:HG23 | 2.12 | 0.50 |
| 8:CI:20:ILE:HD12 | 8:CI:20:ILE:N | 2.24 | 0.50 |
| 12:CM:29:SER:O | 12:CM:33:LEU:HG | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CN:26:LEU:HA | 13:CN:29:ILE:HB | 1.94 | 0.50 |
| 13:CN:60:ARG:HE | 13:CN:62:ARG:HG2 | 1.76 | 0.50 |
| 14:CO:55:LEU:O | 14:CO:59:VAL:HG23 | 2.11 | 0.50 |
| 17:CR:42:ARG:HG3 | 17:CR:43:ILE:N | 2.27 | 0.50 |
| 18:CS:35:ARG:HB3 | 18:CS:50:VAL:HG13 | 1.91 | 0.50 |
| 22:DA:3:C:H2' | 22:DA:4:C:C6 | 2.47 | 0.50 |
| 22:DA:43:C:O2' | 28:DF:91:ARG:HD2 | 2.12 | 0.50 |
| 23:DB:1064:C:H5'' | 52:DI:87:SER:OG | 2.11 | 0.50 |
| 23:DB:1099:G:H3' | 52:DI:2:LYS:HA | 1.93 | 0.50 |
| 23:DB:1210:G:C5' | 23:DB:1212:G:H5'' | 2.42 | 0.50 |
| 23:DB:1229:C:H2' | 23:DB:1230:A:C8 | 2.47 | 0.50 |
| 23:DB:1794:A:O2' | 23:DB:1795:C:H5' | 2.12 | 0.50 |
| 23:DB:204:A:H4' | 23:DB:205:G:OP1 | 2.11 | 0.50 |
| 23:DB:288:U:C2' | 23:DB:289:G:H5' | 2.41 | 0.50 |
| 23:DB:490:C:H3' | 23:DB:491:G:H5'' | 1.94 | 0.50 |
| 26:DD:148:GLN:HG3 | 26:DD:152:PRO:CB | 2.42 | 0.50 |
| 28:DF:33:ILE:HG12 | 28:DF:155:ILE:HG13 | 1.94 | 0.50 |
| 28:DF:71:LYS:O | 28:DF:72:SER:HB3 | 2.11 | 0.50 |
| 29:DG:116:LEU:HD23 | 29:DG:121:THR:HA | 1.94 | 0.50 |
| 29:DG:26:LYS:CA | 29:DG:32:LEU:H | 2.16 | 0.50 |
| 31:DJ:36:LEU:HD13 | 31:DJ:121:LYS:HE3 | 1.93 | 0.50 |
| 35:DN:55:ALA:HA | 35:DN:80:PHE:CE1 | 2.47 | 0.50 |
| 41:DT:57:VAL:HG22 | 41:DT:58:VAL:N | 2.20 | 0.50 |
| 41:DT:66:LYS:N | 41:DT:76:ARG:NH2 | 2.59 | 0.50 |
| 30:DH:27:ARG:CZ | 46:DZ:60:ASP:HA | 2.41 | 0.50 |
| 1:AA:1029:U:H5'' | 1:AA:1030:U:C5 | 2.47 | 0.50 |
| 1:AA:1118:U:H1' | 1:AA:1179:A:C4 | 2.47 | 0.50 |
| 1:AA:114:U:H2' | 1:AA:115:G:C8 | 2.47 | 0.50 |
| 1:AA:390:U:H2' | 1:AA:391:G:H8 | 1.76 | 0.50 |
| 20:AB:10:LYS:O | 20:AB:13:VAL:HG23 | 2.12 | 0.50 |
| 3:AD:149:LYS:HB2 | 3:AD:177:MET:HG3 | 1.94 | 0.50 |
| 6:AG:67:ASN:HB2 | 6:AG:134:VAL:HG12 | 1.93 | 0.50 |
| 6:AG:21:LEU:HG | 6:AG:22:LEU:H | 1.76 | 0.50 |
| 12:AM:17:ALA:HB2 | 12:AM:44:ILE:HD11 | 1.93 | 0.50 |
| 14:AO:80:LEU:O | 14:AO:84:LEU:HD13 | 2.11 | 0.50 |
| 17:AR:42:ARG:HG3 | 17:AR:43:ILE:N | 2.27 | 0.50 |
| 23:BB:1163:G:O2' | 23:BB:1164:C:H5' | 2.12 | 0.50 |
| 23:BB:1403:A:H2' | 23:BB:1404:C:C6 | 2.46 | 0.50 |
| 23:BB:1482:G:H2' | 23:BB:1483:G:H8 | 1.76 | 0.50 |
| 23:BB:2072:C:O2' | 23:BB:2073:C:H5' | 2.12 | 0.50 |
| 23:BB:219:A:O2' | 23:BB:220:G:H5' | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:338:G:N2 | 23:BB:339:U:H1' | 2.26 | 0.50 |
| 25:BC:90:ILE:HD12 | 25:BC:102:TYR:HB3 | 1.93 | 0.50 |
| 26:BD:104:VAL:HA | 26:BD:106:LYS:HZ1 | 1.77 | 0.50 |
| 27:BE:5:LEU:CD1 | 27:BE:10:SER:HB2 | 2.41 | 0.50 |
| 23:BB:626:A:H2' | 33:BL:78:ARG:NH1 | 2.27 | 0.50 |
| 35:BN:38:LEU:CB | 35:BN:39:PRO:HD3 | 2.37 | 0.50 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:C6 | 2.46 | 0.50 |
| 1:CA:1459:G:H2' | 1:CA:1460:C:C6 | 2.45 | 0.50 |
| 1:CA:312:C:H2' | 1:CA:313:A:H8 | 1.77 | 0.50 |
| 1:CA:724:G:O2' | 1:CA:725:G:H5' | 2.10 | 0.50 |
| 1:CA:86:G:H1' | 1:CA:87:C:O4' | 2.12 | 0.50 |
| 3:CD:55:ARG:NH1 | 3:CD:55:ARG:HG3 | 2.26 | 0.50 |
| 4:CE:87:VAL:HG22 | 4:CE:88:HIS:N | 2.26 | 0.50 |
| 6:CG:12:LEU:HD22 | 6:CG:13:PRO:HD2 | 1.94 | 0.50 |
| 12:CM:3:ILE:HD12 | 12:CM:9:PRO:HD2 | 1.93 | 0.50 |
| 48:D1:6:GLU:HB2 | 48:D1:52:LYS:CE | 2.42 | 0.50 |
| 23:DB:1047:G:H1' | 23:DB:1111:A:N6 | 2.27 | 0.50 |
| 23:DB:1779:U:C5 | 23:DB:1784:A:N7 | 2.79 | 0.50 |
| 23:DB:1812:U:O2' | 25:DC:43:ASN:ND2 | 2.44 | 0.50 |
| 23:DB:1841:U:C2 | 23:DB:1842:G:C8 | 3.00 | 0.50 |
| 23:DB:1857:G:H2' | 23:DB:1884:G:H22 | 1.76 | 0.50 |
| 23:DB:2294:G:P | 36:DO:94:ARG:HH11 | 2.35 | 0.50 |
| 23:DB:2341:G:H2' | 23:DB:2342:C:C6 | 2.46 | 0.50 |
| 23:DB:279:A:N6 | 23:DB:361:G:O2' | 2.44 | 0.50 |
| 23:DB:41:C:H2' | 23:DB:42:A:C8 | 2.45 | 0.50 |
| 23:DB:475:C:H4' | 23:DB:509:C:H2' | 1.94 | 0.50 |
| 23:DB:688:U:O2' | 23:DB:689:A:H5' | 2.12 | 0.50 |
| 23:DB:696:G:O2' | 23:DB:697:G:H5' | 2.11 | 0.50 |
| 26:DD:56:LYS:HG3 | 26:DD:58:ASN:HB2 | 1.93 | 0.50 |
| 27:DE:5:LEU:CD1 | 27:DE:10:SER:HB2 | 2.42 | 0.50 |
| 27:DE:67:ARG:HD2 | 27:DE:68:ALA:O | 2.11 | 0.50 |
| 12:CM:70:ARG:CZ | 28:DF:142:TYR:HB2 | 2.42 | 0.50 |
| 52:DI:1:ALA:C | 52:DI:2:LYS:HD2 | 2.32 | 0.50 |
| 34:DM:73:ILE:HG13 | 34:DM:93:VAL:HB | 1.94 | 0.50 |
| 38:DQ:80:ASN:ND2 | 38:DQ:81:GLY:H | 2.09 | 0.50 |
| 39:DR:19:THR:CG2 | 39:DR:97:LYS:HD2 | 2.42 | 0.50 |
| 39:DR:16:GLU:CA | 39:DR:98:ILE:HG22 | 2.39 | 0.50 |
| 41:DT:68:LYS:O | 41:DT:69:ARG:CB | 2.59 | 0.50 |
| 41:DT:9:LYS:HG2 | 41:DT:9:LYS:O | 2.12 | 0.50 |
| 24:DV:30:ILE:HG23 | 24:DV:72:VAL:HG11 | 1.92 | 0.50 |
| 1:AA:452:A:H2' | 1:AA:453:G:O4' | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:767:A:H2' | 1:AA:768:A:C8 | 2.47 | 0.50 |
| 2:AC:146:LYS:HD3 | 2:AC:204:GLY:HA2 | 1.92 | 0.50 |
| 3:AD:16:THR:HG22 | 3:AD:17:ASP:N | 2.27 | 0.50 |
| 8:AI:109:GLN:NE2 | 8:AI:110:VAL:H | 2.09 | 0.50 |
| 12:AM:21:ILE:HG22 | 12:AM:23:GLY:H | 1.76 | 0.50 |
| 12:AM:29:SER:O | 12:AM:33:LEU:HG | 2.12 | 0.50 |
| 17:AR:42:ARG:HG3 | 17:AR:43:ILE:H | 1.76 | 0.50 |
| 18:AS:39:ILE:HG21 | 18:AS:61:VAL:HG13 | 1.92 | 0.50 |
| 47:B0:47:TYR:O | 47:B0:48:TYR:HB2 | 2.11 | 0.50 |
| 23:BB:1117:C:H2' | 23:BB:1118:C:C6 | 2.46 | 0.50 |
| 23:BB:1141:U:H5'' | 31:BJ:27:ARG:HH21 | 1.76 | 0.50 |
| 23:BB:1563:U:O2' | 23:BB:1564:C:H5' | 2.11 | 0.50 |
| 23:BB:2269:G:H4' | 43:BW:19:ARG:NH1 | 2.22 | 0.50 |
| 23:BB:2577:A:H5'' | 23:BB:2578:G:H5' | 1.94 | 0.50 |
| 23:BB:588:U:H2' | 23:BB:589:U:C6 | 2.46 | 0.50 |
| 23:BB:671:C:O2' | 23:BB:672:C:H5' | 2.12 | 0.50 |
| 23:BB:692:C:H2' | 23:BB:693:A:H8 | 1.77 | 0.50 |
| 23:BB:784:G:OP1 | 23:BB:2588:G:H5'' | 2.12 | 0.50 |
| 26:BD:106:LYS:O | 26:BD:107:VAL:HB | 2.12 | 0.50 |
| 26:BD:10:GLY:O | 26:BD:11:MET:HB2 | 2.11 | 0.50 |
| 26:BD:9:VAL:HG13 | 26:BD:9:VAL:O | 2.11 | 0.50 |
| 28:BF:134:GLN:O | 28:BF:136:ILE:N | 2.44 | 0.50 |
| 28:BF:47:LYS:HA | 28:BF:50:ASP:OD1 | 2.11 | 0.50 |
| 32:BK:34:GLY:O | 32:BK:36:GLY:N | 2.44 | 0.50 |
| 34:BM:35:ALA:O | 34:BM:36:VAL:HB | 2.12 | 0.50 |
| 36:BO:7:ARG:O | 36:BO:96:GLY:HA3 | 2.11 | 0.50 |
| 37:BP:31:VAL:O | 37:BP:32:VAL:HG12 | 2.12 | 0.50 |
| 38:BQ:63:ARG:CZ | 38:BQ:96:ASP:HA | 2.41 | 0.50 |
| 42:BU:11:ILE:HA | 42:BU:21:ARG:HG2 | 1.94 | 0.50 |
| 24:BV:53:LYS:HD2 | 24:BV:55:GLU:OE1 | 2.12 | 0.50 |
| 23:BB:2355:G:O3' | 43:BW:20:LEU:HD13 | 2.11 | 0.50 |
| 1:CA:9:G:H2' | 1:CA:10:A:H8 | 1.77 | 0.50 |
| 1:CA:1254:A:H2' | 1:CA:1255:G:C8 | 2.47 | 0.50 |
| 1:CA:1530:G:H2' | 1:CA:1531:A:H8 | 1.77 | 0.50 |
| 1:CA:216:U:H2' | 1:CA:217:C:C6 | 2.47 | 0.50 |
| 1:CA:399:G:H2' | 1:CA:400:C:C6 | 2.47 | 0.50 |
| 1:CA:453:G:H2' | 1:CA:454:G:C8 | 2.47 | 0.50 |
| 1:CA:643:C:H2' | 1:CA:644:U:H6 | 1.77 | 0.50 |
| 4:CE:95:MET:HA | 4:CE:124:ALA:HB2 | 1.94 | 0.50 |
| 6:CG:3:ARG:HG3 | 6:CG:3:ARG:HH11 | 1.76 | 0.50 |
| 13:CN:11:LYS:N | 13:CN:11:LYS:HZ3 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:CO:16:ARG:HA | 14:CO:16:ARG:HH11 | 1.76 | 0.50 |
| 18:CS:51:HIS:HB2 | 18:CS:56:HIS:CE1 | 2.47 | 0.50 |
| 19:CT:65:LEU:HG | 19:CT:66:ILE:HD13 | 1.93 | 0.50 |
| 19:CT:66:ILE:HG23 | 19:CT:70:LYS:HB3 | 1.92 | 0.50 |
| 48:D1:29:LYS:N | 48:D1:30:PRO:HD3 | 2.26 | 0.50 |
| 23:DB:1049:C:O2 | 23:DB:1113:U:H4' | 2.12 | 0.50 |
| 23:DB:1747:U:H2' | 23:DB:1748:C:H6 | 1.76 | 0.50 |
| 23:DB:2246:G:H2' | 23:DB:2247:A:C8 | 2.47 | 0.50 |
| 23:DB:2487:G:H2' | 23:DB:2488:G:H8 | 1.77 | 0.50 |
| 23:DB:2519:U:C6 | 23:DB:2542:A:N6 | 2.80 | 0.50 |
| 23:DB:2734:A:H2' | 23:DB:2735:G:C5' | 2.40 | 0.50 |
| 23:DB:315:G:H2' | 23:DB:316:C:C6 | 2.46 | 0.50 |
| 23:DB:358:U:O5' | 23:DB:358:U:H6 | 1.94 | 0.50 |
| 23:DB:817:C:H2' | 23:DB:818:G:O4' | 2.12 | 0.50 |
| 23:DB:992:C:H2' | 23:DB:993:G:H8 | 1.76 | 0.50 |
| 26:DD:149:ASN:C | 26:DD:152:PRO:HD2 | 2.32 | 0.50 |
| 28:DF:62:GLN:HB2 | 28:DF:91:ARG:HE | 1.77 | 0.50 |
| 29:DG:42:VAL:HG23 | 29:DG:50:THR:O | 2.12 | 0.50 |
| 29:DG:51:PHE:CD2 | 29:DG:68:ARG:HG2 | 2.47 | 0.50 |
| 52:DI:128:ILE:HA | 52:DI:131:THR:CG2 | 2.41 | 0.50 |
| 52:DI:131:THR:O | 52:DI:135:MET:HG3 | 2.11 | 0.50 |
| 31:DJ:36:LEU:O | 31:DJ:51:GLY:HA3 | 2.11 | 0.50 |
| 31:DJ:52:ASP:O | 31:DJ:54:ILE:HG22 | 2.11 | 0.50 |
| 32:DK:18:ARG:O | 32:DK:45:GLU:HB2 | 2.11 | 0.50 |
| 33:DL:120:VAL:HG12 | 33:DL:121:THR:N | 2.27 | 0.50 |
| 1:AA:493:A:H3' | 1:AA:494:G:C8 | 2.47 | 0.50 |
| 1:AA:657:U:O2' | 1:AA:658:C:H5' | 2.11 | 0.50 |
| 20:AB:216:VAL:O | 20:AB:220:VAL:HG23 | 2.12 | 0.50 |
| 2:AC:139:ASN:O | 2:AC:143:LEU:HD23 | 2.11 | 0.50 |
| 3:AD:77:GLU:OE2 | 3:AD:81:LEU:HD21 | 2.12 | 0.50 |
| 3:AD:71:PHE:CE1 | 3:AD:89:LEU:HD11 | 2.46 | 0.50 |
| 4:AE:35:LEU:HD21 | 4:AE:136:VAL:HG11 | 1.93 | 0.50 |
| 4:AE:55:VAL:N | 4:AE:56:PRO:HD2 | 2.26 | 0.50 |
| 7:AH:51:GLU:HB3 | 7:AH:57:GLU:HB3 | 1.94 | 0.50 |
| 10:AK:103:GLY:HA2 | 2:CC:74:ILE:HD13 | 1.93 | 0.50 |
| 11:AL:13:ARG:HG2 | 11:AL:14:LYS:H | 1.77 | 0.50 |
| 11:AL:14:LYS:HG2 | 11:AL:15:VAL:N | 2.27 | 0.50 |
| 16:AQ:3:LYS:HE2 | 16:AQ:3:LYS:HA | 1.92 | 0.50 |
| 12:AM:82:LEU:HD11 | 18:AS:64:GLU:HB2 | 1.92 | 0.50 |
| 51:B4:4:ARG:N | 51:B4:37:GLN:HE22 | 2.09 | 0.50 |
| 23:BB:1259:G:H2' | 23:BB:1260:A:C8 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:2034:U:O2' | 23:BB:2035:G:H5' | 2.12 | 0.50 |
| 23:BB:2798:U:H5'' | 23:BB:2799:A:OP1 | 2.10 | 0.50 |
| 23:BB:598:U:H2' | 23:BB:599:A:H8 | 1.76 | 0.50 |
| 28:BF:102:LEU:HA | 28:BF:106:ALA:HB3 | 1.92 | 0.50 |
| 31:BJ:44:TYR:O | 31:BJ:45:THR:HB | 2.12 | 0.50 |
| 31:BJ:64:VAL:HG11 | 31:BJ:69:ARG:HB2 | 1.93 | 0.50 |
| 32:BK:118:LEU:O | 32:BK:120:PRO:HD2 | 2.12 | 0.50 |
| 36:BO:24:THR:O | 36:BO:90:VAL:HB | 2.12 | 0.50 |
| 1:CA:1005:A:H4' | 1:CA:1037:C:O2 | 2.12 | 0.50 |
| 1:CA:1121:U:O2' | 1:CA:1122:U:H5' | 2.11 | 0.50 |
| 1:CA:490:C:H2' | 1:CA:491:G:H8 | 1.75 | 0.50 |
| 1:CA:613:C:H2' | 1:CA:614:C:C6 | 2.46 | 0.50 |
| 1:CA:632:U:H3' | 1:CA:633:G:H5' | 1.94 | 0.50 |
| 1:CA:640:A:O2' | 1:CA:641:U:H5' | 2.12 | 0.50 |
| 1:CA:893:C:H2' | 1:CA:894:G:C8 | 2.47 | 0.50 |
| 20:CB:128:LEU:HD23 | 20:CB:132:GLU:HB3 | 1.94 | 0.50 |
| 20:CB:16:GLY:HA2 | 20:CB:40:ILE:CG1 | 2.42 | 0.50 |
| 8:CI:56:MET:O | 8:CI:57:VAL:HB | 2.10 | 0.50 |
| 9:CJ:12:ALA:CB | 9:CJ:96:VAL:HG12 | 2.41 | 0.50 |
| 15:CP:25:ARG:CD | 15:CP:25:ARG:H | 2.21 | 0.50 |
| 16:CQ:30:HIS:HE1 | 16:CQ:32:ILE:HG22 | 1.77 | 0.50 |
| 49:D2:34:ARG:NE | 49:D2:39:ARG:HG2 | 2.26 | 0.50 |
| 23:DB:132:G:O2' | 23:DB:133:U:H5' | 2.11 | 0.50 |
| 23:DB:1349:C:H2' | 23:DB:1350:C:H6 | 1.77 | 0.50 |
| 23:DB:1746:A:H2' | 23:DB:1747:U:C6 | 2.46 | 0.50 |
| 23:DB:1992:G:N2 | 23:DB:1996:C:O2' | 2.45 | 0.50 |
| 23:DB:2783:U:H2' | 23:DB:2784:U:C6 | 2.47 | 0.50 |
| 23:DB:291:G:H2' | 23:DB:292:U:C6 | 2.46 | 0.50 |
| 23:DB:704:G:H1' | 23:DB:727:A:N6 | 2.26 | 0.50 |
| 23:DB:710:U:H2' | 23:DB:711:G:H8 | 1.77 | 0.50 |
| 23:DB:968:C:H2' | 23:DB:969:G:C8 | 2.46 | 0.50 |
| 25:DC:77:VAL:HG23 | 25:DC:112:GLY:N | 2.08 | 0.50 |
| 26:DD:117:GLY:O | 26:DD:119:ALA:N | 2.44 | 0.50 |
| 28:DF:107:VAL:N | 28:DF:108:PRO:CD | 2.75 | 0.50 |
| 23:DB:2305:U:H4' | 28:DF:132:ARG:NE | 2.27 | 0.50 |
| 28:DF:134:GLN:O | 28:DF:136:ILE:N | 2.43 | 0.50 |
| 29:DG:87:GLN:HG2 | 29:DG:164:ALA:HA | 1.94 | 0.50 |
| 29:DG:93:TYR:O | 29:DG:94:ARG:HG3 | 2.12 | 0.50 |
| 30:DH:77:THR:HG22 | 30:DH:143:ILE:HB | 1.92 | 0.50 |
| 30:DH:31:VAL:CB | 30:DH:32:PRO:HD3 | 2.33 | 0.50 |
| 52:DI:102:ARG:HG3 | 52:DI:141:ASP:HB2 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:DI:21:PRO:CB | 52:DI:22:PRO:HD3 | 2.38 | 0.50 |
| 31:DJ:104:ALA:O | 31:DJ:108:MET:HG2 | 2.12 | 0.50 |
| 36:DO:51:ALA:CB | 36:DO:81:ARG:HH11 | 2.25 | 0.50 |
| 38:DQ:81:GLY:HA3 | 38:DQ:116:LEU:CD1 | 2.42 | 0.50 |
| 39:DR:2:TYR:HB2 | 39:DR:42:ALA:CB | 2.40 | 0.50 |
| 41:DT:43:ILE:O | 41:DT:47:VAL:HG23 | 2.12 | 0.50 |
| 42:DU:78:LYS:CD | 42:DU:79:ALA:H | 2.24 | 0.50 |
| 1:AA:1081:A:O2' | 1:AA:1082:A:H5' | 2.12 | 0.50 |
| 1:AA:1432:G:O2' | 1:AA:1468:A:N6 | 2.45 | 0.50 |
| 1:AA:1451:U:O2 | 1:AA:1451:U:H2' | 2.12 | 0.50 |
| 20:AB:8:MET:HB3 | 20:AB:46:VAL:HB | 1.93 | 0.50 |
| 1:AA:1057:G:O3' | 2:AC:196:GLY:HA3 | 2.11 | 0.50 |
| 5:AF:80:PHE:CZ | 25:BC:123:ILE:HG12 | 2.47 | 0.50 |
| 8:AI:56:MET:O | 8:AI:57:VAL:HB | 2.12 | 0.50 |
| 1:AA:538:G:OP2 | 11:AL:111:GLN:HB2 | 2.12 | 0.50 |
| 1:AA:528:C:H41 | 11:AL:45:ASN:CG | 2.16 | 0.50 |
| 13:AN:61:ASN:HB3 | 13:AN:72:PHE:CE2 | 2.47 | 0.50 |
| 18:AS:20:LYS:O | 18:AS:23:GLU:HG3 | 2.11 | 0.50 |
| 22:BA:32:U:C4' | 22:BA:52:A:H62 | 2.22 | 0.50 |
| 22:BA:78:A:H2' | 22:BA:79:G:O4' | 2.12 | 0.50 |
| 23:BB:1173:U:HO2' | 23:BB:1176:U:H3 | 1.60 | 0.50 |
| 23:BB:1395:A:H4' | 23:BB:1397:U:C5 | 2.47 | 0.50 |
| 23:BB:1509:A:H5'' | 23:BB:1509:A:C8 | 2.46 | 0.50 |
| 23:BB:1742:U:H2' | 23:BB:1743:G:C8 | 2.47 | 0.50 |
| 23:BB:1794:A:H2' | 23:BB:1795:C:H6 | 1.77 | 0.50 |
| 23:BB:1817:G:OP1 | 25:BC:86:ARG:NH2 | 2.45 | 0.50 |
| 23:BB:1911:U:H2' | 23:BB:1918:A:N1 | 2.27 | 0.50 |
| 23:BB:2295:C:O2' | 23:BB:2296:U:H5' | 2.12 | 0.50 |
| 23:BB:2405:G:H1' | 23:BB:2412:A:N6 | 2.26 | 0.50 |
| 23:BB:24:G:H1' | 40:BS:77:ASP:HB3 | 1.94 | 0.50 |
| 23:BB:2519:U:C6 | 23:BB:2542:A:N6 | 2.80 | 0.50 |
| 23:BB:2527:C:O3' | 51:B4:31:PRO:HB2 | 2.12 | 0.50 |
| 23:BB:2720:U:H2' | 23:BB:2721:A:C8 | 2.47 | 0.50 |
| 23:BB:2872:A:H1' | 23:BB:2873:A:C8 | 2.47 | 0.50 |
| 23:BB:601:C:H2' | 23:BB:602:A:H8 | 1.76 | 0.50 |
| 25:BC:119:VAL:HA | 25:BC:133:ASN:ND2 | 2.27 | 0.50 |
| 29:BG:84:LYS:HG3 | 29:BG:131:VAL:HA | 1.94 | 0.50 |
| 29:BG:148:ARG:HD3 | 29:BG:152:ARG:NE | 2.27 | 0.50 |
| 34:BM:74:THR:O | 34:BM:75:GLU:HB2 | 2.11 | 0.50 |
| 36:BO:56:LYS:C | 36:BO:60:GLU:HG2 | 2.32 | 0.50 |
| 31:BJ:44:TYR:CE2 | 38:BQ:59:LEU:HD11 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:BW:50:VAL:HG23 | 43:BW:61:LYS:HE3 | 1.92 | 0.50 |
| 44:BX:18:LEU:O | 44:BX:22:LEU:HB3 | 2.12 | 0.50 |
| 45:BY:37:ARG:HG2 | 45:BY:43:ILE:CD1 | 2.42 | 0.50 |
| 1:CA:1437:A:H2' | 1:CA:1438:G:C8 | 2.46 | 0.50 |
| 1:CA:658:C:H2' | 1:CA:659:U:C6 | 2.44 | 0.50 |
| 20:CB:46:VAL:O | 20:CB:49:PHE:HB2 | 2.12 | 0.50 |
| 2:CC:149:LYS:HE3 | 2:CC:166:TRP:CH2 | 2.47 | 0.50 |
| 2:CC:14:VAL:O | 2:CC:15:LYS:HD2 | 2.11 | 0.50 |
| 4:CE:28:ARG:CZ | 4:CE:30:PHE:HB3 | 2.42 | 0.50 |
| 5:CF:5:GLU:HA | 5:CF:63:ASN:HA | 1.94 | 0.50 |
| 1:CA:1379:G:O6 | 6:CG:2:ARG:HD3 | 2.12 | 0.50 |
| 7:CH:111:THR:H | 7:CH:114:ALA:HB3 | 1.76 | 0.50 |
| 8:CI:30:ASN:O | 8:CI:31:GLN:HB2 | 2.11 | 0.50 |
| 8:CI:56:MET:SD | 8:CI:57:VAL:HG23 | 2.52 | 0.50 |
| 9:CJ:36:VAL:HA | 9:CJ:76:ILE:HA | 1.94 | 0.50 |
| 1:CA:528:C:H41 | 11:CL:45:ASN:CG | 2.15 | 0.50 |
| 12:CM:89:ARG:HB3 | 12:CM:96:VAL:HG22 | 1.94 | 0.50 |
| 22:DA:71:C:H2' | 22:DA:72:G:O4' | 2.11 | 0.50 |
| 23:DB:1283:G:N2 | 23:DB:1285:A:H3' | 2.27 | 0.50 |
| 23:DB:1439:A:N7 | 23:DB:1440:U:N1 | 2.59 | 0.50 |
| 23:DB:1487:U:H2' | 23:DB:1488:C:H6 | 1.76 | 0.50 |
| 23:DB:156:A:O2' | 23:DB:157:C:H5' | 2.12 | 0.50 |
| 23:DB:1678:A:H2' | 23:DB:1679:A:C8 | 2.47 | 0.50 |
| 23:DB:1838:C:H4' | 23:DB:1839:G:H8 | 1.76 | 0.50 |
| 23:DB:1948:G:O2' | 23:DB:1949:G:H5' | 2.12 | 0.50 |
| 23:DB:2196:C:O2' | 23:DB:2197:U:H5' | 2.11 | 0.50 |
| 23:DB:2835:A:N6 | 23:DB:2878:U:H2' | 2.26 | 0.50 |
| 23:DB:747:U:OP2 | 40:DS:90:LYS:NZ | 2.43 | 0.50 |
| 25:DC:119:VAL:HA | 25:DC:133:ASN:ND2 | 2.27 | 0.50 |
| 25:DC:250:GLN:CD | 25:DC:254:LYS:HG2 | 2.33 | 0.50 |
| 27:DE:112:LEU:C | 27:DE:114:ARG:H | 2.14 | 0.50 |
| 28:DF:111:ARG:HH22 | 28:DF:113:PHE:HB2 | 1.76 | 0.50 |
| 28:DF:43:ILE:HA | 28:DF:46:LYS:CE | 2.42 | 0.50 |
| 31:DJ:19:ASP:CG | 31:DJ:57:LEU:HB3 | 2.31 | 0.50 |
| 32:DK:61:VAL:HG11 | 32:DK:112:PHE:CZ | 2.47 | 0.50 |
| 37:DP:3:ILE:C | 37:DP:3:ILE:HD13 | 2.32 | 0.50 |
| 24:DV:53:LYS:HD2 | 24:DV:55:GLU:OE1 | 2.12 | 0.50 |
| 43:DW:37:VAL:HG12 | 43:DW:38:ARG:N | 2.22 | 0.50 |
| 1:AA:1317:C:H3' | 1:AA:1318:A:H8 | 1.76 | 0.49 |
| 1:AA:512:U:O2' | 1:AA:513:C:H5' | 2.12 | 0.49 |
| 1:AA:636:U:H2' | 1:AA:637:C:H6 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:9:G:H2' | 1:AA:10:A:H8 | 1.76 | 0.49 |
| 20:AB:212:TYR:O | 20:AB:216:VAL:HG13 | 2.12 | 0.49 |
| 2:AC:155:ARG:NH2 | 2:AC:192:TYR:HB2 | 2.26 | 0.49 |
| 5:AF:2:ARG:O | 5:AF:65:GLU:HA | 2.12 | 0.49 |
| 7:AH:113:ARG:NH2 | 7:AH:114:ALA:HA | 2.27 | 0.49 |
| 8:AI:46:VAL:HG23 | 8:AI:47:VAL:H | 1.77 | 0.49 |
| 9:AJ:36:VAL:HA | 9:AJ:76:ILE:HA | 1.93 | 0.49 |
| 10:AK:30:ILE:HG22 | 10:AK:45:THR:CB | 2.42 | 0.49 |
| 15:AP:43:ALA:CA | 15:AP:46:LYS:HE3 | 2.42 | 0.49 |
| 18:AS:44:ILE:O | 18:AS:44:ILE:HG23 | 2.11 | 0.49 |
| 23:BB:1173:U:H6 | 23:BB:1173:U:O5' | 1.95 | 0.49 |
| 23:BB:1175:A:H2' | 23:BB:1176:U:H5' | 1.94 | 0.49 |
| 23:BB:138:U:H2' | 23:BB:140:C:O4' | 2.11 | 0.49 |
| 23:BB:1436:G:O2' | 23:BB:1437:C:H5' | 2.12 | 0.49 |
| 23:BB:2215:C:H2' | 23:BB:2216:G:H8 | 1.77 | 0.49 |
| 23:BB:2760:C:O2' | 23:BB:2761:A:H5' | 2.12 | 0.49 |
| 23:BB:2885:G:H2' | 23:BB:2886:A:C4' | 2.42 | 0.49 |
| 23:BB:45:G:C5' | 23:BB:46:G:H5' | 2.40 | 0.49 |
| 23:BB:934:U:H2' | 23:BB:935:C:H6 | 1.77 | 0.49 |
| 25:BC:106:PRO:O | 25:BC:109:LEU:HD13 | 2.12 | 0.49 |
| 23:BB:2786:U:C5' | 26:BD:70:LYS:HG3 | 2.42 | 0.49 |
| 28:BF:71:LYS:HD3 | 28:BF:73:VAL:O | 2.12 | 0.49 |
| 28:BF:86:CYS:O | 28:BF:88:VAL:HG23 | 2.12 | 0.49 |
| 32:BK:113:MET:HA | 32:BK:116:ILE:HD11 | 1.94 | 0.49 |
| 32:BK:40:LYS:NZ | 32:BK:59:LYS:HE3 | 2.26 | 0.49 |
| 32:BK:43:ILE:CG2 | 32:BK:46:ALA:HB2 | 2.42 | 0.49 |
| 33:BL:120:VAL:HG12 | 33:BL:121:THR:N | 2.26 | 0.49 |
| 33:BL:6:LEU:H | 33:BL:6:LEU:CD2 | 2.20 | 0.49 |
| 41:BT:68:LYS:O | 41:BT:69:ARG:CB | 2.59 | 0.49 |
| 42:BU:64:ILE:HG13 | 42:BU:68:ASN:HD22 | 1.77 | 0.49 |
| 43:BW:30:VAL:O | 43:BW:30:VAL:HG13 | 2.12 | 0.49 |
| 1:CA:239:U:H6 | 1:CA:239:U:H5' | 1.76 | 0.49 |
| 1:CA:772:U:H2' | 1:CA:773:G:C8 | 2.46 | 0.49 |
| 4:CE:53:ARG:HB3 | 4:CE:53:ARG:CZ | 2.42 | 0.49 |
| 8:CI:78:ILE:HG22 | 8:CI:82:ILE:HD11 | 1.92 | 0.49 |
| 9:CJ:6:ILE:HB | 9:CJ:76:ILE:HD11 | 1.94 | 0.49 |
| 11:CL:17:LYS:HZ1 | 11:CL:17:LYS:N | 2.11 | 0.49 |
| 12:CM:44:ILE:HA | 12:CM:47:LEU:HD23 | 1.93 | 0.49 |
| 15:CP:28:ARG:HD3 | 15:CP:29:ASN:HD22 | 1.76 | 0.49 |
| 18:CS:10:ILE:HG22 | 18:CS:37:SER:HB3 | 1.94 | 0.49 |
| 18:CS:11:ASP:OD1 | 18:CS:34:SER:HA | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1145:C:O2' | 23:DB:1146:C:H5' | 2.10 | 0.49 |
| 23:DB:1820:U:H3 | 25:DC:197:ALA:HA | 1.76 | 0.49 |
| 23:DB:2216:G:H2' | 23:DB:2217:G:C8 | 2.47 | 0.49 |
| 23:DB:2234:G:O2' | 23:DB:2235:G:H5' | 2.13 | 0.49 |
| 23:DB:2332:C:H1' | 23:DB:2336:A:C8 | 2.47 | 0.49 |
| 23:DB:2556:C:H2' | 23:DB:2557:G:O4' | 2.12 | 0.49 |
| 23:DB:264:C:O2' | 23:DB:265:A:H5'' | 2.12 | 0.49 |
| 23:DB:272:A:H2' | 23:DB:273:G:C8 | 2.47 | 0.49 |
| 25:DC:36:ASN:ND2 | 25:DC:85:ASN:HD21 | 2.08 | 0.49 |
| 28:DF:155:ILE:HG22 | 28:DF:156:THR:N | 2.26 | 0.49 |
| 28:DF:113:PHE:CZ | 28:DF:175:PRO:HB2 | 2.48 | 0.49 |
| 28:DF:31:GLU:C | 28:DF:32:LYS:HD3 | 2.33 | 0.49 |
| 28:DF:55:ASP:O | 28:DF:59:ILE:HG13 | 2.12 | 0.49 |
| 29:DG:91:VAL:O | 29:DG:93:TYR:N | 2.44 | 0.49 |
| 23:DB:142:A:N3 | 41:DT:2:ILE:HG22 | 2.27 | 0.49 |
| 42:DU:81:ARG:HB2 | 42:DU:96:LYS:HG2 | 1.94 | 0.49 |
| 1:AA:113:G:O4' | 1:AA:354:G:H4' | 2.12 | 0.49 |
| 1:AA:921:U:H2' | 1:AA:922:G:H8 | 1.75 | 0.49 |
| 20:AB:59:ILE:HG21 | 20:AB:158:ASP:HB3 | 1.94 | 0.49 |
| 2:AC:161:ILE:N | 2:AC:161:ILE:HD12 | 2.27 | 0.49 |
| 4:AE:113:VAL:HG23 | 4:AE:114:LEU:N | 2.27 | 0.49 |
| 4:AE:53:ARG:CZ | 4:AE:53:ARG:HB3 | 2.41 | 0.49 |
| 8:AI:30:ASN:O | 8:AI:31:GLN:HB2 | 2.12 | 0.49 |
| 51:B4:8:LYS:O | 51:B4:25:VAL:HG21 | 2.12 | 0.49 |
| 23:BB:1386:C:H2' | 23:BB:1387:A:H8 | 1.72 | 0.49 |
| 23:BB:1590:A:H2' | 23:BB:1591:A:C8 | 2.48 | 0.49 |
| 23:BB:1843:C:H5'' | 25:BC:250:GLN:NE2 | 2.25 | 0.49 |
| 23:BB:2394:C:OP1 | 33:BL:63:LYS:HG2 | 2.12 | 0.49 |
| 23:BB:2805:C:O2' | 23:BB:2806:C:H5' | 2.12 | 0.49 |
| 23:BB:685:A:H1' | 23:BB:688:U:O4 | 2.13 | 0.49 |
| 23:BB:729:G:H5'' | 23:BB:730:A:H5'' | 1.93 | 0.49 |
| 23:BB:925:A:O2' | 23:BB:926:G:H5' | 2.12 | 0.49 |
| 25:BC:20:ASN:OD1 | 25:BC:22:GLU:HG2 | 2.12 | 0.49 |
| 26:BD:174:SER:O | 26:BD:175:LEU:HB2 | 2.11 | 0.49 |
| 27:BE:161:ALA:CA | 27:BE:164:LEU:HB2 | 2.37 | 0.49 |
| 52:BI:72:THR:HG21 | 52:BI:111:THR:O | 2.12 | 0.49 |
| 35:BN:63:ARG:O | 35:BN:66:ALA:HB3 | 2.11 | 0.49 |
| 37:BP:3:ILE:CD1 | 37:BP:7:LEU:HD11 | 2.42 | 0.49 |
| 41:BT:29:THR:CG2 | 41:BT:86:THR:HG22 | 2.42 | 0.49 |
| 43:BW:37:VAL:CG1 | 43:BW:38:ARG:HH11 | 2.24 | 0.49 |
| 44:BX:55:THR:O | 44:BX:58:ASN:HB3 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BZ:21:ALA:HB3 | 46:BZ:23:ASN:HD21 | 1.77 | 0.49 |
| 1:CA:1134:G:N2 | 1:CA:1135:U:H1' | 2.26 | 0.49 |
| 1:CA:1317:C:H3' | 1:CA:1318:A:H8 | 1.77 | 0.49 |
| 1:CA:643:C:H2' | 1:CA:644:U:C6 | 2.47 | 0.49 |
| 3:CD:120:LYS:O | 3:CD:145:ARG:HG3 | 2.12 | 0.49 |
| 4:CE:15:ILE:HB | 4:CE:35:LEU:O | 2.12 | 0.49 |
| 1:CA:1069:C:H5'' | 4:CE:25:LYS:NZ | 2.27 | 0.49 |
| 7:CH:108:GLY:O | 7:CH:110:MET:HG3 | 2.12 | 0.49 |
| 8:CI:34:LEU:HD21 | 8:CI:48:ARG:NH2 | 2.18 | 0.49 |
| 10:CK:75:GLU:N | 10:CK:75:GLU:CD | 2.66 | 0.49 |
| 10:CK:90:PRO:C | 10:CK:92:ARG:H | 2.16 | 0.49 |
| 11:CL:13:ARG:HG2 | 11:CL:14:LYS:H | 1.76 | 0.49 |
| 12:CM:43:LYS:N | 12:CM:43:LYS:HD2 | 2.26 | 0.49 |
| 15:CP:36:VAL:O | 15:CP:36:VAL:HG13 | 2.12 | 0.49 |
| 16:CQ:29:LYS:HG3 | 16:CQ:34:GLY:O | 2.12 | 0.49 |
| 17:CR:56:ARG:O | 17:CR:60:ARG:HG2 | 2.12 | 0.49 |
| 18:CS:10:ILE:HB | 18:CS:14:LEU:HD11 | 1.94 | 0.49 |
| 50:D3:54:LEU:CG | 50:D3:58:ILE:HD11 | 2.42 | 0.49 |
| 23:DB:140:C:H5' | 23:DB:141:G:C5 | 2.47 | 0.49 |
| 23:DB:1511:G:H2' | 23:DB:1512:C:C6 | 2.48 | 0.49 |
| 23:DB:1541:C:H2' | 23:DB:1542:U:O4' | 2.12 | 0.49 |
| 23:DB:2143:C:N3 | 23:DB:2144:G:H1' | 2.26 | 0.49 |
| 23:DB:2684:U:H2' | 23:DB:2685:G:O4' | 2.12 | 0.49 |
| 23:DB:311:A:H3' | 23:DB:312:G:H8 | 1.77 | 0.49 |
| 23:DB:502:A:H5' | 23:DB:503:A:OP2 | 2.11 | 0.49 |
| 23:DB:861:A:H2' | 23:DB:862:G:O4' | 2.12 | 0.49 |
| 25:DC:105:ALA:HB1 | 25:DC:109:LEU:CD1 | 2.42 | 0.49 |
| 26:DD:108:ASP:OD2 | 26:DD:206:ALA:HA | 2.12 | 0.49 |
| 31:DJ:13:ARG:HB3 | 31:DJ:53:TYR:CD2 | 2.46 | 0.49 |
| 23:DB:7:G:H4' | 31:DJ:15:TRP:CZ2 | 2.47 | 0.49 |
| 32:DK:108:ARG:O | 32:DK:113:MET:HE3 | 2.12 | 0.49 |
| 34:DM:35:ALA:O | 34:DM:36:VAL:HB | 2.11 | 0.49 |
| 35:DN:117:ASP:C | 35:DN:117:ASP:OD2 | 2.51 | 0.49 |
| 36:DO:84:GLU:C | 36:DO:86:GLY:H | 2.14 | 0.49 |
| 39:DR:39:LEU:HD23 | 39:DR:39:LEU:N | 2.26 | 0.49 |
| 39:DR:61:ALA:HB1 | 39:DR:96:VAL:HB | 1.94 | 0.49 |
| 42:DU:26:ASN:ND2 | 42:DU:26:ASN:N | 2.61 | 0.49 |
| 46:DZ:56:MET:O | 46:DZ:59:ILE:HG12 | 2.12 | 0.49 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:H8 | 1.77 | 0.49 |
| 1:AA:1464:U:H2' | 1:AA:1465:A:C8 | 2.47 | 0.49 |
| 1:AA:1480:A:H2' | 1:AA:1481:U:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1522:U:H2' | 1:AA:1523:G:H8 | 1.77 | 0.49 |
| 1:AA:393:A:O2' | 1:AA:394:G:H5' | 2.12 | 0.49 |
| 1:AA:411:A:N6 | 1:AA:413:G:H21 | 2.09 | 0.49 |
| 2:AC:14:VAL:O | 2:AC:15:LYS:HD2 | 2.12 | 0.49 |
| 3:AD:120:LYS:O | 3:AD:145:ARG:HG3 | 2.12 | 0.49 |
| 4:AE:136:VAL:HG13 | 4:AE:137:ARG:N | 2.27 | 0.49 |
| 6:AG:144:ALA:O | 6:AG:146:ALA:N | 2.38 | 0.49 |
| 8:AI:56:MET:HA | 8:AI:59:LYS:HB2 | 1.94 | 0.49 |
| 10:AK:90:PRO:C | 10:AK:92:ARG:H | 2.15 | 0.49 |
| 11:AL:34:THR:O | 11:AL:35:ARG:HD2 | 2.12 | 0.49 |
| 12:AM:90:HIS:CE1 | 12:AM:96:VAL:HG21 | 2.47 | 0.49 |
| 16:AQ:29:LYS:HG3 | 16:AQ:34:GLY:O | 2.12 | 0.49 |
| 17:AR:63:TYR:N | 17:AR:63:TYR:HD2 | 2.10 | 0.49 |
| 47:B0:42:ILE:HG22 | 47:B0:43:THR:O | 2.12 | 0.49 |
| 22:BA:55:U:H2' | 22:BA:56:G:C8 | 2.47 | 0.49 |
| 23:BB:1789:A:OP1 | 25:BC:220:ARG:HD3 | 2.12 | 0.49 |
| 23:BB:1893:C:H2' | 23:BB:1894:C:O4' | 2.12 | 0.49 |
| 23:BB:1914:C:H2' | 23:BB:1915:U:C6 | 2.47 | 0.49 |
| 23:BB:2247:A:H3' | 56:BB:3266:HOH:O | 2.11 | 0.49 |
| 23:BB:2443:C:O2' | 23:BB:2444:G:H5' | 2.13 | 0.49 |
| 23:BB:37:C:O2' | 23:BB:38:A:H5' | 2.13 | 0.49 |
| 23:BB:725:G:H2' | 23:BB:726:G:Cl' | 2.43 | 0.49 |
| 23:BB:764:A:H5'' | 25:BC:208:GLY:HA2 | 1.94 | 0.49 |
| 23:BB:853:C:O2' | 23:BB:854:C:H5' | 2.11 | 0.49 |
| 26:BD:204:LYS:HB2 | 26:BD:205:PRO:HD2 | 1.93 | 0.49 |
| 28:BF:169:LEU:HB3 | 28:BF:174:PHE:CD1 | 2.47 | 0.49 |
| 29:BG:10:VAL:CG1 | 29:BG:16:VAL:HG21 | 2.41 | 0.49 |
| 29:BG:148:ARG:HB2 | 29:BG:152:ARG:HH11 | 1.76 | 0.49 |
| 30:BH:73:ASN:ND2 | 30:BH:74:ALA:N | 2.56 | 0.49 |
| 31:BJ:106:LYS:HE3 | 31:BJ:106:LYS:HA | 1.94 | 0.49 |
| 31:BJ:35:ARG:HA | 31:BJ:40:HIS:NE2 | 2.27 | 0.49 |
| 34:BM:40:ARG:HB3 | 34:BM:95:LEU:HD12 | 1.93 | 0.49 |
| 35:BN:108:ALA:O | 35:BN:110:MET:HE3 | 2.12 | 0.49 |
| 39:BR:5:PHE:HB2 | 39:BR:37:GLU:OE1 | 2.12 | 0.49 |
| 40:BS:23:LEU:HD21 | 47:B0:21:LEU:HB3 | 1.93 | 0.49 |
| 41:BT:43:ILE:O | 41:BT:46:ALA:HB3 | 2.13 | 0.49 |
| 41:BT:4:GLU:OE1 | 41:BT:5:GLU:HG2 | 2.12 | 0.49 |
| 42:BU:73:ASN:C | 42:BU:75:ALA:H | 2.16 | 0.49 |
| 1:CA:1029:U:H5'' | 1:CA:1030:U:C5 | 2.47 | 0.49 |
| 1:CA:1030:U:H4' | 1:CA:1031:C:OP2 | 2.12 | 0.49 |
| 1:CA:1163:A:H2' | 1:CA:1164:G:H8 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1250:A:H2 | 1:CA:1370:G:H1' | 1.77 | 0.49 |
| 1:CA:1432:G:O2' | 1:CA:1468:A:N6 | 2.45 | 0.49 |
| 1:CA:1510:C:H2' | 1:CA:1511:G:C8 | 2.47 | 0.49 |
| 1:CA:429:U:OP2 | 3:CD:31:CYS:HB2 | 2.13 | 0.49 |
| 2:CC:142:ARG:HH21 | 2:CC:143:LEU:HD21 | 1.77 | 0.49 |
| 7:CH:27:PRO:HA | 7:CH:56:PRO:O | 2.12 | 0.49 |
| 7:CH:45:ILE:HB | 7:CH:61:THR:O | 2.13 | 0.49 |
| 10:CK:106:ILE:HG13 | 10:CK:107:THR:N | 2.23 | 0.49 |
| 10:CK:30:ILE:HG22 | 10:CK:45:THR:CB | 2.42 | 0.49 |
| 16:CQ:74:LEU:HD13 | 16:CQ:75:VAL:N | 2.28 | 0.49 |
| 22:DA:52:A:H4' | 22:DA:52:A:OP1 | 2.12 | 0.49 |
| 23:DB:2295:C:OP2 | 36:DO:10:ARG:HG2 | 2.12 | 0.49 |
| 23:DB:2328:A:H2' | 23:DB:2329:U:H6 | 1.73 | 0.49 |
| 23:DB:2636:C:H2' | 23:DB:2637:U:C6 | 2.47 | 0.49 |
| 23:DB:2814:A:H2' | 23:DB:2815:C:C6 | 2.48 | 0.49 |
| 23:DB:345:A:H1' | 23:DB:346:A:C2 | 2.48 | 0.49 |
| 23:DB:765:C:H2' | 23:DB:766:U:H6 | 1.77 | 0.49 |
| 23:DB:785:G:H2' | 23:DB:786:C:C6 | 2.47 | 0.49 |
| 23:DB:851:C:H2' | 23:DB:852:U:C6 | 2.48 | 0.49 |
| 25:DC:90:ILE:HD12 | 25:DC:102:TYR:HB3 | 1.93 | 0.49 |
| 25:DC:131:MET:HE2 | 25:DC:143:VAL:HG13 | 1.93 | 0.49 |
| 25:DC:175:LEU:HD11 | 25:DC:181:ARG:HG3 | 1.94 | 0.49 |
| 23:DB:2598:A:OP1 | 25:DC:233:GLY:HA3 | 2.12 | 0.49 |
| 26:DD:69:ALA:CA | 26:DD:73:VAL:HB | 2.41 | 0.49 |
| 27:DE:153:LEU:HG | 27:DE:154:ASP:H | 1.76 | 0.49 |
| 28:DF:29:ARG:H | 28:DF:29:ARG:CD | 2.25 | 0.49 |
| 31:DJ:75:TYR:CD1 | 31:DJ:86:GLN:HB3 | 2.47 | 0.49 |
| 33:DL:142:ILE:N | 33:DL:142:ILE:HD12 | 2.28 | 0.49 |
| 35:DN:97:ILE:HD12 | 35:DN:98:LEU:N | 2.21 | 0.49 |
| 36:DO:7:ARG:O | 36:DO:96:GLY:HA3 | 2.12 | 0.49 |
| 44:DX:55:THR:O | 44:DX:58:ASN:HB3 | 2.12 | 0.49 |
| 1:AA:1124:G:H5'' | 9:AJ:37:ARG:O | 2.13 | 0.49 |
| 1:AA:1314:C:H3' | 18:AS:5:LYS:NZ | 2.26 | 0.49 |
| 1:AA:55:A:OP2 | 1:AA:352:C:N4 | 2.44 | 0.49 |
| 1:AA:898:G:N2 | 1:AA:900:A:H3' | 2.28 | 0.49 |
| 20:AB:128:LEU:HD13 | 20:AB:129:THR:H | 1.77 | 0.49 |
| 9:AJ:15:HIS:O | 9:AJ:18:ILE:HG22 | 2.13 | 0.49 |
| 15:AP:46:LYS:C | 15:AP:48:GLU:H | 2.16 | 0.49 |
| 17:AR:56:ARG:O | 17:AR:60:ARG:HG2 | 2.12 | 0.49 |
| 22:BA:88:C:H1' | 22:BA:89:U:C5 | 2.46 | 0.49 |
| 23:BB:2027:G:C6 | 23:BB:2028:U:C4 | 3.00 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:2353:G:H1' | 43:BW:30:VAL:HG12 | 1.91 | 0.49 |
| 23:BB:2838:G:H2' | 23:BB:2839:G:H8 | 1.77 | 0.49 |
| 23:BB:2899:A:H5' | 31:BJ:136:GLN:OE1 | 2.12 | 0.49 |
| 23:BB:289:G:H2' | 23:BB:290:U:O4' | 2.12 | 0.49 |
| 23:BB:337:C:H2' | 23:BB:338:G:O4' | 2.12 | 0.49 |
| 31:BJ:13:ARG:HB3 | 31:BJ:53:TYR:CD2 | 2.45 | 0.49 |
| 38:BQ:57:ARG:HA | 38:BQ:60:TRP:CE3 | 2.47 | 0.49 |
| 23:BB:329:G:O6 | 42:BU:16:LYS:HG2 | 2.11 | 0.49 |
| 42:BU:48:VAL:O | 42:BU:48:VAL:HG13 | 2.12 | 0.49 |
| 46:BZ:7:VAL:HG13 | 46:BZ:8:THR:CG2 | 2.39 | 0.49 |
| 1:CA:1127:G:O2' | 1:CA:1128:C:H5' | 2.12 | 0.49 |
| 1:CA:1118:U:H1' | 1:CA:1179:A:C5 | 2.47 | 0.49 |
| 1:CA:1413:A:O2' | 1:CA:1414:U:H5' | 2.12 | 0.49 |
| 1:CA:320:A:H2' | 1:CA:321:A:C8 | 2.47 | 0.49 |
| 1:CA:429:U:H3' | 3:CD:8:LEU:HD23 | 1.93 | 0.49 |
| 1:CA:464:U:H2' | 1:CA:466:A:OP2 | 2.11 | 0.49 |
| 1:CA:634:C:H2' | 1:CA:635:A:H8 | 1.77 | 0.49 |
| 1:CA:636:U:H2' | 1:CA:637:C:H6 | 1.78 | 0.49 |
| 1:CA:767:A:H2' | 1:CA:768:A:C8 | 2.47 | 0.49 |
| 7:CH:47:ASP:CG | 7:CH:48:PHE:H | 2.16 | 0.49 |
| 1:CA:598:U:H4' | 7:CH:85:TYR:CG | 2.46 | 0.49 |
| 9:CJ:15:HIS:O | 9:CJ:18:ILE:HG22 | 2.11 | 0.49 |
| 12:CM:50:GLY:O | 12:CM:54:THR:HG23 | 2.11 | 0.49 |
| 47:D0:42:ILE:HG22 | 47:D0:43:THR:O | 2.12 | 0.49 |
| 47:D0:43:THR:HG21 | 47:D0:47:TYR:HB2 | 1.93 | 0.49 |
| 22:DA:91:C:H2' | 22:DA:92:C:H6 | 1.77 | 0.49 |
| 23:DB:1040:A:H2' | 23:DB:1041:G:O4' | 2.12 | 0.49 |
| 23:DB:1083:U:H2' | 23:DB:1085:A:OP2 | 2.12 | 0.49 |
| 23:DB:1655:A:H2' | 23:DB:1656:C:O4' | 2.11 | 0.49 |
| 23:DB:175:G:O2' | 23:DB:176:A:H5' | 2.12 | 0.49 |
| 23:DB:2461:A:H2' | 23:DB:2462:C:H6 | 1.77 | 0.49 |
| 25:DC:69:ASN:O | 25:DC:70:LYS:C | 2.50 | 0.49 |
| 28:DF:45:ASP:HB3 | 28:DF:48:LEU:CD2 | 2.42 | 0.49 |
| 30:DH:114:GLU:HB3 | 30:DH:133:GLN:HG3 | 1.94 | 0.49 |
| 30:DH:25:TYR:CG | 30:DH:30:LEU:HG | 2.47 | 0.49 |
| 31:DJ:64:VAL:HG11 | 31:DJ:69:ARG:HB2 | 1.92 | 0.49 |
| 37:DP:50:ARG:HB3 | 37:DP:57:ALA:H | 1.77 | 0.49 |
| 38:DQ:26:ALA:C | 38:DQ:28:SER:H | 2.14 | 0.49 |
| 31:DJ:44:TYR:CD2 | 38:DQ:59:LEU:HD21 | 2.47 | 0.49 |
| 39:DR:95:ASP:O | 39:DR:96:VAL:HG13 | 2.13 | 0.49 |
| 24:DV:75:GLN:HA | 24:DV:75:GLN:OE1 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1030:U:H4' | 1:AA:1031:C:OP2 | 2.12 | 0.49 |
| 1:AA:106:C:O2' | 1:AA:107:G:H5' | 2.13 | 0.49 |
| 1:AA:233:C:H2' | 1:AA:234:C:H6 | 1.77 | 0.49 |
| 2:AC:190:THR:HG22 | 2:AC:191:THR:H | 1.75 | 0.49 |
| 2:AC:72:PRO:O | 2:AC:76:ILE:HG12 | 2.12 | 0.49 |
| 3:AD:97:LEU:HD13 | 3:AD:136:VAL:HG11 | 1.93 | 0.49 |
| 3:AD:29:THR:HB | 3:AD:30:LYS:HZ3 | 1.77 | 0.49 |
| 5:AF:2:ARG:HB3 | 5:AF:92:THR:OG1 | 2.11 | 0.49 |
| 6:AG:113:LYS:HB3 | 6:AG:113:LYS:HZ2 | 1.77 | 0.49 |
| 9:AJ:41:PRO:O | 9:AJ:42:LEU:HB2 | 2.12 | 0.49 |
| 22:BA:14:U:H4' | 22:BA:70:C:O2 | 2.13 | 0.49 |
| 23:BB:1229:C:H2' | 23:BB:1230:A:H8 | 1.76 | 0.49 |
| 23:BB:1531:C:H2' | 23:BB:1532:A:H8 | 1.78 | 0.49 |
| 23:BB:1729:U:C2' | 23:BB:1730:C:H4' | 2.36 | 0.49 |
| 23:BB:2088:A:H2' | 23:BB:2089:C:H6 | 1.76 | 0.49 |
| 23:BB:211:C:O2' | 23:BB:212:G:H5' | 2.12 | 0.49 |
| 23:BB:2813:A:H2' | 23:BB:2814:A:H8 | 1.76 | 0.49 |
| 23:BB:83:A:OP1 | 42:BU:91:LYS:HD2 | 2.12 | 0.49 |
| 23:BB:991:C:H5' | 23:BB:991:C:H6 | 1.78 | 0.49 |
| 28:BF:31:GLU:HB3 | 28:BF:156:THR:O | 2.13 | 0.49 |
| 29:BG:94:ARG:HG2 | 29:BG:127:GLN:HE21 | 1.78 | 0.49 |
| 30:BH:53:GLU:HG3 | 30:BH:57:LYS:HD3 | 1.94 | 0.49 |
| 31:BJ:12:LYS:HG3 | 31:BJ:41:LYS:NZ | 2.27 | 0.49 |
| 31:BJ:35:ARG:HA | 31:BJ:40:HIS:CD2 | 2.47 | 0.49 |
| 32:BK:105:ARG:HD2 | 32:BK:122:VAL:HG11 | 1.94 | 0.49 |
| 33:BL:3:LEU:O | 33:BL:5:THR:HG23 | 2.13 | 0.49 |
| 35:BN:115:LEU:O | 35:BN:117:ASP:N | 2.45 | 0.49 |
| 43:BW:49:ASN:HA | 43:BW:61:LYS:HB2 | 1.94 | 0.49 |
| 1:CA:1101:A:H62 | 20:CB:173:LYS:HE3 | 1.77 | 0.49 |
| 1:CA:1500:A:C2' | 1:CA:1501:C:H5' | 2.42 | 0.49 |
| 1:CA:366:A:O2' | 1:CA:394:G:N2 | 2.45 | 0.49 |
| 1:CA:50:A:N6 | 1:CA:361:G:H4' | 2.28 | 0.49 |
| 1:CA:984:C:O2' | 1:CA:985:C:H5' | 2.12 | 0.49 |
| 2:CC:129:PHE:CE2 | 2:CC:156:LEU:HD13 | 2.47 | 0.49 |
| 3:CD:160:LEU:HA | 3:CD:163:GLN:CG | 2.41 | 0.49 |
| 3:CD:77:GLU:OE2 | 3:CD:81:LEU:HD21 | 2.12 | 0.49 |
| 8:CI:109:GLN:CD | 8:CI:110:VAL:H | 2.16 | 0.49 |
| 10:CK:86:LYS:HB2 | 10:CK:113:THR:HA | 1.94 | 0.49 |
| 12:CM:22:TYR:CD1 | 12:CM:65:GLU:HA | 2.46 | 0.49 |
| 13:CN:50:LEU:H | 13:CN:51:PRO:CD | 2.22 | 0.49 |
| 15:CP:6:LEU:HD12 | 15:CP:6:LEU:N | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:664:G:H5'' | 17:CR:52:ARG:HE | 1.77 | 0.49 |
| 51:D4:15:LYS:O | 51:D4:16:ILE:HB | 2.13 | 0.49 |
| 23:DB:1175:A:H2' | 23:DB:1176:U:H5' | 1.94 | 0.49 |
| 23:DB:1210:G:H1' | 23:DB:1212:G:C2 | 2.48 | 0.49 |
| 23:DB:1262:A:N3 | 47:D0:6:LYS:HE3 | 2.27 | 0.49 |
| 23:DB:1386:C:OP2 | 23:DB:1396:U:H5 | 1.94 | 0.49 |
| 23:DB:1531:C:H2' | 23:DB:1532:A:H8 | 1.77 | 0.49 |
| 23:DB:1745:A:H2' | 23:DB:1746:A:O4' | 2.12 | 0.49 |
| 23:DB:1973:G:O2' | 23:DB:1974:C:H5' | 2.13 | 0.49 |
| 23:DB:201:C:H1' | 23:DB:250:G:O6 | 2.13 | 0.49 |
| 23:DB:263:G:H2' | 23:DB:264:C:O4' | 2.11 | 0.49 |
| 23:DB:274:C:H2' | 23:DB:275:C:O4' | 2.13 | 0.49 |
| 23:DB:2882:A:H3' | 23:DB:2883:A:H5'' | 1.93 | 0.49 |
| 23:DB:904:G:H2' | 23:DB:905:A:H8 | 1.78 | 0.49 |
| 27:DE:48:THR:C | 27:DE:50:ALA:H | 2.16 | 0.49 |
| 29:DG:89:VAL:HG12 | 29:DG:90:GLY:N | 2.27 | 0.49 |
| 52:DI:92:PRO:O | 52:DI:93:ASN:HB2 | 2.12 | 0.49 |
| 32:DK:61:VAL:HG11 | 32:DK:112:PHE:CE2 | 2.48 | 0.49 |
| 38:DQ:80:ASN:O | 38:DQ:116:LEU:HD11 | 2.13 | 0.49 |
| 38:DQ:24:TYR:CG | 38:DQ:25:GLY:N | 2.80 | 0.49 |
| 41:DT:39:THR:HG23 | 41:DT:39:THR:O | 2.12 | 0.49 |
| 45:DY:4:ILE:HG22 | 45:DY:56:VAL:CG1 | 2.43 | 0.49 |
| 1:AA:1163:A:H2' | 1:AA:1164:G:H8 | 1.77 | 0.49 |
| 1:AA:1346:A:N1 | 1:AA:1374:A:H5'' | 2.27 | 0.49 |
| 1:AA:252:U:H2' | 1:AA:253:A:H8 | 1.77 | 0.49 |
| 1:AA:847:G:H2' | 1:AA:848:C:C6 | 2.47 | 0.49 |
| 2:AC:59:PRO:HD2 | 2:AC:62:SER:O | 2.11 | 0.49 |
| 2:AC:96:VAL:HB | 2:AC:97:PRO:HD2 | 1.93 | 0.49 |
| 10:AK:28:ASN:ND2 | 10:AK:29:THR:H | 2.11 | 0.49 |
| 11:AL:2:THR:HG22 | 11:AL:5:GLN:NE2 | 2.27 | 0.49 |
| 19:AT:4:LYS:HZ1 | 19:AT:6:ALA:CB | 2.25 | 0.49 |
| 23:BB:1080:A:O2' | 23:BB:1081:U:H5' | 2.12 | 0.49 |
| 23:BB:1230:A:H2' | 23:BB:1231:U:H6 | 1.77 | 0.49 |
| 23:BB:230:G:H2' | 23:BB:231:A:H8 | 1.76 | 0.49 |
| 23:BB:2617:U:C2' | 23:BB:2618:G:H5' | 2.42 | 0.49 |
| 23:BB:418:C:H2' | 23:BB:419:U:H6 | 1.78 | 0.49 |
| 23:BB:785:G:H2' | 23:BB:786:C:C6 | 2.46 | 0.49 |
| 25:BC:141:HIS:NE2 | 25:BC:194:VAL:HB | 2.28 | 0.49 |
| 26:BD:148:GLN:HG3 | 26:BD:152:PRO:HB3 | 1.95 | 0.49 |
| 28:BF:102:LEU:O | 28:BF:103:ILE:HB | 2.11 | 0.49 |
| 29:BG:132:LEU:HD12 | 29:BG:140:ILE:HG22 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BH:21:VAL:HG22 | 30:BH:22:LYS:N | 2.28 | 0.49 |
| 34:BM:31:PHE:HB3 | 34:BM:130:PHE:CZ | 2.48 | 0.49 |
| 34:BM:69:PRO:HA | 34:BM:94:ALA:HA | 1.94 | 0.49 |
| 36:BO:66:GLY:HA2 | 36:BO:102:ARG:NE | 2.27 | 0.49 |
| 36:BO:93:ASP:C | 36:BO:95:SER:H | 2.16 | 0.49 |
| 42:BU:62:ALA:O | 42:BU:63:ALA:HB3 | 2.12 | 0.49 |
| 23:BB:989:G:OP2 | 45:BY:13:ILE:HD11 | 2.12 | 0.49 |
| 46:BZ:53:ALA:O | 46:BZ:55:GLY:N | 2.36 | 0.49 |
| 1:CA:1085:U:H3' | 1:CA:1086:U:C6 | 2.48 | 0.49 |
| 1:CA:602:A:H2' | 1:CA:603:U:C6 | 2.47 | 0.49 |
| 1:CA:602:A:O2' | 1:CA:603:U:H5' | 2.12 | 0.49 |
| 2:CC:120:THR:HG22 | 2:CC:188:ALA:HB2 | 1.94 | 0.49 |
| 1:CA:1057:G:O3' | 2:CC:196:GLY:HA3 | 2.13 | 0.49 |
| 2:CC:16:PRO:CG | 2:CC:53:ARG:HH12 | 2.23 | 0.49 |
| 3:CD:22:SER:N | 3:CD:109:THR:HG22 | 2.28 | 0.49 |
| 12:CM:90:HIS:HA | 12:CM:108:ARG:HH22 | 1.74 | 0.49 |
| 12:CM:14:ALA:HB2 | 12:CM:42:VAL:HG23 | 1.95 | 0.49 |
| 16:CQ:83:LEU:HD13 | 16:CQ:83:LEU:N | 2.27 | 0.49 |
| 18:CS:40:PHE:O | 18:CS:43:MET:HG3 | 2.11 | 0.49 |
| 19:CT:49:ALA:C | 19:CT:52:GLU:HB3 | 2.33 | 0.49 |
| 22:DA:88:C:H1' | 22:DA:89:U:C5 | 2.47 | 0.49 |
| 23:DB:1306:C:O2' | 23:DB:1307:A:H5' | 2.12 | 0.49 |
| 23:DB:2636:C:O2' | 23:DB:2637:U:H5' | 2.13 | 0.49 |
| 23:DB:2729:G:H2' | 23:DB:2730:C:C6 | 2.48 | 0.49 |
| 23:DB:725:G:H2' | 23:DB:726:G:C1' | 2.42 | 0.49 |
| 25:DC:4:LYS:HD2 | 25:DC:5:CYS:H | 1.75 | 0.49 |
| 26:DD:187:LEU:O | 26:DD:188:LEU:HD23 | 2.13 | 0.49 |
| 23:DB:2786:U:O2' | 26:DD:66:GLY:HA3 | 2.12 | 0.49 |
| 28:DF:19:PHE:CE2 | 28:DF:164:GLU:HG2 | 2.47 | 0.49 |
| 28:DF:91:ARG:HD3 | 28:DF:91:ARG:N | 2.27 | 0.49 |
| 30:DH:114:GLU:HB2 | 30:DH:133:GLN:O | 2.12 | 0.49 |
| 30:DH:27:ARG:HH21 | 30:DH:27:ARG:HG2 | 1.78 | 0.49 |
| 30:DH:39:ALA:C | 30:DH:41:LYS:H | 2.16 | 0.49 |
| 30:DH:97:ARG:HB3 | 30:DH:112:LYS:HG2 | 1.94 | 0.49 |
| 35:DN:98:LEU:HG | 47:D0:42:ILE:HD11 | 1.95 | 0.49 |
| 36:DO:56:LYS:C | 36:DO:60:GLU:HG2 | 2.33 | 0.49 |
| 37:DP:24:THR:HB | 37:DP:86:LYS:HB3 | 1.93 | 0.49 |
| 37:DP:26:GLU:HB3 | 37:DP:84:SER:HB3 | 1.94 | 0.49 |
| 39:DR:35:PHE:C | 39:DR:58:VAL:HG23 | 2.33 | 0.49 |
| 42:DU:32:LYS:HG3 | 42:DU:65:GLN:HA | 1.95 | 0.49 |
| 43:DW:19:ARG:H | 43:DW:19:ARG:CD | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1005:A:H4' | 1:AA:1037:C:O2 | 2.13 | 0.49 |
| 1:AA:1159:U:O4' | 1:AA:1182:G:N2 | 2.45 | 0.49 |
| 1:AA:1299:A:H2' | 1:AA:1301:U:H1' | 1.95 | 0.49 |
| 1:AA:724:G:H2' | 1:AA:725:G:H8 | 1.78 | 0.49 |
| 1:AA:728:A:H2' | 1:AA:729:A:H8 | 1.78 | 0.49 |
| 1:AA:784:A:H2' | 1:AA:785:G:H8 | 1.77 | 0.49 |
| 1:AA:80:A:H3' | 1:AA:81:A:C8 | 2.44 | 0.49 |
| 5:AF:53:LYS:HB2 | 5:AF:54:LEU:HD22 | 1.94 | 0.49 |
| 7:AH:115:ALA:O | 7:AH:120:LEU:HD23 | 2.13 | 0.49 |
| 8:AI:78:ILE:O | 8:AI:82:ILE:HG13 | 2.12 | 0.49 |
| 12:AM:64:VAL:HA | 12:AM:68:LEU:CD1 | 2.40 | 0.49 |
| 13:AN:25:GLU:O | 13:AN:29:ILE:HG13 | 2.12 | 0.49 |
| 16:AQ:30:HIS:HB3 | 16:AQ:33:TYR:HB2 | 1.93 | 0.49 |
| 18:AS:48:ILE:O | 18:AS:58:PRO:HA | 2.12 | 0.49 |
| 21:AU:43:GLU:HA | 21:AU:46:ARG:NE | 2.28 | 0.49 |
| 50:B3:7:ARG:HG3 | 50:B3:7:ARG:NH1 | 2.28 | 0.49 |
| 23:BB:1057:A:H62 | 23:BB:1086:A:H2' | 1.78 | 0.49 |
| 23:BB:931:U:H3 | 23:BB:1166:G:N2 | 2.11 | 0.49 |
| 23:BB:1294:U:C2' | 23:BB:1295:C:H5' | 2.42 | 0.49 |
| 23:BB:1584:U:H5'' | 23:BB:1585:C:C5 | 2.47 | 0.49 |
| 23:BB:1794:A:H2' | 23:BB:1795:C:C6 | 2.47 | 0.49 |
| 23:BB:2836:U:H2' | 23:BB:2837:A:H8 | 1.77 | 0.49 |
| 23:BB:582:A:H2' | 23:BB:583:G:H8 | 1.78 | 0.49 |
| 23:BB:2590:A:H5'' | 25:BC:237:ARG:NH2 | 2.27 | 0.49 |
| 25:BC:43:ASN:HD22 | 25:BC:44:ASN:N | 2.10 | 0.49 |
| 26:BD:59:ARG:O | 26:BD:59:ARG:HD3 | 2.13 | 0.49 |
| 28:BF:160:LYS:HG3 | 28:BF:161:SER:N | 2.28 | 0.49 |
| 28:BF:76:PHE:HD2 | 28:BF:78:ILE:HD13 | 1.77 | 0.49 |
| 29:BG:42:VAL:HG23 | 29:BG:50:THR:O | 2.12 | 0.49 |
| 29:BG:71:LEU:HD13 | 29:BG:74:MET:SD | 2.53 | 0.49 |
| 30:BH:12:LEU:O | 30:BH:12:LEU:HG | 2.13 | 0.49 |
| 52:BI:21:PRO:CB | 52:BI:22:PRO:HD3 | 2.39 | 0.49 |
| 52:BI:56:VAL:CG2 | 52:BI:68:PHE:HB2 | 2.43 | 0.49 |
| 52:BI:74:PRO:O | 52:BI:77:VAL:HG22 | 2.13 | 0.49 |
| 32:BK:98:ARG:C | 32:BK:99:ILE:HD12 | 2.33 | 0.49 |
| 36:BO:58:ILE:O | 36:BO:62:LEU:HB2 | 2.13 | 0.49 |
| 43:BW:27:GLY:O | 43:BW:63:ASP:HA | 2.12 | 0.49 |
| 43:BW:58:LEU:HG | 43:BW:79:ILE:HD12 | 1.94 | 0.49 |
| 46:BZ:7:VAL:HG11 | 46:BZ:51:VAL:HG13 | 1.93 | 0.49 |
| 1:CA:1009:U:H2' | 1:CA:1010:U:C6 | 2.48 | 0.49 |
| 1:CA:1527:U:O2' | 1:CA:1528:U:H5' | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:376:G:H2' | 1:CA:377:G:C8 | 2.45 | 0.49 |
| 6:CG:14:ASP:OD2 | 6:CG:22:LEU:HB3 | 2.11 | 0.49 |
| 7:CH:113:ARG:NH2 | 7:CH:114:ALA:HA | 2.28 | 0.49 |
| 7:CH:4:ASP:OD1 | 7:CH:7:ALA:HB2 | 2.13 | 0.49 |
| 9:CJ:8:ILE:HD11 | 9:CJ:76:ILE:HG13 | 1.93 | 0.49 |
| 12:CM:86:ARG:HA | 12:CM:96:VAL:CG1 | 2.42 | 0.49 |
| 13:CN:25:GLU:O | 13:CN:29:ILE:HG13 | 2.12 | 0.49 |
| 13:CN:29:ILE:HB | 13:CN:30:ILE:HD12 | 1.93 | 0.49 |
| 21:CU:13:VAL:O | 21:CU:13:VAL:HG13 | 2.12 | 0.49 |
| 48:D1:7:LYS:HD3 | 50:D3:33:THR:HG21 | 1.94 | 0.49 |
| 23:DB:1099:G:C8 | 52:DI:3:LYS:HB2 | 2.48 | 0.49 |
| 23:DB:1433:A:H2' | 23:DB:1434:A:O4' | 2.12 | 0.49 |
| 23:DB:1838:C:H4' | 23:DB:1839:G:C8 | 2.48 | 0.49 |
| 23:DB:19:A:H2' | 23:DB:20:C:C6 | 2.47 | 0.49 |
| 23:DB:2295:C:O2' | 23:DB:2296:U:H5' | 2.12 | 0.49 |
| 23:DB:278:A:O3' | 23:DB:279:A:H8 | 1.95 | 0.49 |
| 26:DD:55:LYS:HB2 | 26:DD:60:VAL:HG13 | 1.94 | 0.49 |
| 27:DE:173:THR:HA | 27:DE:199:MET:HE1 | 1.95 | 0.49 |
| 28:DF:87:LYS:CG | 28:DF:88:VAL:H | 2.24 | 0.49 |
| 33:DL:77:ILE:HG12 | 33:DL:95:LEU:HD22 | 1.95 | 0.49 |
| 35:DN:75:ILE:O | 35:DN:79:LEU:HD12 | 2.12 | 0.49 |
| 36:DO:106:LEU:HG | 36:DO:107:ALA:N | 2.28 | 0.49 |
| 39:DR:10:LYS:N | 39:DR:10:LYS:HD2 | 2.27 | 0.49 |
| 40:DS:4:ILE:CG2 | 40:DS:106:VAL:HG13 | 2.41 | 0.49 |
| 40:DS:47:VAL:HG23 | 40:DS:48:LYS:N | 2.27 | 0.49 |
| 42:DU:40:LEU:HA | 42:DU:60:LYS:O | 2.13 | 0.49 |
| 45:DY:20:LYS:HA | 45:DY:23:LEU:HB2 | 1.93 | 0.49 |
| 46:DZ:7:VAL:HG23 | 46:DZ:67:VAL:HG11 | 1.94 | 0.49 |
| 1:AA:1343:G:H2' | 1:AA:1344:C:H6 | 1.76 | 0.49 |
| 1:AA:17:U:H1' | 1:AA:1080:A:N3 | 2.28 | 0.49 |
| 1:AA:420:U:H2' | 1:AA:422:C:C5 | 2.47 | 0.49 |
| 1:AA:79:G:C2 | 1:AA:80:A:N6 | 2.80 | 0.49 |
| 1:AA:844:G:H3' | 1:AA:844:G:OP2 | 2.13 | 0.49 |
| 1:AA:846:G:H2' | 1:AA:846:G:N3 | 2.27 | 0.49 |
| 1:AA:1074:G:H4' | 20:AB:102:ASN:HB2 | 1.94 | 0.49 |
| 2:AC:78:LYS:HE3 | 2:AC:79:LYS:NZ | 2.28 | 0.49 |
| 4:AE:92:ARG:NH1 | 4:AE:92:ARG:HB3 | 2.27 | 0.49 |
| 10:AK:83:VAL:HB | 10:AK:109:ILE:HG23 | 1.93 | 0.49 |
| 10:AK:60:PHE:O | 10:AK:64:VAL:HG12 | 2.13 | 0.49 |
| 16:AQ:74:LEU:HD13 | 16:AQ:75:VAL:N | 2.28 | 0.49 |
| 22:BA:52:A:H3' | 22:BA:53:A:H8 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1470:A:H3' | 23:BB:1471:G:H8 | 1.77 | 0.49 |
| 23:BB:2015:A:H2' | 23:BB:2016:U:O4' | 2.13 | 0.49 |
| 23:BB:2734:A:H2' | 23:BB:2735:G:C5' | 2.41 | 0.49 |
| 23:BB:2875:C:H2' | 23:BB:2876:G:C8 | 2.47 | 0.49 |
| 23:BB:454:A:H3' | 23:BB:455:C:H5' | 1.95 | 0.49 |
| 23:BB:670:A:H4' | 23:BB:671:C:O5' | 2.13 | 0.49 |
| 23:BB:751:A:C5' | 40:BS:90:LYS:HA | 2.42 | 0.49 |
| 23:BB:817:C:H2' | 23:BB:818:G:O4' | 2.13 | 0.49 |
| 26:BD:107:VAL:HA | 26:BD:204:LYS:O | 2.13 | 0.49 |
| 27:BE:170:ARG:NH2 | 27:BE:176:ASP:HB2 | 2.28 | 0.49 |
| 28:BF:111:ARG:N | 28:BF:111:ARG:HD2 | 2.28 | 0.49 |
| 28:BF:165:GLY:O | 28:BF:169:LEU:HD12 | 2.12 | 0.49 |
| 28:BF:3:LEU:HD11 | 28:BF:172:PHE:CG | 2.47 | 0.49 |
| 28:BF:45:ASP:HB3 | 28:BF:48:LEU:CD2 | 2.43 | 0.49 |
| 38:BQ:80:ASN:ND2 | 38:BQ:81:GLY:N | 2.61 | 0.49 |
| 39:BR:35:PHE:C | 39:BR:58:VAL:HG23 | 2.33 | 0.49 |
| 41:BT:43:ILE:O | 41:BT:47:VAL:HG23 | 2.13 | 0.49 |
| 23:BB:309:A:H4' | 42:BU:15:GLY:CA | 2.42 | 0.49 |
| 43:BW:32:ALA:C | 43:BW:34:SER:H | 2.16 | 0.49 |
| 46:BZ:33:LEU:O | 46:BZ:34:HIS:CG | 2.66 | 0.49 |
| 1:CA:1206:G:H4' | 2:CC:191:THR:O | 2.13 | 0.49 |
| 1:CA:1320:C:N4 | 18:CS:35:ARG:HD3 | 2.28 | 0.49 |
| 1:CA:1339:A:H2' | 1:CA:1340:A:O4' | 2.12 | 0.49 |
| 1:CA:1423:G:H2' | 1:CA:1424:U:C6 | 2.48 | 0.49 |
| 1:CA:1511:G:O2' | 1:CA:1512:U:H5' | 2.12 | 0.49 |
| 1:CA:398:U:H2' | 1:CA:399:G:C8 | 2.47 | 0.49 |
| 1:CA:780:A:O2' | 1:CA:781:A:H5'' | 2.13 | 0.49 |
| 20:CB:128:LEU:HD23 | 20:CB:132:GLU:CB | 2.42 | 0.49 |
| 3:CD:16:THR:HG22 | 3:CD:17:ASP:N | 2.28 | 0.49 |
| 5:CF:18:VAL:HG21 | 5:CF:58:HIS:CE1 | 2.48 | 0.49 |
| 5:CF:51:ILE:O | 5:CF:51:ILE:HG23 | 2.12 | 0.49 |
| 5:CF:53:LYS:HB2 | 5:CF:54:LEU:HD22 | 1.93 | 0.49 |
| 7:CH:95:MET:HG2 | 7:CH:98:LEU:HB2 | 1.93 | 0.49 |
| 9:CJ:76:ILE:HD12 | 9:CJ:76:ILE:O | 2.11 | 0.49 |
| 12:CM:21:ILE:HG22 | 12:CM:23:GLY:H | 1.77 | 0.49 |
| 13:CN:50:LEU:N | 13:CN:51:PRO:CD | 2.76 | 0.49 |
| 18:CS:40:PHE:HB2 | 18:CS:43:MET:HE3 | 1.95 | 0.49 |
| 48:D1:33:LEU:HB3 | 48:D1:51:ALA:CB | 2.40 | 0.49 |
| 22:DA:28:C:H2' | 22:DA:29:A:C8 | 2.48 | 0.49 |
| 23:DB:1168:G:O2' | 23:DB:1169:A:H5' | 2.11 | 0.49 |
| 23:DB:1580:A:H2' | 23:DB:1581:G:O4' | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1792:G:OP1 | 25:DC:204:LEU:HD12 | 2.13 | 0.49 |
| 23:DB:1985:C:O2' | 23:DB:1986:C:H5' | 2.13 | 0.49 |
| 23:DB:2221:G:O2' | 23:DB:2222:C:H5' | 2.13 | 0.49 |
| 23:DB:2818:U:H4' | 23:DB:2837:A:O4' | 2.13 | 0.49 |
| 23:DB:616:A:H3' | 23:DB:617:G:C8 | 2.43 | 0.49 |
| 23:DB:655:A:H4' | 23:DB:656:G:H5' | 1.95 | 0.49 |
| 26:DD:149:ASN:O | 26:DD:152:PRO:HD2 | 2.12 | 0.49 |
| 26:DD:51:THR:HG23 | 26:DD:78:GLY:O | 2.12 | 0.49 |
| 26:DD:36:GLN:HB3 | 26:DD:67:HIS:HE1 | 1.78 | 0.49 |
| 23:DB:37:C:H1' | 27:DE:45:ALA:HB2 | 1.93 | 0.49 |
| 28:DF:71:LYS:HD3 | 28:DF:73:VAL:O | 2.13 | 0.49 |
| 29:DG:11:PRO:O | 29:DG:14:VAL:HG22 | 2.13 | 0.49 |
| 29:DG:84:LYS:HG3 | 29:DG:131:VAL:C | 2.32 | 0.49 |
| 30:DH:65:ALA:HB1 | 30:DH:138:VAL:HG11 | 1.94 | 0.49 |
| 52:DI:24:GLY:HA2 | 52:DI:34:ILE:HD12 | 1.95 | 0.49 |
| 35:DN:12:ARG:HG3 | 35:DN:13:ASN:H | 1.78 | 0.49 |
| 37:DP:24:THR:N | 37:DP:87:ARG:O | 2.46 | 0.49 |
| 39:DR:16:GLU:H | 39:DR:101:ILE:CG1 | 2.23 | 0.49 |
| 39:DR:72:VAL:HG23 | 39:DR:89:HIS:O | 2.12 | 0.49 |
| 42:DU:53:GLN:N | 42:DU:54:PRO:CD | 2.76 | 0.49 |
| 43:DW:9:THR:O | 43:DW:10:ARG:HB2 | 2.12 | 0.49 |
| 46:DZ:5:CYS:HG | 46:DZ:52:SER:HG | 1.61 | 0.49 |
| 1:AA:1060:U:H2' | 1:AA:1061:G:H8 | 1.77 | 0.49 |
| 1:AA:66:A:H5' | 1:AA:173:U:O4 | 2.13 | 0.49 |
| 1:AA:34:C:H2' | 1:AA:35:G:H8 | 1.77 | 0.49 |
| 1:AA:36:C:O3' | 11:AL:119:LYS:HA | 2.12 | 0.49 |
| 1:AA:715:A:H2' | 1:AA:716:A:H8 | 1.78 | 0.49 |
| 20:AB:186:VAL:O | 20:AB:200:PRO:HA | 2.13 | 0.49 |
| 3:AD:2:ARG:HG3 | 3:AD:114:ARG:NH1 | 2.28 | 0.49 |
| 8:AI:46:VAL:HG23 | 8:AI:47:VAL:N | 2.27 | 0.49 |
| 10:AK:108:ASN:HD21 | 21:AU:6:ARG:HD2 | 1.78 | 0.49 |
| 18:AS:10:ILE:HB | 18:AS:14:LEU:HD11 | 1.95 | 0.49 |
| 21:AU:20:ARG:H | 21:AU:20:ARG:HD2 | 1.78 | 0.49 |
| 49:B2:34:ARG:HE | 49:B2:39:ARG:HG2 | 1.78 | 0.49 |
| 23:BB:2394:C:H2' | 23:BB:2395:C:C6 | 2.48 | 0.49 |
| 23:BB:245:G:H2' | 23:BB:246:C:H6 | 1.77 | 0.49 |
| 23:BB:2462:C:H2' | 23:BB:2463:C:C6 | 2.48 | 0.49 |
| 23:BB:256:A:H2' | 23:BB:257:C:H6 | 1.78 | 0.49 |
| 23:BB:2589:A:H2' | 23:BB:2590:A:H8 | 1.77 | 0.49 |
| 23:BB:2863:C:O2' | 23:BB:2864:G:H5' | 2.12 | 0.49 |
| 23:BB:704:G:H1' | 23:BB:727:A:N6 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:784:G:HO2' | 23:BB:785:G:H5'' | 1.77 | 0.49 |
| 23:BB:922:C:H1' | 43:BW:22:VAL:HG21 | 1.94 | 0.49 |
| 25:BC:153:LEU:HD13 | 25:BC:175:LEU:HD21 | 1.94 | 0.49 |
| 25:BC:92:LEU:HG | 25:BC:93:VAL:H | 1.78 | 0.49 |
| 26:BD:108:ASP:OD2 | 26:BD:206:ALA:HA | 2.12 | 0.49 |
| 27:BE:118:LEU:O | 27:BE:119:ILE:HD13 | 2.12 | 0.49 |
| 28:BF:62:GLN:HB2 | 28:BF:91:ARG:HH11 | 1.78 | 0.49 |
| 22:BA:42:C:C5 | 28:BF:65:LEU:HD22 | 2.47 | 0.49 |
| 29:BG:84:LYS:H | 29:BG:85:LYS:HD2 | 1.77 | 0.49 |
| 29:BG:89:VAL:HG12 | 29:BG:90:GLY:N | 2.26 | 0.49 |
| 30:BH:9:VAL:CG1 | 30:BH:12:LEU:HG | 2.43 | 0.49 |
| 23:BB:670:A:C4' | 33:BL:42:SER:HB2 | 2.42 | 0.49 |
| 36:BO:106:LEU:HG | 36:BO:107:ALA:N | 2.26 | 0.49 |
| 41:BT:15:HIS:O | 41:BT:16:VAL:C | 2.51 | 0.49 |
| 24:BV:30:ILE:O | 24:BV:37:PRO:HA | 2.12 | 0.49 |
| 1:CA:104:G:O2' | 1:CA:105:G:H5' | 2.13 | 0.49 |
| 1:CA:1216:A:H2' | 1:CA:1217:C:C6 | 2.47 | 0.49 |
| 1:CA:1297:G:H1' | 1:CA:1298:U:C5 | 2.44 | 0.49 |
| 1:CA:137:U:H2' | 1:CA:138:G:H8 | 1.78 | 0.49 |
| 1:CA:394:G:O2' | 1:CA:395:C:H5' | 2.13 | 0.49 |
| 1:CA:502:A:H2' | 1:CA:503:C:H6 | 1.76 | 0.49 |
| 1:CA:69:G:N2 | 1:CA:71:A:N6 | 2.61 | 0.49 |
| 1:CA:916:U:O2' | 1:CA:917:G:H5' | 2.12 | 0.49 |
| 2:CC:156:LEU:CD1 | 2:CC:165:GLU:HB2 | 2.43 | 0.49 |
| 4:CE:88:HIS:CE1 | 4:CE:137:ARG:HD2 | 2.48 | 0.49 |
| 5:CF:6:ILE:HG13 | 5:CF:6:ILE:O | 2.13 | 0.49 |
| 8:CI:22:PRO:HA | 8:CI:60:LEU:CB | 2.43 | 0.49 |
| 13:CN:79:SER:O | 13:CN:83:VAL:HG23 | 2.13 | 0.49 |
| 16:CQ:60:ILE:HD13 | 16:CQ:60:ILE:H | 1.78 | 0.49 |
| 23:DB:1033:U:H5 | 51:D4:15:LYS:HE2 | 1.78 | 0.49 |
| 23:DB:1099:G:H4' | 52:DI:4:VAL:HG12 | 1.95 | 0.49 |
| 23:DB:1150:C:O2' | 23:DB:1151:A:H5' | 2.12 | 0.49 |
| 23:DB:222:A:N1 | 23:DB:233:A:H5'' | 2.28 | 0.49 |
| 23:DB:2443:C:O2' | 23:DB:2444:G:H5' | 2.13 | 0.49 |
| 23:DB:2756:U:C1' | 23:DB:2757:A:H5'' | 2.40 | 0.49 |
| 23:DB:303:G:H2' | 23:DB:304:U:H6 | 1.78 | 0.49 |
| 25:DC:138:SER:O | 25:DC:162:GLN:HA | 2.13 | 0.49 |
| 25:DC:149:LYS:HD3 | 25:DC:152:GLN:HE22 | 1.78 | 0.49 |
| 25:DC:264:LYS:HG3 | 25:DC:265:PHE:CD2 | 2.48 | 0.49 |
| 28:DF:126:ASN:ND2 | 28:DF:156:THR:HG23 | 2.06 | 0.49 |
| 28:DF:103:ILE:HD11 | 28:DF:174:PHE:HA | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2307:G:O6 | 28:DF:40:GLY:HA3 | 2.12 | 0.49 |
| 32:DK:113:MET:HA | 32:DK:116:ILE:HD11 | 1.95 | 0.49 |
| 38:DQ:89:ILE:C | 38:DQ:91:ARG:H | 2.16 | 0.49 |
| 40:DS:25:ARG:HE | 40:DS:74:ILE:CG2 | 2.25 | 0.49 |
| 43:DW:18:LYS:HG3 | 43:DW:19:ARG:H | 1.77 | 0.49 |
| 1:AA:1114:C:O2' | 1:AA:1115:U:H5' | 2.13 | 0.49 |
| 1:AA:1464:U:H2' | 1:AA:1465:A:H8 | 1.77 | 0.49 |
| 1:AA:153:C:H2' | 1:AA:154:U:H6 | 1.78 | 0.49 |
| 1:AA:242:G:H2' | 1:AA:243:A:H5'' | 1.94 | 0.49 |
| 1:AA:382:A:H2' | 1:AA:383:A:C8 | 2.48 | 0.49 |
| 1:AA:50:A:N6 | 1:AA:361:G:H4' | 2.28 | 0.49 |
| 1:AA:602:A:H2' | 1:AA:603:U:C6 | 2.48 | 0.49 |
| 1:AA:674:G:H2' | 1:AA:675:A:C8 | 2.40 | 0.49 |
| 20:AB:31:PHE:HB2 | 20:AB:41:ASN:HA | 1.94 | 0.49 |
| 2:AC:165:GLU:HG3 | 2:AC:166:TRP:H | 1.77 | 0.49 |
| 3:AD:192:ALA:C | 3:AD:194:ILE:H | 2.16 | 0.49 |
| 3:AD:90:LEU:HD13 | 3:AD:93:LEU:HD12 | 1.94 | 0.49 |
| 4:AE:15:ILE:HB | 4:AE:35:LEU:O | 2.13 | 0.49 |
| 5:AF:54:LEU:N | 5:AF:54:LEU:HD22 | 2.28 | 0.49 |
| 7:AH:111:THR:H | 7:AH:114:ALA:HB3 | 1.76 | 0.49 |
| 9:AJ:76:ILE:O | 9:AJ:76:ILE:HD12 | 2.13 | 0.49 |
| 12:AM:44:ILE:O | 12:AM:47:LEU:HB2 | 2.12 | 0.49 |
| 12:AM:68:LEU:O | 12:AM:72:ILE:HG22 | 2.13 | 0.49 |
| 13:AN:50:LEU:N | 13:AN:51:PRO:CD | 2.76 | 0.49 |
| 16:AQ:28:VAL:O | 16:AQ:36:PHE:HA | 2.13 | 0.49 |
| 50:B3:25:HIS:HB2 | 50:B3:43:LEU:O | 2.13 | 0.49 |
| 23:BB:1444:G:H2' | 23:BB:1445:G:C8 | 2.47 | 0.49 |
| 23:BB:150:U:H2' | 23:BB:151:C:H6 | 1.76 | 0.49 |
| 23:BB:1951:U:H2' | 23:BB:1953:A:OP2 | 2.13 | 0.49 |
| 23:BB:2101:A:H2' | 23:BB:2102:G:O4' | 2.13 | 0.49 |
| 23:BB:2284:A:OP1 | 48:B1:4:ILE:HG12 | 2.12 | 0.49 |
| 23:BB:2721:A:H2' | 23:BB:2722:G:C8 | 2.48 | 0.49 |
| 23:BB:311:A:H3' | 23:BB:312:G:H8 | 1.78 | 0.49 |
| 23:BB:392:U:H2' | 23:BB:393:C:H6 | 1.78 | 0.49 |
| 23:BB:2073:C:C5' | 25:BC:227:VAL:HG12 | 2.43 | 0.49 |
| 25:BC:77:VAL:HG23 | 25:BC:112:GLY:N | 2.08 | 0.49 |
| 26:BD:30:GLU:OE1 | 26:BD:53:GLY:HA2 | 2.13 | 0.49 |
| 27:BE:176:ASP:OD1 | 27:BE:178:VAL:HG12 | 2.12 | 0.49 |
| 28:BF:102:LEU:HD13 | 28:BF:103:ILE:HB | 1.93 | 0.49 |
| 29:BG:42:VAL:HA | 29:BG:50:THR:O | 2.13 | 0.49 |
| 31:BJ:110:PRO:HB2 | 31:BJ:111:LYS:HE3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BL:105:ILE:HG22 | 33:BL:106:GLU:N | 2.28 | 0.49 |
| 27:BE:181:ILE:HG13 | 33:BL:2:ARG:HE | 1.78 | 0.49 |
| 38:BQ:63:ARG:HH21 | 38:BQ:64:ILE:HD13 | 1.78 | 0.49 |
| 1:CA:1225:A:H5' | 1:CA:1226:C:OP2 | 2.13 | 0.49 |
| 1:CA:1238:A:C8 | 1:CA:1303:C:H1' | 2.48 | 0.49 |
| 1:CA:660:C:H2' | 1:CA:661:G:O4' | 2.13 | 0.49 |
| 1:CA:847:G:H2' | 1:CA:848:C:C6 | 2.48 | 0.49 |
| 20:CB:14:HIS:HD2 | 20:CB:202:ASN:H | 1.60 | 0.49 |
| 3:CD:106:PHE:CE1 | 3:CD:158:LEU:HD21 | 2.48 | 0.49 |
| 4:CE:132:PRO:HG2 | 4:CE:133:ILE:H | 1.78 | 0.49 |
| 4:CE:136:VAL:HG13 | 4:CE:137:ARG:H | 1.78 | 0.49 |
| 11:CL:81:ILE:HG23 | 11:CL:94:TYR:HB3 | 1.95 | 0.49 |
| 15:CP:72:ALA:HA | 15:CP:75:ILE:HD12 | 1.95 | 0.49 |
| 47:D0:47:TYR:O | 47:D0:48:TYR:HB2 | 2.12 | 0.49 |
| 50:D3:15:LYS:HA | 50:D3:21:PHE:HA | 1.95 | 0.49 |
| 23:DB:138:U:H2' | 23:DB:140:C:C4' | 2.42 | 0.49 |
| 23:DB:2223:G:C2' | 23:DB:2224:G:H5' | 2.43 | 0.49 |
| 23:DB:2240:U:O2' | 23:DB:2241:A:H5' | 2.12 | 0.49 |
| 23:DB:545:U:H5'' | 23:DB:546:U:C4' | 2.19 | 0.49 |
| 23:DB:545:U:H2' | 23:DB:547:A:OP1 | 2.13 | 0.49 |
| 23:DB:626:A:H2' | 33:DL:78:ARG:NH1 | 2.28 | 0.49 |
| 23:DB:2772:C:H4' | 26:DD:171:THR:HG21 | 1.95 | 0.49 |
| 23:DB:1256:G:H21 | 27:DE:77:ILE:CG2 | 2.26 | 0.49 |
| 28:DF:33:ILE:HB | 28:DF:90:LEU:HG | 1.95 | 0.49 |
| 29:DG:154:GLU:CD | 29:DG:156:TYR:HB2 | 2.33 | 0.49 |
| 52:DI:19:PRO:HB2 | 52:DI:22:PRO:HD2 | 1.95 | 0.49 |
| 31:DJ:16:TYR:CD2 | 31:DJ:140:LEU:HD12 | 2.48 | 0.49 |
| 31:DJ:38:GLY:HA3 | 31:DJ:50:THR:O | 2.13 | 0.49 |
| 33:DL:125:LEU:H | 33:DL:143:GLU:HG3 | 1.78 | 0.49 |
| 35:DN:90:ARG:HB3 | 35:DN:94:TYR:HE1 | 1.78 | 0.49 |
| 39:DR:71:LYS:HG2 | 39:DR:73:LYS:HZ1 | 1.76 | 0.49 |
| 43:DW:51:GLY:N | 43:DW:59:PHE:HB2 | 2.28 | 0.49 |
| 44:DX:21:LEU:HD23 | 44:DX:21:LEU:H | 1.78 | 0.49 |
| 46:DZ:68:LEU:HB3 | 46:DZ:78:TYR:HE1 | 1.76 | 0.49 |
| 1:AA:1109:C:H2' | 1:AA:1110:A:O4' | 2.13 | 0.48 |
| 1:AA:1221:G:O2' | 1:AA:1222:G:H5' | 2.13 | 0.48 |
| 1:AA:1239:A:H4' | 1:AA:1240:U:C5' | 2.43 | 0.48 |
| 1:AA:1254:A:H2' | 1:AA:1255:G:C8 | 2.48 | 0.48 |
| 1:AA:815:A:H4' | 1:AA:817:C:C4 | 2.48 | 0.48 |
| 1:AA:922:G:H2' | 1:AA:923:A:C8 | 2.49 | 0.48 |
| 20:AB:23:ASN:C | 20:AB:25:LYS:H | 2.16 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:AD:22:SER:HB2 | 3:AD:109:THR:HG22 | 1.94 | 0.48 |
| 1:AA:598:U:H4' | 7:AH:85:TYR:CG | 2.48 | 0.48 |
| 7:AH:9:MET:O | 7:AH:13:ILE:HG13 | 2.13 | 0.48 |
| 8:AI:44:ARG:HE | 8:AI:48:ARG:HH22 | 1.61 | 0.48 |
| 10:AK:86:LYS:HB2 | 10:AK:113:THR:HA | 1.94 | 0.48 |
| 12:AM:86:ARG:HA | 12:AM:96:VAL:CG1 | 2.43 | 0.48 |
| 13:AN:79:SER:O | 13:AN:83:VAL:HG23 | 2.13 | 0.48 |
| 47:B0:18:HIS:HD1 | 47:B0:18:HIS:H | 1.59 | 0.48 |
| 23:BB:1729:U:O4 | 23:BB:1733:G:H1' | 2.12 | 0.48 |
| 23:BB:1985:C:O2' | 23:BB:1986:C:H5' | 2.13 | 0.48 |
| 23:BB:2070:A:H2' | 23:BB:2071:A:C8 | 2.49 | 0.48 |
| 23:BB:2234:G:O2' | 23:BB:2235:G:H5' | 2.13 | 0.48 |
| 23:BB:2783:U:H2' | 23:BB:2784:U:C6 | 2.47 | 0.48 |
| 23:BB:2849:U:H4' | 23:BB:2850:A:C5' | 2.43 | 0.48 |
| 23:BB:796:C:H2' | 23:BB:797:G:H8 | 1.78 | 0.48 |
| 23:BB:904:G:H2' | 23:BB:905:A:H8 | 1.77 | 0.48 |
| 23:BB:992:C:H2' | 23:BB:993:G:H8 | 1.78 | 0.48 |
| 28:BF:33:ILE:HB | 28:BF:90:LEU:HG | 1.95 | 0.48 |
| 29:BG:116:LEU:HD23 | 29:BG:121:THR:HA | 1.94 | 0.48 |
| 29:BG:93:TYR:O | 29:BG:94:ARG:HG3 | 2.11 | 0.48 |
| 30:BH:108:VAL:HG12 | 30:BH:109:GLU:H | 1.78 | 0.48 |
| 30:BH:53:GLU:HA | 30:BH:53:GLU:OE1 | 2.12 | 0.48 |
| 30:BH:66:ASN:N | 30:BH:66:ASN:HD22 | 2.12 | 0.48 |
| 30:BH:80:ILE:H | 30:BH:145:ASN:H | 1.61 | 0.48 |
| 52:BI:89:SER:HA | 52:BI:97:VAL:CG2 | 2.43 | 0.48 |
| 34:BM:86:LYS:HG3 | 34:BM:87:GLY:N | 2.27 | 0.48 |
| 34:BM:35:ALA:HB3 | 34:BM:99:GLY:H | 1.78 | 0.48 |
| 38:BQ:35:PHE:O | 38:BQ:39:ILE:HG12 | 2.13 | 0.48 |
| 38:BQ:80:ASN:C | 38:BQ:82:LEU:H | 2.17 | 0.48 |
| 41:BT:50:LEU:N | 41:BT:50:LEU:HD22 | 2.28 | 0.48 |
| 44:BX:3:ALA:O | 44:BX:6:LEU:HB2 | 2.12 | 0.48 |
| 1:CA:591:U:H2' | 1:CA:592:G:H8 | 1.78 | 0.48 |
| 1:CA:724:G:H2' | 1:CA:725:G:H8 | 1.77 | 0.48 |
| 1:CA:728:A:H2' | 1:CA:729:A:H8 | 1.77 | 0.48 |
| 20:CB:113:LEU:HD23 | 20:CB:114:LYS:N | 2.28 | 0.48 |
| 20:CB:40:ILE:HD13 | 20:CB:201:GLY:HA2 | 1.93 | 0.48 |
| 7:CH:12:ARG:HH11 | 7:CH:12:ARG:HG3 | 1.78 | 0.48 |
| 12:CM:9:PRO:HB2 | 12:CM:17:ALA:HB1 | 1.95 | 0.48 |
| 16:CQ:10:ARG:NH2 | 16:CQ:55:GLY:HA2 | 2.28 | 0.48 |
| 50:D3:25:HIS:HB2 | 50:D3:43:LEU:O | 2.13 | 0.48 |
| 22:DA:39:A:O2' | 22:DA:40:U:H5' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:74:U:H2' | 22:DA:75:G:C8 | 2.48 | 0.48 |
| 23:DB:1348:C:H2' | 23:DB:1349:C:H5' | 1.94 | 0.48 |
| 23:DB:1794:A:H2' | 23:DB:1795:C:C6 | 2.48 | 0.48 |
| 23:DB:1826:G:H2' | 23:DB:1827:U:C6 | 2.48 | 0.48 |
| 23:DB:1939:U:O2 | 23:DB:1967:C:H4' | 2.13 | 0.48 |
| 23:DB:2405:G:H1' | 23:DB:2412:A:H61 | 1.78 | 0.48 |
| 23:DB:519:U:H2' | 23:DB:520:G:C8 | 2.48 | 0.48 |
| 23:DB:685:A:H1' | 23:DB:688:U:O4 | 2.13 | 0.48 |
| 25:DC:239:PHE:HD1 | 25:DC:241:LYS:H | 1.59 | 0.48 |
| 26:DD:171:THR:HG23 | 26:DD:172:VAL:H | 1.77 | 0.48 |
| 28:DF:79:ARG:HB2 | 28:DF:82:TYR:CE2 | 2.48 | 0.48 |
| 32:DK:35:VAL:H | 32:DK:65:THR:HG21 | 1.78 | 0.48 |
| 35:DN:90:ARG:HB3 | 35:DN:94:TYR:CE1 | 2.48 | 0.48 |
| 38:DQ:91:ARG:HE | 38:DQ:94:LEU:HD23 | 1.77 | 0.48 |
| 1:AA:1001:C:H2' | 1:AA:1002:G:H8 | 1.78 | 0.48 |
| 1:AA:1234:C:H1' | 1:AA:1364:U:O2 | 2.14 | 0.48 |
| 1:AA:1414:U:H2' | 1:AA:1415:G:C8 | 2.48 | 0.48 |
| 1:AA:1424:U:H2' | 1:AA:1425:U:C6 | 2.47 | 0.48 |
| 1:AA:317:U:H2' | 1:AA:318:G:H8 | 1.78 | 0.48 |
| 1:AA:908:A:H2' | 1:AA:909:A:H8 | 1.78 | 0.48 |
| 2:AC:13:ILE:HD13 | 2:AC:13:ILE:N | 2.29 | 0.48 |
| 2:AC:149:LYS:O | 2:AC:200:TRP:HE3 | 1.95 | 0.48 |
| 3:AD:24:VAL:O | 3:AD:27:ILE:HG13 | 2.13 | 0.48 |
| 4:AE:148:SER:HB2 | 4:AE:150:GLU:OE1 | 2.13 | 0.48 |
| 4:AE:71:ILE:HG21 | 4:AE:144:GLU:OE2 | 2.12 | 0.48 |
| 6:AG:120:ALA:O | 6:AG:123:LEU:HB2 | 2.13 | 0.48 |
| 6:AG:12:LEU:HD22 | 6:AG:13:PRO:HD2 | 1.94 | 0.48 |
| 6:AG:136:LYS:O | 6:AG:140:VAL:HG23 | 2.13 | 0.48 |
| 8:AI:127:SER:O | 8:AI:129:ARG:HG3 | 2.12 | 0.48 |
| 12:AM:90:HIS:HA | 12:AM:108:ARG:HH22 | 1.76 | 0.48 |
| 14:AO:55:LEU:O | 14:AO:58:MET:HG2 | 2.14 | 0.48 |
| 1:AA:264:C:HO2' | 16:AQ:65:PRO:HG2 | 1.78 | 0.48 |
| 18:AS:62:THR:O | 18:AS:66:VAL:HG13 | 2.13 | 0.48 |
| 50:B3:58:ILE:HG13 | 50:B3:58:ILE:H | 1.39 | 0.48 |
| 22:BA:91:C:H2' | 22:BA:92:C:C6 | 2.48 | 0.48 |
| 23:BB:1059:G:H2' | 23:BB:1060:U:C5 | 2.48 | 0.48 |
| 23:BB:1210:G:H1' | 23:BB:1212:G:C2 | 2.48 | 0.48 |
| 23:BB:1716:U:H2' | 23:BB:1717:A:H8 | 1.78 | 0.48 |
| 23:BB:1838:C:H4' | 23:BB:1839:G:C8 | 2.48 | 0.48 |
| 23:BB:2282:G:OP1 | 23:BB:2283:C:H1' | 2.13 | 0.48 |
| 23:BB:2569:G:O2' | 23:BB:2570:G:H5' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2820:A:H4' | 35:BN:3:HIS:CG | 2.48 | 0.48 |
| 23:BB:623:C:H2' | 23:BB:624:C:C6 | 2.48 | 0.48 |
| 23:BB:710:U:H2' | 23:BB:711:G:H8 | 1.79 | 0.48 |
| 23:BB:851:C:H2' | 23:BB:852:U:H6 | 1.78 | 0.48 |
| 25:BC:69:ASN:O | 25:BC:70:LYS:C | 2.51 | 0.48 |
| 26:BD:116:LYS:HB3 | 26:BD:118:PHE:CZ | 2.47 | 0.48 |
| 26:BD:55:LYS:HB2 | 26:BD:60:VAL:HG13 | 1.94 | 0.48 |
| 23:BB:2531:A:H4' | 29:BG:156:TYR:CD1 | 2.48 | 0.48 |
| 30:BH:64:ALA:O | 30:BH:65:ALA:HB2 | 2.13 | 0.48 |
| 31:BJ:75:TYR:CD1 | 31:BJ:86:GLN:HB3 | 2.48 | 0.48 |
| 32:BK:35:VAL:H | 32:BK:65:THR:HG21 | 1.78 | 0.48 |
| 35:BN:11:ASN:O | 35:BN:12:ARG:HB2 | 2.13 | 0.48 |
| 36:BO:39:VAL:HB | 36:BO:49:VAL:HG22 | 1.96 | 0.48 |
| 37:BP:24:THR:N | 37:BP:87:ARG:O | 2.47 | 0.48 |
| 39:BR:61:ALA:HB1 | 39:BR:96:VAL:HB | 1.95 | 0.48 |
| 40:BS:17:VAL:HG11 | 40:BS:103:ILE:HG12 | 1.93 | 0.48 |
| 45:BY:29:ARG:H | 45:BY:33:HIS:CD2 | 2.30 | 0.48 |
| 46:BZ:76:GLU:HG3 | 46:BZ:77:LYS:H | 1.77 | 0.48 |
| 1:CA:114:U:H2' | 1:CA:115:G:C8 | 2.48 | 0.48 |
| 1:CA:386:C:C2' | 1:CA:387:U:H5' | 2.44 | 0.48 |
| 1:CA:820:U:H4' | 1:CA:821:G:OP2 | 2.12 | 0.48 |
| 1:CA:846:G:H2' | 1:CA:846:G:N3 | 2.28 | 0.48 |
| 20:CB:75:ALA:C | 20:CB:79:VAL:HG23 | 2.33 | 0.48 |
| 20:CB:93:HIS:O | 20:CB:94:ARG:O | 2.30 | 0.48 |
| 2:CC:155:ARG:H | 2:CC:162:ALA:HA | 1.78 | 0.48 |
| 3:CD:8:LEU:HD12 | 3:CD:31:CYS:SG | 2.53 | 0.48 |
| 5:CF:68:GLN:HA | 5:CF:71:ILE:HD11 | 1.95 | 0.48 |
| 8:CI:50:PRO:HD3 | 8:CI:79:ARG:CG | 2.43 | 0.48 |
| 14:CO:68:TYR:HA | 14:CO:71:ARG:HE | 1.77 | 0.48 |
| 1:CA:734:G:O2' | 17:CR:59:LYS:HD3 | 2.13 | 0.48 |
| 23:DB:1387:A:H5' | 23:DB:1469:A:H1' | 1.95 | 0.48 |
| 23:DB:1445:G:H2' | 23:DB:1446:C:O4' | 2.13 | 0.48 |
| 23:DB:1467:U:O2' | 23:DB:1468:U:H5' | 2.13 | 0.48 |
| 23:DB:1794:A:H2' | 23:DB:1795:C:H6 | 1.77 | 0.48 |
| 23:DB:1885:A:H2' | 23:DB:1886:U:O4' | 2.14 | 0.48 |
| 23:DB:2466:C:O2' | 23:DB:2467:C:H5' | 2.12 | 0.48 |
| 23:DB:492:A:H2' | 23:DB:493:G:O4' | 2.13 | 0.48 |
| 23:DB:636:G:H3' | 33:DL:128:THR:CG2 | 2.42 | 0.48 |
| 23:DB:796:C:O2' | 23:DB:797:G:H5' | 2.13 | 0.48 |
| 31:DJ:16:TYR:N | 31:DJ:137:PRO:HB3 | 2.29 | 0.48 |
| 33:DL:125:LEU:HD23 | 33:DL:126:ARG:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DQ:60:TRP:C | 38:DQ:64:ILE:HG12 | 2.33 | 0.48 |
| 38:DQ:80:ASN:ND2 | 38:DQ:81:GLY:N | 2.61 | 0.48 |
| 40:DS:76:VAL:HG12 | 40:DS:103:ILE:HA | 1.95 | 0.48 |
| 41:DT:14:PRO:HA | 41:DT:32:LEU:CB | 2.44 | 0.48 |
| 1:AA:251:G:N3 | 1:AA:266:G:O6 | 2.46 | 0.48 |
| 3:AD:31:CYS:SG | 3:AD:33:ILE:HB | 2.53 | 0.48 |
| 1:AA:1178:G:H3' | 8:AI:98:ARG:NH2 | 2.29 | 0.48 |
| 12:AM:15:VAL:HG22 | 12:AM:33:LEU:CD1 | 2.44 | 0.48 |
| 15:AP:6:LEU:HD12 | 15:AP:6:LEU:N | 2.28 | 0.48 |
| 23:BB:2539:C:H4' | 51:B4:36:ARG:HH21 | 1.77 | 0.48 |
| 23:BB:1711:A:O2' | 23:BB:1712:U:H5' | 2.13 | 0.48 |
| 23:BB:204:A:H4' | 23:BB:205:G:OP1 | 2.13 | 0.48 |
| 23:BB:2083:G:H2' | 23:BB:2084:C:C6 | 2.48 | 0.48 |
| 23:BB:2385:C:H2' | 23:BB:2386:A:C8 | 2.47 | 0.48 |
| 23:BB:2472:G:C2' | 23:BB:2475:C:H42 | 2.27 | 0.48 |
| 23:BB:286:U:O2' | 23:BB:287:G:H5' | 2.12 | 0.48 |
| 23:BB:464:U:H2' | 23:BB:465:G:O4' | 2.13 | 0.48 |
| 23:BB:571:U:O2' | 23:BB:573:U:O5' | 2.31 | 0.48 |
| 23:BB:598:U:H2' | 23:BB:599:A:C8 | 2.47 | 0.48 |
| 23:BB:816:C:O2' | 23:BB:817:C:H5' | 2.13 | 0.48 |
| 25:BC:12:ARG:HA | 25:BC:15:VAL:CG2 | 2.44 | 0.48 |
| 23:BB:320:A:H2' | 27:BE:131:THR:OG1 | 2.13 | 0.48 |
| 28:BF:105:ILE:C | 28:BF:108:PRO:HD2 | 2.34 | 0.48 |
| 28:BF:43:ILE:HA | 28:BF:46:LYS:HE2 | 1.95 | 0.48 |
| 28:BF:62:GLN:HG3 | 28:BF:91:ARG:NH1 | 2.29 | 0.48 |
| 29:BG:154:GLU:CD | 29:BG:156:TYR:HB2 | 2.33 | 0.48 |
| 29:BG:28:LYS:HG2 | 29:BG:79:THR:HA | 1.95 | 0.48 |
| 30:BH:5:LEU:HD13 | 30:BH:13:GLY:HA2 | 1.94 | 0.48 |
| 34:BM:10:ARG:HH21 | 34:BM:10:ARG:HG3 | 1.78 | 0.48 |
| 38:BQ:68:ALA:O | 38:BQ:71:ASN:HB3 | 2.13 | 0.48 |
| 38:BQ:91:ARG:HE | 38:BQ:94:LEU:HD23 | 1.77 | 0.48 |
| 39:BR:10:LYS:HD2 | 39:BR:10:LYS:N | 2.27 | 0.48 |
| 40:BS:25:ARG:HE | 40:BS:74:ILE:HG23 | 1.79 | 0.48 |
| 42:BU:11:ILE:O | 42:BU:11:ILE:HD13 | 2.12 | 0.48 |
| 42:BU:26:ASN:N | 42:BU:26:ASN:ND2 | 2.62 | 0.48 |
| 42:BU:41:VAL:O | 42:BU:59:GLU:HA | 2.13 | 0.48 |
| 46:BZ:40:VAL:CG2 | 46:BZ:43:GLU:HB3 | 2.34 | 0.48 |
| 46:BZ:45:ARG:HE | 46:BZ:47:VAL:HG12 | 1.77 | 0.48 |
| 1:CA:1001:C:H2' | 1:CA:1002:G:H8 | 1.77 | 0.48 |
| 1:CA:794:A:H2' | 1:CA:795:C:C6 | 2.48 | 0.48 |
| 1:CA:908:A:H2' | 1:CA:909:A:H8 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:CB:209:VAL:HG23 | 20:CB:210:THR:N | 2.27 | 0.48 |
| 2:CC:149:LYS:HG3 | 2:CC:168:ARG:HB2 | 1.96 | 0.48 |
| 2:CC:129:PHE:HD2 | 2:CC:156:LEU:HD22 | 1.78 | 0.48 |
| 3:CD:129:VAL:HG12 | 3:CD:131:ILE:H | 1.78 | 0.48 |
| 4:CE:53:ARG:HB3 | 4:CE:53:ARG:NH1 | 2.28 | 0.48 |
| 6:CG:67:ASN:HB2 | 6:CG:134:VAL:HG12 | 1.95 | 0.48 |
| 6:CG:70:PRO:O | 6:CG:95:ARG:HG3 | 2.13 | 0.48 |
| 11:CL:42:LYS:HB3 | 11:CL:44:PRO:HD2 | 1.94 | 0.48 |
| 13:CN:5:MET:SD | 13:CN:8:ARG:HD3 | 2.53 | 0.48 |
| 17:CR:42:ARG:HG3 | 17:CR:43:ILE:H | 1.78 | 0.48 |
| 22:DA:30:C:H2' | 22:DA:31:C:H5' | 1.95 | 0.48 |
| 23:DB:1290:C:O2' | 23:DB:1291:C:H5' | 2.13 | 0.48 |
| 23:DB:1292:G:H2' | 23:DB:1293:C:H6 | 1.77 | 0.48 |
| 23:DB:1793:C:H2' | 23:DB:1794:A:C8 | 2.48 | 0.48 |
| 23:DB:2074:U:O2' | 23:DB:2075:U:H5' | 2.13 | 0.48 |
| 23:DB:2391:G:HO2' | 23:DB:2424:C:H41 | 1.61 | 0.48 |
| 23:DB:2663:G:H2' | 23:DB:2664:G:O4' | 2.13 | 0.48 |
| 23:DB:2675:A:N1 | 23:DB:2732:G:O6 | 2.47 | 0.48 |
| 23:DB:2708:G:O2' | 23:DB:2709:G:H5' | 2.11 | 0.48 |
| 23:DB:2897:U:H2' | 23:DB:2898:U:H6 | 1.76 | 0.48 |
| 25:DC:43:ASN:HD22 | 25:DC:44:ASN:N | 2.11 | 0.48 |
| 25:DC:57:HIS:CG | 25:DC:58:LYS:H | 2.31 | 0.48 |
| 26:DD:106:LYS:O | 26:DD:107:VAL:HB | 2.13 | 0.48 |
| 26:DD:107:VAL:N | 26:DD:206:ALA:H | 2.11 | 0.48 |
| 30:DH:113:SER:N | 30:DH:132:PHE:HZ | 2.11 | 0.48 |
| 30:DH:87:GLU:HB2 | 30:DH:89:LYS:NZ | 2.27 | 0.48 |
| 52:DI:11:GLN:HA | 52:DI:55:PRO:HA | 1.94 | 0.48 |
| 52:DI:100:ILE:O | 52:DI:139:VAL:HA | 2.14 | 0.48 |
| 31:DJ:64:VAL:O | 31:DJ:68:LYS:HD2 | 2.12 | 0.48 |
| 34:DM:55:ARG:HH22 | 34:DM:58:LYS:HA | 1.78 | 0.48 |
| 1:AA:1390:U:O2' | 1:AA:1391:U:H5' | 2.14 | 0.48 |
| 1:AA:175:C:H2' | 1:AA:176:C:H6 | 1.78 | 0.48 |
| 1:AA:56:U:H2' | 1:AA:57:G:H8 | 1.79 | 0.48 |
| 1:AA:591:U:OP2 | 7:AH:30:LYS:HE2 | 2.14 | 0.48 |
| 1:AA:624:C:H2' | 1:AA:625:U:C6 | 2.48 | 0.48 |
| 1:AA:814:A:H5' | 1:AA:1511:G:H4' | 1.96 | 0.48 |
| 1:AA:87:C:H2' | 1:AA:88:U:O3' | 2.13 | 0.48 |
| 2:AC:149:LYS:HE3 | 2:AC:166:TRP:CH2 | 2.49 | 0.48 |
| 3:AD:104:MET:SD | 3:AD:179:GLY:HA3 | 2.54 | 0.48 |
| 4:AE:87:VAL:HG22 | 4:AE:88:HIS:N | 2.28 | 0.48 |
| 11:AL:33:CYS:HA | 11:AL:54:VAL:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:AR:58:ILE:O | 17:AR:62:ARG:HG3 | 2.14 | 0.48 |
| 21:AU:39:LYS:HD3 | 21:AU:39:LYS:H | 1.78 | 0.48 |
| 23:BB:1387:A:H5' | 23:BB:1469:A:H1' | 1.95 | 0.48 |
| 23:BB:2286:G:H4' | 23:BB:2287:A:O4' | 2.13 | 0.48 |
| 23:BB:235:U:H2' | 23:BB:236:C:C6 | 2.47 | 0.48 |
| 23:BB:2557:G:H2' | 23:BB:2558:C:H6 | 1.74 | 0.48 |
| 23:BB:2716:C:H2' | 23:BB:2717:C:C6 | 2.48 | 0.48 |
| 23:BB:392:U:O2' | 23:BB:393:C:H5' | 2.14 | 0.48 |
| 23:BB:783:A:H2' | 23:BB:784:G:O5' | 2.12 | 0.48 |
| 23:BB:812:C:H5' | 23:BB:1250:G:O2' | 2.12 | 0.48 |
| 23:BB:939:G:O2' | 23:BB:940:G:H5' | 2.13 | 0.48 |
| 23:BB:979:A:H2' | 23:BB:982:C:N4 | 2.20 | 0.48 |
| 26:BD:171:THR:HG23 | 26:BD:172:VAL:H | 1.78 | 0.48 |
| 28:BF:126:ASN:ND2 | 28:BF:156:THR:HG23 | 2.05 | 0.48 |
| 28:BF:70:ARG:HA | 28:BF:80:GLN:NE2 | 2.29 | 0.48 |
| 29:BG:10:VAL:HG23 | 29:BG:48:THR:HA | 1.94 | 0.48 |
| 31:BJ:125:TYR:HH | 31:BJ:132:HIS:CE1 | 2.32 | 0.48 |
| 33:BL:73:ILE:HD12 | 33:BL:106:GLU:HB2 | 1.95 | 0.48 |
| 23:BB:196:A:H5'' | 33:BL:47:ARG:HH12 | 1.78 | 0.48 |
| 33:BL:77:ILE:HG12 | 33:BL:95:LEU:HD22 | 1.94 | 0.48 |
| 24:BV:77:VAL:CG1 | 34:BM:136:MET:HB3 | 2.43 | 0.48 |
| 36:BO:49:VAL:HG11 | 36:BO:82:ALA:CA | 2.41 | 0.48 |
| 42:BU:53:GLN:N | 42:BU:54:PRO:CD | 2.76 | 0.48 |
| 42:BU:82:VAL:CG1 | 42:BU:93:ARG:HB3 | 2.43 | 0.48 |
| 24:BV:72:VAL:HG21 | 24:BV:91:PHE:CG | 2.48 | 0.48 |
| 43:BW:30:VAL:HA | 43:BW:60:ALA:O | 2.12 | 0.48 |
| 46:BZ:56:MET:O | 46:BZ:59:ILE:HG12 | 2.13 | 0.48 |
| 1:CA:1060:U:H5'' | 9:CJ:53:ILE:HG12 | 1.94 | 0.48 |
| 1:CA:233:C:H2' | 1:CA:234:C:H6 | 1.78 | 0.48 |
| 1:CA:308:C:H2' | 1:CA:309:A:H8 | 1.78 | 0.48 |
| 1:CA:475:C:H2' | 1:CA:476:U:H6 | 1.78 | 0.48 |
| 1:CA:474:G:O2' | 1:CA:475:C:H5' | 2.13 | 0.48 |
| 1:CA:586:C:H2' | 1:CA:587:G:H5' | 1.95 | 0.48 |
| 1:CA:775:G:H2' | 1:CA:776:G:H8 | 1.78 | 0.48 |
| 1:CA:815:A:H4' | 1:CA:817:C:C4 | 2.49 | 0.48 |
| 5:CF:21:MET:HB3 | 5:CF:25:TYR:CZ | 2.48 | 0.48 |
| 5:CF:6:ILE:HG23 | 5:CF:62:MET:HB3 | 1.95 | 0.48 |
| 11:CL:98:ARG:HD2 | 11:CL:103:CYS:SG | 2.53 | 0.48 |
| 11:CL:2:THR:HG22 | 11:CL:5:GLN:HE21 | 1.79 | 0.48 |
| 13:CN:97:LYS:NZ | 13:CN:97:LYS:HB3 | 2.28 | 0.48 |
| 47:D0:18:HIS:H | 47:D0:18:HIS:HD1 | 1.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1369:G:O2' | 23:DB:1370:C:H5' | 2.14 | 0.48 |
| 23:DB:1436:G:O2' | 23:DB:1437:C:H5' | 2.13 | 0.48 |
| 23:DB:1716:U:H2' | 23:DB:1717:A:H8 | 1.78 | 0.48 |
| 23:DB:1729:U:O4 | 23:DB:1733:G:H1' | 2.13 | 0.48 |
| 23:DB:2144:G:H2' | 23:DB:2145:C:O3' | 2.13 | 0.48 |
| 23:DB:2462:C:H2' | 23:DB:2463:C:C6 | 2.47 | 0.48 |
| 23:DB:2617:U:O2' | 23:DB:2618:G:H5' | 2.13 | 0.48 |
| 25:DC:14:HIS:O | 25:DC:16:VAL:HG23 | 2.13 | 0.48 |
| 25:DC:259:ASN:C | 25:DC:261:ARG:H | 2.16 | 0.48 |
| 25:DC:35:LYS:HG2 | 25:DC:36:ASN:N | 2.25 | 0.48 |
| 25:DC:64:VAL:HG11 | 25:DC:66:PHE:CE2 | 2.49 | 0.48 |
| 25:DC:93:VAL:HG13 | 25:DC:94:LEU:H | 1.77 | 0.48 |
| 26:DD:171:THR:HG23 | 26:DD:172:VAL:N | 2.28 | 0.48 |
| 26:DD:25:THR:HG21 | 26:DD:193:VAL:CG2 | 2.39 | 0.48 |
| 26:DD:33:ARG:HG2 | 26:DD:33:ARG:HH21 | 1.78 | 0.48 |
| 27:DE:188:MET:HE2 | 27:DE:193:VAL:HG22 | 1.94 | 0.48 |
| 27:DE:106:LYS:CE | 27:DE:200:LEU:HB3 | 2.42 | 0.48 |
| 29:DG:166:GLU:CG | 29:DG:168:VAL:HG23 | 2.43 | 0.48 |
| 30:DH:47:PHE:CE1 | 30:DH:51:ARG:HD3 | 2.48 | 0.48 |
| 23:DB:1098:A:C3' | 52:DI:3:LYS:HA | 2.26 | 0.48 |
| 33:DL:95:LEU:HD12 | 33:DL:95:LEU:H | 1.78 | 0.48 |
| 36:DO:67:ASN:O | 36:DO:69:ASP:N | 2.46 | 0.48 |
| 37:DP:52:ARG:NH1 | 37:DP:52:ARG:HG2 | 2.27 | 0.48 |
| 23:DB:559:G:H21 | 38:DQ:51:GLN:NE2 | 2.11 | 0.48 |
| 38:DQ:56:PHE:O | 38:DQ:59:LEU:HB3 | 2.12 | 0.48 |
| 24:DV:14:LYS:HE3 | 24:DV:18:ARG:NH2 | 2.29 | 0.48 |
| 1:AA:1320:C:N4 | 18:AS:35:ARG:HD3 | 2.28 | 0.48 |
| 1:AA:309:A:O2' | 1:AA:310:G:H5' | 2.12 | 0.48 |
| 1:AA:36:C:O2' | 1:AA:37:U:H5' | 2.14 | 0.48 |
| 1:AA:409:U:OP1 | 3:AD:23:GLY:HA3 | 2.13 | 0.48 |
| 1:AA:69:G:H2' | 1:AA:70:U:C6 | 2.48 | 0.48 |
| 1:AA:957:U:H2' | 1:AA:959:A:OP2 | 2.13 | 0.48 |
| 20:AB:63:LYS:HA | 20:AB:224:ARG:NH1 | 2.29 | 0.48 |
| 2:AC:21:TRP:CH2 | 2:AC:31:ASN:HB3 | 2.49 | 0.48 |
| 2:AC:91:ALA:HB2 | 2:AC:98:ALA:H | 1.78 | 0.48 |
| 3:AD:10:LEU:HD12 | 3:AD:20:LEU:HD11 | 1.96 | 0.48 |
| 4:AE:80:LEU:HA | 4:AE:146:MET:HE1 | 1.95 | 0.48 |
| 7:AH:7:ALA:O | 7:AH:11:THR:HG23 | 2.14 | 0.48 |
| 7:AH:95:MET:HG2 | 7:AH:98:LEU:HB2 | 1.95 | 0.48 |
| 8:AI:32:ARG:HD3 | 8:AI:37:TYR:CD1 | 2.49 | 0.48 |
| 12:AM:89:ARG:CB | 12:AM:96:VAL:HG22 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AN:29:ILE:HB | 13:AN:30:ILE:HD12 | 1.95 | 0.48 |
| 15:AP:36:VAL:HG13 | 15:AP:36:VAL:O | 2.14 | 0.48 |
| 16:AQ:60:ILE:HG22 | 16:AQ:74:LEU:HA | 1.95 | 0.48 |
| 19:AT:61:ALA:HB1 | 19:AT:67:HIS:HA | 1.95 | 0.48 |
| 21:AU:33:ARG:HG2 | 21:AU:34:ARG:N | 2.27 | 0.48 |
| 23:BB:1606:C:H5'' | 23:BB:1607:C:OP1 | 2.14 | 0.48 |
| 23:BB:1678:A:H2' | 23:BB:1679:A:C8 | 2.45 | 0.48 |
| 23:BB:1682:G:H2' | 23:BB:1683:U:C6 | 2.49 | 0.48 |
| 23:BB:1848:A:H2' | 23:BB:1849:G:C8 | 2.47 | 0.48 |
| 23:BB:2025:C:H2' | 23:BB:2026:U:H6 | 1.77 | 0.48 |
| 23:BB:2305:U:H2' | 23:BB:2306:C:C6 | 2.47 | 0.48 |
| 23:BB:2471:A:O2' | 23:BB:2472:G:O5' | 2.30 | 0.48 |
| 23:BB:2583:G:H2' | 23:BB:2584:U:O4' | 2.14 | 0.48 |
| 23:BB:2835:A:N6 | 23:BB:2878:U:H2' | 2.29 | 0.48 |
| 25:BC:105:ALA:HB1 | 25:BC:109:LEU:CD1 | 2.43 | 0.48 |
| 25:BC:54:GLY:O | 25:BC:214:GLY:HA2 | 2.14 | 0.48 |
| 25:BC:43:ASN:HB2 | 25:BC:49:THR:CG2 | 2.43 | 0.48 |
| 26:BD:36:GLN:HB3 | 26:BD:67:HIS:HE1 | 1.79 | 0.48 |
| 28:BF:33:ILE:O | 28:BF:90:LEU:HB2 | 2.14 | 0.48 |
| 29:BG:88:LEU:O | 29:BG:88:LEU:HD12 | 2.13 | 0.48 |
| 30:BH:9:VAL:HG11 | 30:BH:12:LEU:HG | 1.95 | 0.48 |
| 30:BH:26:ALA:C | 30:BH:28:ASN:N | 2.66 | 0.48 |
| 30:BH:48:GLU:HG2 | 30:BH:49:ALA:N | 2.29 | 0.48 |
| 23:BB:1059:G:O2' | 52:BI:112:LYS:HE2 | 2.14 | 0.48 |
| 1:CA:546:A:P | 3:CD:68:GLU:HB3 | 2.53 | 0.48 |
| 1:CA:923:A:H2' | 1:CA:924:C:H6 | 1.77 | 0.48 |
| 20:CB:10:LYS:O | 20:CB:13:VAL:HG23 | 2.13 | 0.48 |
| 2:CC:59:PRO:HD2 | 2:CC:62:SER:O | 2.13 | 0.48 |
| 8:CI:32:ARG:HD3 | 8:CI:37:TYR:CD1 | 2.47 | 0.48 |
| 11:CL:66:ILE:N | 11:CL:66:ILE:HD12 | 2.28 | 0.48 |
| 13:CN:68:ARG:HG2 | 13:CN:68:ARG:HH11 | 1.78 | 0.48 |
| 19:CT:70:LYS:O | 19:CT:74:HIS:HB2 | 2.13 | 0.48 |
| 48:D1:49:LYS:O | 48:D1:50:GLU:HB3 | 2.14 | 0.48 |
| 23:DB:1309:G:OP1 | 49:D2:9:VAL:HG12 | 2.14 | 0.48 |
| 23:DB:1199:U:H5'' | 56:DB:3623:HOH:O | 2.12 | 0.48 |
| 23:DB:1247:A:O2' | 23:DB:1248:G:H5' | 2.13 | 0.48 |
| 23:DB:1266:G:OP1 | 47:D0:15:ARG:NE | 2.42 | 0.48 |
| 23:DB:1403:A:H2' | 23:DB:1404:C:C6 | 2.49 | 0.48 |
| 23:DB:1534:U:H2' | 23:DB:1536:C:C5 | 2.49 | 0.48 |
| 23:DB:2811:G:OP1 | 26:DD:61:THR:HB | 2.12 | 0.48 |
| 23:DB:48:G:HO2' | 23:DB:49:A:H2 | 1.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:69:C:H2' | 23:DB:70:G:H8 | 1.78 | 0.48 |
| 23:DB:969:G:H2' | 23:DB:970:U:C6 | 2.49 | 0.48 |
| 23:DB:2590:A:H5'' | 25:DC:237:ARG:NH2 | 2.28 | 0.48 |
| 27:DE:34:ALA:HA | 27:DE:94:GLN:NE2 | 2.28 | 0.48 |
| 29:DG:25:ILE:HD12 | 29:DG:25:ILE:N | 2.29 | 0.48 |
| 29:DG:49:LEU:HD23 | 29:DG:51:PHE:CZ | 2.48 | 0.48 |
| 31:DJ:3:THR:HG21 | 38:DQ:60:TRP:HE1 | 1.78 | 0.48 |
| 39:DR:34:GLU:HB3 | 39:DR:58:VAL:HG21 | 1.95 | 0.48 |
| 42:DU:78:LYS:CG | 42:DU:79:ALA:H | 2.27 | 0.48 |
| 23:DB:2336:A:H61 | 43:DW:40:ARG:HD2 | 1.75 | 0.48 |
| 43:DW:49:ASN:CB | 43:DW:61:LYS:H | 2.25 | 0.48 |
| 46:DZ:45:ARG:HE | 46:DZ:47:VAL:HG12 | 1.77 | 0.48 |
| 46:DZ:5:CYS:SG | 46:DZ:8:THR:HG23 | 2.54 | 0.48 |
| 1:AA:1530:G:HO2' | 1:AA:1531:A:H8 | 1.62 | 0.48 |
| 1:AA:517:G:H22 | 1:AA:533:A:P | 2.37 | 0.48 |
| 1:AA:660:C:H2' | 1:AA:661:G:O4' | 2.13 | 0.48 |
| 3:AD:160:LEU:H | 3:AD:160:LEU:CD1 | 2.16 | 0.48 |
| 3:AD:10:LEU:HD13 | 3:AD:62:ARG:HD3 | 1.95 | 0.48 |
| 6:AG:4:ARG:CG | 6:AG:5:VAL:H | 2.22 | 0.48 |
| 8:AI:12:LYS:HA | 8:AI:109:GLN:HG2 | 1.94 | 0.48 |
| 8:AI:17:ARG:HB2 | 8:AI:65:THR:HB | 1.95 | 0.48 |
| 11:AL:33:CYS:H | 11:AL:54:VAL:HG13 | 1.79 | 0.48 |
| 11:AL:65:TYR:HB3 | 11:AL:95:HIS:CD2 | 2.48 | 0.48 |
| 11:AL:81:ILE:HG23 | 11:AL:94:TYR:HB3 | 1.95 | 0.48 |
| 12:AM:52:ILE:HA | 12:AM:55:LEU:HG | 1.96 | 0.48 |
| 16:AQ:3:LYS:HG3 | 16:AQ:4:ILE:H | 1.78 | 0.48 |
| 22:BA:76:G:H1 | 22:BA:101:A:H61 | 1.60 | 0.48 |
| 23:BB:1196:C:H2' | 23:BB:1197:G:H8 | 1.78 | 0.48 |
| 23:BB:1463:C:H2' | 23:BB:1464:G:C8 | 2.49 | 0.48 |
| 23:BB:1508:A:H3' | 23:BB:1509:A:C2 | 2.48 | 0.48 |
| 23:BB:1655:A:H2' | 23:BB:1656:C:O4' | 2.13 | 0.48 |
| 23:BB:1945:G:H2' | 23:BB:1946:U:C6 | 2.49 | 0.48 |
| 23:BB:2027:G:O2' | 23:BB:2028:U:H5' | 2.13 | 0.48 |
| 23:BB:2150:C:O2' | 23:BB:2151:U:H5' | 2.13 | 0.48 |
| 23:BB:2273:A:H2' | 23:BB:2274:A:C8 | 2.48 | 0.48 |
| 23:BB:2385:C:H2' | 23:BB:2386:A:H8 | 1.78 | 0.48 |
| 23:BB:2391:G:HO2' | 23:BB:2392:A:P | 2.36 | 0.48 |
| 23:BB:543:G:H2' | 23:BB:544:C:C5' | 2.43 | 0.48 |
| 26:BD:107:VAL:N | 26:BD:206:ALA:H | 2.11 | 0.48 |
| 27:BE:172:ALA:HB2 | 27:BE:195:GLN:NE2 | 2.29 | 0.48 |
| 28:BF:31:GLU:C | 28:BF:32:LYS:HD3 | 2.34 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BF:55:ASP:O | 28:BF:59:ILE:HG13 | 2.13 | 0.48 |
| 30:BH:131:SER:HA | 30:BH:142:VAL:N | 2.27 | 0.48 |
| 52:BI:124:MET:O | 52:BI:128:ILE:HG12 | 2.13 | 0.48 |
| 31:BJ:98:GLU:HB3 | 31:BJ:124:VAL:HG21 | 1.95 | 0.48 |
| 23:BB:2723:C:H5' | 35:BN:1:MET:HE2 | 1.94 | 0.48 |
| 23:BB:2821:A:OP2 | 35:BN:3:HIS:NE2 | 2.47 | 0.48 |
| 36:BO:30:ARG:HG3 | 36:BO:30:ARG:NH1 | 2.29 | 0.48 |
| 32:BK:77:ILE:HD11 | 37:BP:71:ARG:CZ | 2.43 | 0.48 |
| 38:BQ:7:VAL:HG23 | 38:BQ:8:ILE:N | 2.29 | 0.48 |
| 41:BT:51:PHE:HB3 | 41:BT:53:VAL:HG23 | 1.95 | 0.48 |
| 41:BT:74:ILE:HG13 | 41:BT:75:GLY:N | 2.29 | 0.48 |
| 44:BX:21:LEU:HD23 | 44:BX:21:LEU:H | 1.77 | 0.48 |
| 46:BZ:7:VAL:HG23 | 46:BZ:67:VAL:HG11 | 1.95 | 0.48 |
| 1:CA:1009:U:H1' | 1:CA:1021:A:C2 | 2.49 | 0.48 |
| 1:CA:113:G:O4' | 1:CA:354:G:H4' | 2.13 | 0.48 |
| 20:CB:68:PHE:HE1 | 20:CB:88:GLN:HB3 | 1.79 | 0.48 |
| 2:CC:146:LYS:HB2 | 2:CC:202:PHE:CD2 | 2.49 | 0.48 |
| 2:CC:71:ARG:O | 2:CC:75:VAL:HG23 | 2.13 | 0.48 |
| 2:CC:78:LYS:C | 2:CC:80:GLY:H | 2.16 | 0.48 |
| 3:CD:149:LYS:HB2 | 3:CD:177:MET:HG3 | 1.94 | 0.48 |
| 4:CE:136:VAL:HG13 | 4:CE:137:ARG:N | 2.28 | 0.48 |
| 4:CE:17:VAL:HG23 | 4:CE:33:THR:O | 2.14 | 0.48 |
| 4:CE:37:VAL:HG11 | 4:CE:113:VAL:CG1 | 2.43 | 0.48 |
| 23:DB:1048:A:H8 | 23:DB:1048:A:P | 2.36 | 0.48 |
| 23:DB:1101:U:O2' | 23:DB:1102:C:H5' | 2.13 | 0.48 |
| 23:DB:1460:U:H3' | 23:DB:1461:C:H5' | 1.96 | 0.48 |
| 23:DB:2063:C:O2 | 23:DB:2450:A:N1 | 2.47 | 0.48 |
| 23:DB:2867:G:N3 | 23:DB:2867:G:C2' | 2.74 | 0.48 |
| 23:DB:470:A:H61 | 41:DT:72:GLN:HE22 | 1.60 | 0.48 |
| 23:DB:659:G:H4' | 27:DE:95:LYS:CD | 2.43 | 0.48 |
| 23:DB:950:G:H2' | 23:DB:951:C:C6 | 2.48 | 0.48 |
| 23:DB:992:C:O2' | 23:DB:993:G:H5' | 2.14 | 0.48 |
| 23:DB:1799:G:C5 | 25:DC:175:LEU:HD13 | 2.49 | 0.48 |
| 26:DD:171:THR:O | 26:DD:172:VAL:HG23 | 2.12 | 0.48 |
| 28:DF:121:PHE:HB3 | 28:DF:127:TYR:CD2 | 2.49 | 0.48 |
| 28:DF:160:LYS:HG3 | 28:DF:161:SER:N | 2.29 | 0.48 |
| 22:DA:42:C:C5 | 28:DF:65:LEU:HD22 | 2.49 | 0.48 |
| 29:DG:10:VAL:HG23 | 29:DG:48:THR:HA | 1.96 | 0.48 |
| 29:DG:42:VAL:HA | 29:DG:50:THR:O | 2.14 | 0.48 |
| 30:DH:4:ILE:HG21 | 30:DH:47:PHE:CE1 | 2.49 | 0.48 |
| 23:DB:1063:G:H5' | 52:DI:135:MET:HG2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:7:G:OP1 | 31:DJ:132:HIS:HE1 | 1.96 | 0.48 |
| 40:DS:20:VAL:C | 40:DS:22:ASP:H | 2.16 | 0.48 |
| 41:DT:50:LEU:HD22 | 41:DT:50:LEU:N | 2.28 | 0.48 |
| 41:DT:29:THR:CG2 | 41:DT:86:THR:HG22 | 2.44 | 0.48 |
| 24:DV:61:LEU:O | 24:DV:71:LYS:HA | 2.14 | 0.48 |
| 24:DV:72:VAL:HG21 | 24:DV:91:PHE:CG | 2.48 | 0.48 |
| 43:DW:48:ALA:HB3 | 43:DW:81:ILE:HG13 | 1.95 | 0.48 |
| 45:DY:29:ARG:H | 45:DY:33:HIS:CD2 | 2.30 | 0.48 |
| 1:AA:1293:C:O2' | 1:AA:1294:G:H5' | 2.13 | 0.48 |
| 1:AA:945:G:H21 | 1:AA:1334:G:H4' | 1.79 | 0.48 |
| 1:AA:1388:C:H2' | 1:AA:1389:C:C6 | 2.48 | 0.48 |
| 1:AA:1479:C:O2' | 1:AA:1480:A:H5' | 2.14 | 0.48 |
| 1:AA:308:C:H2' | 1:AA:309:A:H8 | 1.79 | 0.48 |
| 1:AA:369:G:O2' | 1:AA:370:C:H5' | 2.13 | 0.48 |
| 1:AA:373:A:H2' | 1:AA:374:A:C8 | 2.46 | 0.48 |
| 1:AA:436:C:O2' | 1:AA:437:U:H5' | 2.12 | 0.48 |
| 1:AA:612:C:H2' | 1:AA:613:C:C6 | 2.48 | 0.48 |
| 1:AA:613:C:H2' | 1:AA:614:C:H6 | 1.78 | 0.48 |
| 1:AA:687:A:C2 | 1:AA:704:A:C5 | 3.01 | 0.48 |
| 1:AA:893:C:H2' | 1:AA:894:G:C8 | 2.48 | 0.48 |
| 1:AA:95:C:H2' | 1:AA:96:U:C6 | 2.48 | 0.48 |
| 20:AB:113:LEU:HD23 | 20:AB:114:LYS:N | 2.28 | 0.48 |
| 20:AB:217:ALA:O | 20:AB:221:ARG:HG2 | 2.14 | 0.48 |
| 20:AB:83:ALA:O | 20:AB:88:GLN:HB2 | 2.14 | 0.48 |
| 20:AB:71:THR:HG23 | 20:AB:94:ARG:H | 1.78 | 0.48 |
| 3:AD:129:VAL:HG12 | 3:AD:131:ILE:H | 1.78 | 0.48 |
| 4:AE:37:VAL:HG11 | 4:AE:113:VAL:CG1 | 2.43 | 0.48 |
| 5:AF:85:ILE:HG22 | 5:AF:86:ARG:H | 1.78 | 0.48 |
| 7:AH:45:ILE:HB | 7:AH:61:THR:O | 2.14 | 0.48 |
| 8:AI:16:ALA:HA | 8:AI:66:VAL:HA | 1.96 | 0.48 |
| 8:AI:74:GLN:O | 8:AI:78:ILE:HG13 | 2.13 | 0.48 |
| 12:AM:14:ALA:O | 12:AM:17:ALA:HB3 | 2.14 | 0.48 |
| 12:AM:83:GLY:O | 12:AM:88:LEU:HD21 | 2.14 | 0.48 |
| 23:BB:1940:U:H5'' | 23:BB:1940:U:O2 | 2.14 | 0.48 |
| 23:BB:572:A:C2 | 23:BB:2033:A:C2 | 3.02 | 0.48 |
| 23:BB:2571:U:O3' | 26:BD:151:THR:HB | 2.13 | 0.48 |
| 23:BB:2589:A:H2' | 23:BB:2590:A:C8 | 2.48 | 0.48 |
| 23:BB:2677:G:H2' | 23:BB:2678:C:C6 | 2.49 | 0.48 |
| 23:BB:942:G:O2' | 23:BB:943:A:H5' | 2.14 | 0.48 |
| 28:BF:113:PHE:CZ | 28:BF:175:PRO:HB2 | 2.48 | 0.48 |
| 29:BG:123:GLU:O | 29:BG:125:PRO:HD3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BG:84:LYS:HG3 | 29:BG:131:VAL:C | 2.33 | 0.48 |
| 29:BG:87:GLN:HG2 | 29:BG:164:ALA:HA | 1.94 | 0.48 |
| 32:BK:99:ILE:HD13 | 32:BK:118:LEU:HD22 | 1.96 | 0.48 |
| 32:BK:11:ALA:HB3 | 32:BK:85:VAL:CG2 | 2.43 | 0.48 |
| 33:BL:125:LEU:H | 33:BL:143:GLU:HG3 | 1.78 | 0.48 |
| 34:BM:101:VAL:HG22 | 34:BM:101:VAL:O | 2.13 | 0.48 |
| 40:BS:60:HIS:O | 40:BS:61:ASN:CB | 2.62 | 0.48 |
| 42:BU:13:LEU:HD12 | 42:BU:68:ASN:O | 2.13 | 0.48 |
| 1:CA:1320:C:OP2 | 18:CS:69:LYS:HE3 | 2.13 | 0.48 |
| 1:CA:54:C:H2' | 1:CA:352:C:H41 | 1.78 | 0.48 |
| 1:CA:411:A:C4 | 1:CA:413:G:H1' | 2.49 | 0.48 |
| 1:CA:610:U:O4' | 1:CA:610:U:O2 | 2.30 | 0.48 |
| 1:CA:614:C:O2' | 1:CA:615:G:H5' | 2.14 | 0.48 |
| 4:CE:95:MET:HA | 4:CE:124:ALA:CB | 2.44 | 0.48 |
| 5:CF:2:ARG:O | 5:CF:65:GLU:HA | 2.14 | 0.48 |
| 5:CF:8:PHE:O | 5:CF:60:VAL:HG23 | 2.14 | 0.48 |
| 8:CI:56:MET:SD | 8:CI:57:VAL:N | 2.87 | 0.48 |
| 8:CI:98:ARG:NE | 8:CI:103:VAL:HG21 | 2.28 | 0.48 |
| 10:CK:37:GLN:HB2 | 10:CK:39:ASN:HD22 | 1.79 | 0.48 |
| 12:CM:38:ILE:HD12 | 12:CM:47:LEU:HD11 | 1.95 | 0.48 |
| 23:DB:1060:U:OP1 | 52:DI:75:ALA:HB3 | 2.14 | 0.48 |
| 23:DB:1353:A:H2' | 23:DB:1354:A:H8 | 1.78 | 0.48 |
| 23:DB:141:G:N3 | 23:DB:141:G:H5'' | 2.29 | 0.48 |
| 23:DB:1478:G:O2' | 23:DB:1479:G:H5' | 2.14 | 0.48 |
| 23:DB:2034:U:O2' | 23:DB:2035:G:H5' | 2.13 | 0.48 |
| 23:DB:2073:C:O2' | 23:DB:2074:U:H5' | 2.13 | 0.48 |
| 23:DB:2233:U:H2' | 23:DB:2234:G:C8 | 2.48 | 0.48 |
| 23:DB:2271:G:H2' | 23:DB:2272:U:H6 | 1.77 | 0.48 |
| 23:DB:2355:G:H4' | 43:DW:20:LEU:HD13 | 1.94 | 0.48 |
| 23:DB:2436:G:O2' | 23:DB:2437:G:H5' | 2.13 | 0.48 |
| 23:DB:2589:A:H2' | 23:DB:2590:A:H8 | 1.78 | 0.48 |
| 23:DB:471:A:OP1 | 27:DE:79:ARG:NH1 | 2.47 | 0.48 |
| 23:DB:544:C:H2' | 23:DB:545:U:C4 | 2.48 | 0.48 |
| 14:CO:88:ARG:HH22 | 23:DB:715:A:H5'' | 1.78 | 0.48 |
| 25:DC:144:GLU:OE2 | 25:DC:188:ARG:HG3 | 2.14 | 0.48 |
| 23:DB:1789:A:P | 25:DC:220:ARG:HH11 | 2.36 | 0.48 |
| 26:DD:204:LYS:HB2 | 26:DD:205:PRO:HD2 | 1.96 | 0.48 |
| 26:DD:55:LYS:HZ1 | 26:DD:59:ARG:HD2 | 1.77 | 0.48 |
| 27:DE:118:LEU:O | 27:DE:119:ILE:HD13 | 2.13 | 0.48 |
| 28:DF:102:LEU:HD13 | 28:DF:103:ILE:HB | 1.94 | 0.48 |
| 28:DF:43:ILE:HA | 28:DF:46:LYS:HE2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DH:26:ALA:C | 30:DH:28:ASN:H | 2.15 | 0.48 |
| 23:DB:1063:G:C4' | 52:DI:135:MET:HG2 | 2.44 | 0.48 |
| 31:DJ:110:PRO:HB2 | 31:DJ:111:LYS:HE3 | 1.95 | 0.48 |
| 34:DM:31:PHE:HB3 | 34:DM:130:PHE:CZ | 2.49 | 0.48 |
| 35:DN:83:LEU:HA | 35:DN:86:ARG:HB2 | 1.94 | 0.48 |
| 38:DQ:18:LYS:C | 38:DQ:20:ALA:H | 2.15 | 0.48 |
| 38:DQ:63:ARG:HH21 | 38:DQ:64:ILE:HD13 | 1.78 | 0.48 |
| 39:DR:79:ARG:NE | 39:DR:80:ARG:NH2 | 2.61 | 0.48 |
| 40:DS:73:LYS:HE3 | 40:DS:74:ILE:N | 2.26 | 0.48 |
| 42:DU:98:ASN:OD1 | 42:DU:100:GLU:HB2 | 2.13 | 0.48 |
| 1:AA:1216:A:H2' | 1:AA:1217:C:C6 | 2.48 | 0.48 |
| 1:AA:1459:G:H2' | 1:AA:1460:C:C6 | 2.48 | 0.48 |
| 1:AA:208:U:O2' | 1:AA:209:U:H3' | 2.13 | 0.48 |
| 1:AA:643:C:H2' | 1:AA:644:U:H6 | 1.79 | 0.48 |
| 1:AA:734:G:H2' | 1:AA:735:C:C6 | 2.48 | 0.48 |
| 1:AA:868:C:H2' | 1:AA:869:G:O4' | 2.14 | 0.48 |
| 23:BB:1258:U:H2' | 23:BB:1259:G:C8 | 2.49 | 0.48 |
| 23:BB:1551:A:C3' | 23:BB:1552:A:H5'' | 2.43 | 0.48 |
| 23:BB:1720:U:O2' | 23:BB:1721:G:H5' | 2.13 | 0.48 |
| 23:BB:1841:U:C2 | 23:BB:1842:G:C8 | 3.01 | 0.48 |
| 23:BB:2572:A:OP2 | 26:BD:151:THR:HB | 2.13 | 0.48 |
| 23:BB:405:U:H4' | 23:BB:405:U:OP2 | 2.13 | 0.48 |
| 23:BB:502:A:H5' | 23:BB:503:A:OP2 | 2.13 | 0.48 |
| 23:BB:566:U:H5'' | 33:BL:29:LYS:HZ2 | 1.79 | 0.48 |
| 23:BB:56:A:H2' | 23:BB:57:C:C6 | 2.48 | 0.48 |
| 23:BB:912:C:O2' | 23:BB:913:U:H5' | 2.13 | 0.48 |
| 25:BC:183:VAL:HG22 | 25:BC:187:CYS:SG | 2.53 | 0.48 |
| 26:BD:171:THR:HG23 | 26:BD:172:VAL:N | 2.29 | 0.48 |
| 28:BF:29:ARG:HB2 | 28:BF:158:THR:HG21 | 1.96 | 0.48 |
| 29:BG:37:ASN:HD22 | 29:BG:40:VAL:CB | 2.24 | 0.48 |
| 52:BI:52:LEU:HD12 | 52:BI:52:LEU:N | 2.29 | 0.48 |
| 33:BL:100:ILE:O | 33:BL:100:ILE:HG12 | 2.13 | 0.48 |
| 34:BM:71:LYS:HG2 | 34:BM:93:VAL:HG12 | 1.95 | 0.48 |
| 38:BQ:64:ILE:HD12 | 38:BQ:95:ALA:HB3 | 1.95 | 0.48 |
| 41:BT:66:LYS:N | 41:BT:76:ARG:NH2 | 2.62 | 0.48 |
| 1:CA:1234:C:H1' | 1:CA:1364:U:O2 | 2.13 | 0.48 |
| 1:CA:1263:C:O2' | 1:CA:1264:U:H5' | 2.14 | 0.48 |
| 1:CA:1451:U:O2 | 1:CA:1451:U:H2' | 2.13 | 0.48 |
| 1:CA:1522:U:H2' | 1:CA:1523:G:H8 | 1.79 | 0.48 |
| 1:CA:624:C:H2' | 1:CA:625:U:C6 | 2.48 | 0.48 |
| 20:CB:212:TYR:O | 20:CB:216:VAL:HG13 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:CB:63:LYS:HA | 20:CB:224:ARG:NH1 | 2.29 | 0.48 |
| 20:CB:8:MET:C | 20:CB:9:LEU:HD12 | 2.33 | 0.48 |
| 8:CI:52:GLU:C | 8:CI:53:LEU:HD22 | 2.33 | 0.48 |
| 15:CP:12:LYS:HD2 | 15:CP:13:LYS:HG3 | 1.96 | 0.48 |
| 15:CP:20:VAL:HG21 | 15:CP:32:PHE:CG | 2.48 | 0.48 |
| 15:CP:43:ALA:HA | 15:CP:46:LYS:HE3 | 1.96 | 0.48 |
| 18:CS:62:THR:O | 18:CS:66:VAL:HG13 | 2.14 | 0.48 |
| 21:CU:20:ARG:N | 21:CU:20:ARG:HD2 | 2.29 | 0.48 |
| 23:DB:1230:A:H2' | 23:DB:1231:U:H6 | 1.79 | 0.48 |
| 23:DB:1405:U:H2' | 23:DB:1406:U:C6 | 2.49 | 0.48 |
| 23:DB:1541:C:O2' | 23:DB:1542:U:H5' | 2.13 | 0.48 |
| 23:DB:1786:A:H1' | 23:DB:1938:A:N6 | 2.29 | 0.48 |
| 23:DB:1969:A:H2' | 23:DB:1972:G:H21 | 1.79 | 0.48 |
| 23:DB:2022:U:O2' | 23:DB:2617:U:H5' | 2.14 | 0.48 |
| 23:DB:2301:C:H2' | 23:DB:2302:U:H6 | 1.79 | 0.48 |
| 23:DB:2428:G:H21 | 33:DL:60:ARG:NE | 2.09 | 0.48 |
| 23:DB:324:A:H2' | 23:DB:325:G:O4' | 2.14 | 0.48 |
| 25:DC:106:PRO:O | 25:DC:109:LEU:HD13 | 2.14 | 0.48 |
| 26:DD:118:PHE:O | 26:DD:119:ALA:CB | 2.62 | 0.48 |
| 26:DD:107:VAL:HA | 26:DD:204:LYS:O | 2.14 | 0.48 |
| 27:DE:132:LYS:O | 27:DE:135:ALA:HB3 | 2.13 | 0.48 |
| 27:DE:192:ALA:O | 27:DE:196:VAL:HG23 | 2.14 | 0.48 |
| 28:DF:102:LEU:HA | 28:DF:106:ALA:HB2 | 1.96 | 0.48 |
| 29:DG:84:LYS:HG3 | 29:DG:131:VAL:HA | 1.96 | 0.48 |
| 31:DJ:48:VAL:HG12 | 31:DJ:50:THR:HG23 | 1.96 | 0.48 |
| 33:DL:51:GLU:HG2 | 50:D3:56:LEU:CD2 | 2.43 | 0.48 |
| 23:DB:2485:G:H5'' | 34:DM:125:PRO:HG3 | 1.94 | 0.48 |
| 24:DV:77:VAL:HG12 | 34:DM:136:MET:HG2 | 1.94 | 0.48 |
| 39:DR:20:VAL:HG12 | 39:DR:21:ARG:N | 2.26 | 0.48 |
| 41:DT:23:ALA:C | 41:DT:25:GLU:H | 2.17 | 0.48 |
| 41:DT:40:LYS:HA | 41:DT:43:ILE:HB | 1.95 | 0.48 |
| 43:DW:61:LYS:O | 43:DW:62:ALA:O | 2.31 | 0.48 |
| 1:AA:537:G:H2' | 1:AA:538:G:H8 | 1.78 | 0.48 |
| 1:AA:586:C:H2' | 1:AA:587:G:H5' | 1.95 | 0.48 |
| 1:AA:794:A:H2' | 1:AA:795:C:C6 | 2.48 | 0.48 |
| 1:AA:847:G:H2' | 1:AA:848:C:H6 | 1.79 | 0.48 |
| 1:AA:875:U:O2' | 7:AH:14:ARG:HD2 | 2.14 | 0.48 |
| 20:AB:93:HIS:O | 20:AB:94:ARG:O | 2.32 | 0.48 |
| 6:AG:72:VAL:HG12 | 6:AG:89:GLU:CB | 2.43 | 0.48 |
| 10:AK:122:PRO:HG2 | 21:AU:34:ARG:HA | 1.95 | 0.48 |
| 12:AM:13:HIS:O | 12:AM:17:ALA:HB2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:981:U:C4' | 13:AN:60:ARG:HD2 | 2.37 | 0.48 |
| 13:AN:68:ARG:HH11 | 13:AN:71:GLY:H | 1.60 | 0.48 |
| 15:AP:28:ARG:HD3 | 15:AP:29:ASN:HD22 | 1.77 | 0.48 |
| 18:AS:4:LEU:HD11 | 18:AS:9:PHE:HB3 | 1.96 | 0.48 |
| 23:BB:1349:C:H2' | 23:BB:1350:C:H6 | 1.79 | 0.48 |
| 23:BB:2081:U:OP1 | 46:BZ:19:SER:HB3 | 2.14 | 0.48 |
| 23:BB:2247:A:H2' | 23:BB:2248:C:C6 | 2.48 | 0.48 |
| 23:BB:226:A:H1' | 23:BB:230:G:N2 | 2.29 | 0.48 |
| 23:BB:39:G:H2' | 23:BB:40:U:C6 | 2.49 | 0.48 |
| 23:BB:98:G:H22 | 42:BU:6:ARG:NH1 | 2.11 | 0.48 |
| 23:BB:1789:A:P | 25:BC:220:ARG:HH11 | 2.37 | 0.48 |
| 26:BD:151:THR:HB | 26:BD:152:PRO:HD3 | 1.94 | 0.48 |
| 22:BA:43:C:H1' | 28:BF:91:ARG:NH2 | 2.29 | 0.48 |
| 30:BH:25:TYR:CD1 | 30:BH:30:LEU:HG | 2.49 | 0.48 |
| 30:BH:54:LEU:O | 30:BH:58:LEU:HB3 | 2.13 | 0.48 |
| 30:BH:66:ASN:HA | 30:BH:134:VAL:HG21 | 1.96 | 0.48 |
| 52:BI:89:SER:HB2 | 52:BI:136:GLY:HA3 | 1.95 | 0.48 |
| 35:BN:2:ARG:C | 35:BN:2:ARG:HE | 2.16 | 0.48 |
| 40:BS:17:VAL:C | 40:BS:19:LEU:N | 2.66 | 0.48 |
| 41:BT:9:LYS:HG2 | 41:BT:9:LYS:O | 2.12 | 0.48 |
| 42:BU:10:VAL:HB | 42:BU:69:VAL:HB | 1.96 | 0.48 |
| 1:CA:1004:A:H2' | 1:CA:1005:A:O4' | 2.14 | 0.48 |
| 1:CA:1180:A:OP1 | 8:CI:104:THR:HG22 | 2.14 | 0.48 |
| 1:CA:130:A:H1' | 1:CA:263:A:O2' | 2.13 | 0.48 |
| 1:CA:1406:U:C2' | 1:CA:1407:C:H5' | 2.43 | 0.48 |
| 1:CA:599:C:H4' | 7:CH:121:GLY:HA3 | 1.96 | 0.48 |
| 20:CB:19:THR:HG23 | 20:CB:20:ARG:N | 2.23 | 0.48 |
| 20:CB:23:ASN:C | 20:CB:25:LYS:H | 2.17 | 0.48 |
| 2:CC:139:ASN:O | 2:CC:143:LEU:HD23 | 2.13 | 0.48 |
| 5:CF:52:ASN:HA | 5:CF:53:LYS:HZ3 | 1.79 | 0.48 |
| 8:CI:12:LYS:HA | 8:CI:109:GLN:HG2 | 1.95 | 0.48 |
| 8:CI:129:ARG:HB2 | 8:CI:129:ARG:CZ | 2.43 | 0.48 |
| 8:CI:74:GLN:O | 8:CI:78:ILE:HG13 | 2.14 | 0.48 |
| 12:CM:83:GLY:O | 12:CM:88:LEU:HD21 | 2.14 | 0.48 |
| 13:CN:20:PHE:HB2 | 13:CN:54:SER:OG | 2.13 | 0.48 |
| 49:D2:3:ARG:HH21 | 49:D2:3:ARG:HG2 | 1.78 | 0.48 |
| 23:DB:1163:G:O2' | 23:DB:1164:C:H5' | 2.14 | 0.48 |
| 23:DB:1181:U:H2' | 23:DB:1182:G:H8 | 1.78 | 0.48 |
| 23:DB:1193:G:H2' | 23:DB:1194:A:O4' | 2.14 | 0.48 |
| 23:DB:1196:C:H2' | 23:DB:1197:G:H8 | 1.78 | 0.48 |
| 23:DB:129:C:H2' | 23:DB:130:C:C6 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1374:G:H2' | 23:DB:1375:U:C6 | 2.49 | 0.48 |
| 23:DB:1485:U:O2' | 23:DB:1486:U:H5' | 2.14 | 0.48 |
| 23:DB:1789:A:OP1 | 25:DC:220:ARG:HD3 | 2.14 | 0.48 |
| 23:DB:924:G:H2' | 23:DB:925:A:H8 | 1.79 | 0.48 |
| 25:DC:43:ASN:ND2 | 25:DC:44:ASN:N | 2.60 | 0.48 |
| 28:DF:111:ARG:HD2 | 28:DF:111:ARG:N | 2.29 | 0.48 |
| 30:DH:135:HIS:HB3 | 30:DH:138:VAL:CB | 2.36 | 0.48 |
| 30:DH:131:SER:CB | 30:DH:141:LYS:HA | 2.34 | 0.48 |
| 33:DL:122:VAL:HB | 33:DL:143:GLU:OE1 | 2.13 | 0.48 |
| 33:DL:135:ILE:HG12 | 33:DL:140:GLY:HA3 | 1.96 | 0.48 |
| 33:DL:23:ILE:HD12 | 33:DL:23:ILE:N | 2.29 | 0.48 |
| 33:DL:3:LEU:O | 33:DL:5:THR:HG23 | 2.14 | 0.48 |
| 33:DL:55:MET:HE2 | 33:DL:56:PRO:HD2 | 1.94 | 0.48 |
| 34:DM:30:SER:HA | 34:DM:133:LYS:HB2 | 1.95 | 0.48 |
| 34:DM:74:THR:O | 34:DM:75:GLU:HB2 | 2.14 | 0.48 |
| 40:DS:42:LYS:HG3 | 40:DS:43:ALA:N | 2.28 | 0.48 |
| 43:DW:43:LYS:HB3 | 43:DW:79:ILE:HD11 | 1.96 | 0.48 |
| 1:AA:1009:U:H2' | 1:AA:1010:U:C6 | 2.48 | 0.48 |
| 1:AA:270:A:H2' | 1:AA:271:C:O4' | 2.14 | 0.48 |
| 1:AA:502:A:H2' | 1:AA:503:C:H6 | 1.78 | 0.48 |
| 1:AA:72:A:N6 | 1:AA:99:C:H1' | 2.20 | 0.48 |
| 20:AB:142:LYS:HA | 20:AB:145:ASN:OD1 | 2.13 | 0.48 |
| 2:AC:119:ILE:CG2 | 2:AC:120:THR:N | 2.76 | 0.48 |
| 3:AD:125:ASN:OD1 | 3:AD:140:ASP:HA | 2.14 | 0.48 |
| 1:AA:546:A:P | 3:AD:68:GLU:HB3 | 2.54 | 0.48 |
| 4:AE:17:VAL:HG23 | 4:AE:33:THR:O | 2.14 | 0.48 |
| 1:AA:599:C:H4' | 7:AH:121:GLY:HA3 | 1.94 | 0.48 |
| 7:AH:94:VAL:HG12 | 7:AH:99:GLY:HA3 | 1.96 | 0.48 |
| 9:AJ:80:THR:HG21 | 9:AJ:82:LYS:HZ2 | 1.79 | 0.48 |
| 12:AM:43:LYS:N | 12:AM:43:LYS:HD2 | 2.28 | 0.48 |
| 18:AS:42:ASN:N | 18:AS:42:ASN:ND2 | 2.62 | 0.48 |
| 23:BB:1107:G:H2' | 23:BB:1108:U:C6 | 2.48 | 0.48 |
| 23:BB:1564:C:O2' | 23:BB:1565:C:H5' | 2.13 | 0.48 |
| 23:BB:1826:G:H2' | 23:BB:1827:U:H6 | 1.79 | 0.48 |
| 23:BB:2063:C:O2 | 23:BB:2450:A:N1 | 2.46 | 0.48 |
| 23:BB:2281:A:O2' | 23:BB:2282:G:H5' | 2.13 | 0.48 |
| 23:BB:2341:G:H2' | 23:BB:2342:C:C6 | 2.49 | 0.48 |
| 23:BB:2663:G:H2' | 23:BB:2664:G:O4' | 2.13 | 0.48 |
| 23:BB:299:A:H2' | 23:BB:300:A:C8 | 2.48 | 0.48 |
| 23:BB:942:G:H2' | 23:BB:943:A:H8 | 1.77 | 0.48 |
| 25:BC:129:LEU:HD21 | 25:BC:133:ASN:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BD:171:THR:O | 26:BD:172:VAL:HG23 | 2.13 | 0.48 |
| 26:BD:8:LYS:CA | 26:BD:201:LEU:HD11 | 2.43 | 0.48 |
| 26:BD:33:ARG:HH21 | 26:BD:33:ARG:HG2 | 1.79 | 0.48 |
| 27:BE:58:LYS:CD | 27:BE:58:LYS:H | 2.13 | 0.48 |
| 28:BF:139:GLU:O | 28:BF:141:ASP:N | 2.47 | 0.48 |
| 29:BG:156:TYR:O | 29:BG:157:LYS:HD2 | 2.14 | 0.48 |
| 29:BG:51:PHE:CD2 | 29:BG:68:ARG:HG2 | 2.49 | 0.48 |
| 30:BH:112:LYS:HE3 | 30:BH:112:LYS:C | 2.34 | 0.48 |
| 30:BH:133:GLN:HB2 | 30:BH:139:PHE:HB3 | 1.95 | 0.48 |
| 31:BJ:104:ALA:O | 31:BJ:108:MET:HG2 | 2.14 | 0.48 |
| 23:BB:558:U:OP1 | 31:BJ:113:PRO:HB2 | 2.13 | 0.48 |
| 31:BJ:44:TYR:C | 31:BJ:44:TYR:CD2 | 2.88 | 0.48 |
| 32:BK:19:VAL:HG13 | 32:BK:43:ILE:HA | 1.96 | 0.48 |
| 36:BO:25:ARG:HD2 | 36:BO:93:ASP:HB2 | 1.95 | 0.48 |
| 23:BB:1222:U:P | 39:BR:90:ARG:HH22 | 2.37 | 0.48 |
| 43:BW:70:VAL:O | 43:BW:70:VAL:HG22 | 2.14 | 0.48 |
| 45:BY:4:ILE:HG22 | 45:BY:56:VAL:CG1 | 2.43 | 0.48 |
| 46:BZ:63:GLY:HA3 | 46:BZ:66:THR:OG1 | 2.14 | 0.48 |
| 1:CA:1346:A:N1 | 1:CA:1374:A:H5'' | 2.29 | 0.48 |
| 1:CA:708:C:O2' | 1:CA:709:U:H5' | 2.14 | 0.48 |
| 1:CA:828:U:OP1 | 1:CA:828:U:H4' | 2.14 | 0.48 |
| 5:CF:51:ILE:HD11 | 5:CF:86:ARG:HG3 | 1.96 | 0.48 |
| 8:CI:83:THR:OG1 | 8:CI:97:LEU:HD22 | 2.14 | 0.48 |
| 10:CK:60:PHE:O | 10:CK:64:VAL:HG12 | 2.14 | 0.48 |
| 14:CO:55:LEU:O | 14:CO:58:MET:HG2 | 2.14 | 0.48 |
| 22:DA:102:G:O2' | 22:DA:103:U:H5' | 2.14 | 0.48 |
| 23:DB:1120:G:O2' | 23:DB:1121:C:H5' | 2.14 | 0.48 |
| 23:DB:1274:A:C2 | 23:DB:1297:C:H1' | 2.49 | 0.48 |
| 23:DB:1508:A:H3' | 23:DB:1509:A:C2 | 2.49 | 0.48 |
| 23:DB:1656:C:H2' | 23:DB:1657:U:H6 | 1.79 | 0.48 |
| 23:DB:1700:A:H2' | 23:DB:1701:A:H5' | 1.96 | 0.48 |
| 23:DB:2070:A:C2 | 23:DB:2442:C:C2 | 3.02 | 0.48 |
| 23:DB:2405:G:H1' | 23:DB:2412:A:N6 | 2.29 | 0.48 |
| 23:DB:589:U:H2' | 23:DB:590:A:C8 | 2.49 | 0.48 |
| 23:DB:675:A:H4' | 27:DE:62:GLN:HE22 | 1.79 | 0.48 |
| 23:DB:979:A:H2' | 23:DB:982:C:N4 | 2.23 | 0.48 |
| 25:DC:76:VAL:CG1 | 25:DC:114:GLN:HG2 | 2.44 | 0.48 |
| 25:DC:74:PRO:HG2 | 25:DC:96:LYS:CG | 2.43 | 0.48 |
| 28:DF:36:ASN:ND2 | 28:DF:152:ASP:HB2 | 2.08 | 0.48 |
| 30:DH:14:SER:C | 30:DH:16:GLY:N | 2.67 | 0.48 |
| 52:DI:100:ILE:O | 52:DI:139:VAL:HG13 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DL:75:ALA:HB3 | 33:DL:108:ALA:HB2 | 1.96 | 0.48 |
| 33:DL:93:ASN:O | 33:DL:95:LEU:HD12 | 2.14 | 0.48 |
| 38:DQ:4:LYS:CE | 38:DQ:7:VAL:HG22 | 2.44 | 0.48 |
| 38:DQ:91:ARG:HB2 | 39:DR:11:GLN:CD | 2.35 | 0.48 |
| 39:DR:4:VAL:O | 39:DR:38:VAL:HA | 2.13 | 0.48 |
| 40:DS:15:GLN:HA | 40:DS:18:ARG:CG | 2.43 | 0.48 |
| 43:DW:17:ALA:HB1 | 43:DW:37:VAL:H | 1.78 | 0.48 |
| 1:AA:1016:A:H4' | 1:AA:1218:C:H4' | 1.95 | 0.47 |
| 1:AA:1263:C:O2' | 1:AA:1264:U:H5' | 2.14 | 0.47 |
| 1:AA:1423:G:H2' | 1:AA:1424:U:H6 | 1.77 | 0.47 |
| 1:AA:429:U:H3' | 3:AD:8:LEU:CD2 | 2.44 | 0.47 |
| 1:AA:643:C:H2' | 1:AA:644:U:C6 | 2.49 | 0.47 |
| 1:AA:818:G:C3' | 1:AA:819:A:H5'' | 2.43 | 0.47 |
| 20:AB:75:ALA:C | 20:AB:79:VAL:HG23 | 2.33 | 0.47 |
| 3:AD:106:PHE:CE1 | 3:AD:158:LEU:HD21 | 2.49 | 0.47 |
| 6:AG:104:VAL:O | 6:AG:108:ARG:HG3 | 2.14 | 0.47 |
| 8:AI:98:ARG:NE | 8:AI:103:VAL:HG21 | 2.29 | 0.47 |
| 1:AA:716:A:N3 | 10:AK:118:ASN:O | 2.47 | 0.47 |
| 12:AM:76:ILE:HG23 | 12:AM:79:LEU:HD12 | 1.95 | 0.47 |
| 23:BB:1080:A:H2' | 23:BB:1081:U:H6 | 1.79 | 0.47 |
| 23:BB:1221:C:O2' | 23:BB:1222:U:H5' | 2.13 | 0.47 |
| 23:BB:1416:G:HO2' | 23:BB:1417:C:H6 | 1.60 | 0.47 |
| 23:BB:1745:A:H2' | 23:BB:1746:A:O4' | 2.14 | 0.47 |
| 23:BB:2193:G:H2' | 23:BB:2194:U:C6 | 2.48 | 0.47 |
| 23:BB:2419:U:OP2 | 50:B3:32:LEU:HD13 | 2.14 | 0.47 |
| 23:BB:2439:A:H4' | 23:BB:2440:C:O5' | 2.13 | 0.47 |
| 23:BB:68:G:O2' | 23:BB:69:C:H5' | 2.14 | 0.47 |
| 23:BB:919:U:H2' | 23:BB:920:A:H8 | 1.73 | 0.47 |
| 23:BB:1792:G:P | 25:BC:204:LEU:HD12 | 2.54 | 0.47 |
| 25:BC:74:PRO:HG2 | 25:BC:96:LYS:CG | 2.42 | 0.47 |
| 28:BF:23:SER:O | 28:BF:26:GLN:HB2 | 2.14 | 0.47 |
| 28:BF:62:GLN:HB2 | 28:BF:91:ARG:HE | 1.78 | 0.47 |
| 29:BG:25:ILE:HD12 | 29:BG:25:ILE:N | 2.29 | 0.47 |
| 29:BG:66:THR:O | 29:BG:70:LEU:HB2 | 2.14 | 0.47 |
| 30:BH:114:GLU:HB3 | 30:BH:133:GLN:O | 2.14 | 0.47 |
| 31:BJ:19:ASP:CG | 31:BJ:57:LEU:HB3 | 2.34 | 0.47 |
| 34:BM:29:GLY:HA2 | 34:BM:106:ASP:HB2 | 1.96 | 0.47 |
| 37:BP:24:THR:HB | 37:BP:86:LYS:HB3 | 1.95 | 0.47 |
| 33:BL:23:ILE:HG13 | 39:BR:82:HIS:CE1 | 2.49 | 0.47 |
| 42:BU:78:LYS:CG | 42:BU:79:ALA:H | 2.27 | 0.47 |
| 1:CA:1040:U:H2' | 1:CA:1041:G:C8 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1299:A:H2' | 1:CA:1301:U:H1' | 1.96 | 0.47 |
| 1:CA:454:G:H2' | 1:CA:455:G:H8 | 1.79 | 0.47 |
| 1:CA:468:A:H3' | 1:CA:469:C:C6 | 2.49 | 0.47 |
| 1:CA:754:C:H3' | 1:CA:754:C:O2 | 2.14 | 0.47 |
| 20:CB:116:LEU:O | 20:CB:119:GLN:HB2 | 2.13 | 0.47 |
| 20:CB:204:ASP:O | 20:CB:208:ALA:HB3 | 2.14 | 0.47 |
| 4:CE:132:PRO:O | 4:CE:136:VAL:HG12 | 2.14 | 0.47 |
| 6:CG:129:ASN:HA | 6:CG:134:VAL:CG1 | 2.38 | 0.47 |
| 6:CG:78:ARG:NH1 | 6:CG:80:GLY:H | 2.11 | 0.47 |
| 7:CH:82:LEU:O | 7:CH:82:LEU:HD13 | 2.13 | 0.47 |
| 7:CH:94:VAL:HG21 | 7:CH:100:ILE:O | 2.13 | 0.47 |
| 8:CI:127:SER:O | 8:CI:129:ARG:HG3 | 2.14 | 0.47 |
| 12:CM:14:ALA:O | 12:CM:17:ALA:HB3 | 2.14 | 0.47 |
| 19:CT:3:ILE:HG13 | 19:CT:3:ILE:H | 1.47 | 0.47 |
| 22:DA:35:C:H2' | 22:DA:36:C:O4' | 2.14 | 0.47 |
| 23:DB:1133:A:H5' | 23:DB:1134:A:OP1 | 2.13 | 0.47 |
| 23:DB:1222:U:O2' | 23:DB:1223:G:H5' | 2.14 | 0.47 |
| 23:DB:137:U:O5' | 23:DB:137:U:H6 | 1.97 | 0.47 |
| 23:DB:1439:A:N7 | 23:DB:1440:U:C6 | 2.82 | 0.47 |
| 23:DB:1484:U:H2' | 23:DB:1485:U:H6 | 1.79 | 0.47 |
| 23:DB:1607:C:N4 | 23:DB:1622:G:OP2 | 2.46 | 0.47 |
| 23:DB:1842:G:H2' | 23:DB:1843:C:H6 | 1.78 | 0.47 |
| 23:DB:2286:G:H4' | 23:DB:2287:A:O4' | 2.14 | 0.47 |
| 23:DB:2379:G:H2' | 23:DB:2380:C:C6 | 2.49 | 0.47 |
| 23:DB:2449:U:H4' | 23:DB:2450:A:OP1 | 2.14 | 0.47 |
| 23:DB:2559:C:H2' | 23:DB:2560:A:H8 | 1.79 | 0.47 |
| 23:DB:785:G:H2' | 23:DB:786:C:H6 | 1.79 | 0.47 |
| 23:DB:991:C:H5' | 23:DB:991:C:H6 | 1.78 | 0.47 |
| 25:DC:52:HIS:O | 25:DC:53:ILE:HB | 2.14 | 0.47 |
| 26:DD:141:ARG:O | 26:DD:142:VAL:HG13 | 2.14 | 0.47 |
| 23:DB:1060:U:OP2 | 52:DI:74:PRO:HA | 2.13 | 0.47 |
| 32:DK:26:GLY:O | 32:DK:30:ARG:HD2 | 2.14 | 0.47 |
| 32:DK:77:ILE:HD11 | 37:DP:71:ARG:CZ | 2.44 | 0.47 |
| 37:DP:25:VAL:HA | 37:DP:85:VAL:C | 2.34 | 0.47 |
| 37:DP:4:ILE:O | 37:DP:6:GLN:N | 2.45 | 0.47 |
| 37:DP:77:SER:O | 37:DP:80:VAL:HG12 | 2.14 | 0.47 |
| 38:DQ:51:GLN:O | 38:DQ:55:GLN:HG3 | 2.13 | 0.47 |
| 24:DV:21:ARG:NE | 24:DV:87:GLN:HB3 | 2.28 | 0.47 |
| 44:DX:43:LEU:O | 44:DX:47:ARG:HG3 | 2.14 | 0.47 |
| 1:AA:1004:A:H5' | 1:AA:1024:G:H22 | 1.77 | 0.47 |
| 1:AA:1032:G:N3 | 1:AA:1032:G:H5'' | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1252:A:H2' | 1:AA:1253:G:O4' | 2.14 | 0.47 |
| 1:AA:1436:U:H2' | 1:AA:1437:A:H8 | 1.78 | 0.47 |
| 1:AA:142:G:N3 | 1:AA:196:A:H2 | 2.12 | 0.47 |
| 1:AA:738:C:H2' | 1:AA:739:C:H6 | 1.78 | 0.47 |
| 1:AA:949:A:H2' | 1:AA:950:U:O4' | 2.14 | 0.47 |
| 6:AG:72:VAL:HG12 | 6:AG:89:GLU:CA | 2.43 | 0.47 |
| 7:AH:68:LYS:HG3 | 7:AH:69:ALA:N | 2.29 | 0.47 |
| 8:AI:18:VAL:HA | 8:AI:64:ILE:HA | 1.96 | 0.47 |
| 14:AO:67:ASP:O | 14:AO:71:ARG:HG3 | 2.13 | 0.47 |
| 14:AO:88:ARG:HH11 | 14:AO:88:ARG:CA | 2.22 | 0.47 |
| 22:BA:55:U:H2' | 22:BA:56:G:H8 | 1.79 | 0.47 |
| 22:BA:60:C:O2' | 22:BA:61:G:H5' | 2.13 | 0.47 |
| 23:BB:1046:A:C4' | 23:BB:1047:G:H5'' | 2.44 | 0.47 |
| 23:BB:1274:A:C2 | 23:BB:1297:C:H1' | 2.49 | 0.47 |
| 23:BB:1726:C:H2' | 23:BB:1727:C:C6 | 2.49 | 0.47 |
| 23:BB:786:C:H5'' | 23:BB:1780:A:N7 | 2.28 | 0.47 |
| 23:BB:1958:C:H2' | 23:BB:1959:G:H8 | 1.79 | 0.47 |
| 23:BB:2630:G:O2' | 23:BB:2631:G:H5' | 2.14 | 0.47 |
| 23:BB:2848:G:H1 | 23:BB:2867:G:N2 | 2.11 | 0.47 |
| 23:BB:615:U:O4 | 27:BE:39:ALA:HB2 | 2.14 | 0.47 |
| 28:BF:19:PHE:CE2 | 28:BF:164:GLU:HG2 | 2.48 | 0.47 |
| 52:BI:32:VAL:HG13 | 52:BI:66:PHE:CD2 | 2.49 | 0.47 |
| 35:BN:12:ARG:HG3 | 35:BN:13:ASN:H | 1.78 | 0.47 |
| 38:BQ:33:VAL:HG23 | 38:BQ:34:ALA:H | 1.78 | 0.47 |
| 38:BQ:51:GLN:O | 38:BQ:55:GLN:HG3 | 2.14 | 0.47 |
| 38:BQ:64:ILE:HD12 | 38:BQ:95:ALA:CB | 2.44 | 0.47 |
| 39:BR:43:ASN:CG | 39:BR:45:GLU:H | 2.17 | 0.47 |
| 43:BW:30:VAL:O | 43:BW:30:VAL:HG22 | 2.13 | 0.47 |
| 1:CA:1109:C:H2' | 1:CA:1110:A:O4' | 2.14 | 0.47 |
| 1:CA:1317:C:H3' | 1:CA:1318:A:C8 | 2.49 | 0.47 |
| 1:CA:36:C:O3' | 11:CL:119:LYS:HA | 2.14 | 0.47 |
| 1:CA:443:C:H2' | 1:CA:444:G:H8 | 1.79 | 0.47 |
| 1:CA:549:C:H2' | 1:CA:550:G:C8 | 2.49 | 0.47 |
| 1:CA:898:G:N2 | 1:CA:900:A:H3' | 2.29 | 0.47 |
| 20:CB:216:VAL:O | 20:CB:220:VAL:HG23 | 2.14 | 0.47 |
| 20:CB:8:MET:HG3 | 20:CB:9:LEU:HD12 | 1.95 | 0.47 |
| 2:CC:129:PHE:CD2 | 2:CC:156:LEU:HD22 | 2.48 | 0.47 |
| 3:CD:123:MET:CB | 3:CD:128:VAL:HA | 2.44 | 0.47 |
| 6:CG:125:ASP:HB3 | 6:CG:131:GLY:H | 1.78 | 0.47 |
| 6:CG:75:LYS:HD3 | 6:CG:76:SER:N | 2.28 | 0.47 |
| 7:CH:58:LEU:HD22 | 7:CH:60:LEU:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CJ:13:PHE:CD2 | 9:CJ:69:THR:HG23 | 2.49 | 0.47 |
| 10:CK:74:LYS:HG3 | 10:CK:104:PHE:CZ | 2.49 | 0.47 |
| 11:CL:113:ARG:NE | 11:CL:120:ARG:HA | 2.29 | 0.47 |
| 13:CN:27:LYS:HG3 | 13:CN:28:ALA:H | 1.79 | 0.47 |
| 16:CQ:11:VAL:HG13 | 16:CQ:20:ILE:HG23 | 1.94 | 0.47 |
| 19:CT:49:ALA:O | 19:CT:52:GLU:HB3 | 2.14 | 0.47 |
| 21:CU:20:ARG:HD2 | 21:CU:20:ARG:H | 1.79 | 0.47 |
| 48:D1:6:GLU:HB2 | 48:D1:52:LYS:NZ | 2.29 | 0.47 |
| 22:DA:70:C:O2' | 22:DA:71:C:H5' | 2.14 | 0.47 |
| 23:DB:138:U:H2' | 23:DB:140:C:C1' | 2.44 | 0.47 |
| 23:DB:1470:A:H3' | 23:DB:1471:G:H8 | 1.78 | 0.47 |
| 23:DB:1668:A:N3 | 23:DB:1670:C:C4 | 2.82 | 0.47 |
| 23:DB:786:C:H5'' | 23:DB:1780:A:N7 | 2.29 | 0.47 |
| 23:DB:19:A:H2' | 23:DB:20:C:H6 | 1.79 | 0.47 |
| 23:DB:2273:A:H2' | 23:DB:2274:A:C8 | 2.49 | 0.47 |
| 23:DB:2709:G:H2' | 23:DB:2710:C:C6 | 2.49 | 0.47 |
| 23:DB:275:C:H2' | 23:DB:276:U:C1' | 2.43 | 0.47 |
| 23:DB:364:C:H2' | 23:DB:365:U:C6 | 2.49 | 0.47 |
| 23:DB:531:C:O2' | 23:DB:563:A:H5'' | 2.13 | 0.47 |
| 23:DB:77:G:O2' | 23:DB:78:U:H5' | 2.13 | 0.47 |
| 25:DC:229:HIS:ND1 | 25:DC:230:PRO:HD2 | 2.28 | 0.47 |
| 25:DC:245:THR:OG1 | 25:DC:249:VAL:HG23 | 2.14 | 0.47 |
| 26:DD:101:PHE:O | 26:DD:180:VAL:HG11 | 2.14 | 0.47 |
| 26:DD:30:GLU:OE1 | 26:DD:53:GLY:HA2 | 2.14 | 0.47 |
| 28:DF:115:GLY:HA3 | 28:DF:177:ARG:HB2 | 1.95 | 0.47 |
| 28:DF:137:PHE:CD2 | 28:DF:137:PHE:N | 2.82 | 0.47 |
| 29:DG:94:ARG:HG2 | 29:DG:127:GLN:HE21 | 1.80 | 0.47 |
| 30:DH:122:LEU:HD11 | 30:DH:130:VAL:CG2 | 2.40 | 0.47 |
| 32:DK:12:ASP:OD2 | 32:DK:85:VAL:HG13 | 2.15 | 0.47 |
| 23:DB:1190:G:OP1 | 33:DL:32:GLY:HA2 | 2.14 | 0.47 |
| 34:DM:86:LYS:HG3 | 34:DM:87:GLY:N | 2.29 | 0.47 |
| 36:DO:28:VAL:HG12 | 36:DO:93:ASP:O | 2.14 | 0.47 |
| 36:DO:52:SER:C | 36:DO:54:VAL:H | 2.17 | 0.47 |
| 38:DQ:111:LYS:H | 39:DR:48:LYS:HZ3 | 1.62 | 0.47 |
| 38:DQ:91:ARG:NH1 | 39:DR:10:LYS:HB3 | 2.25 | 0.47 |
| 41:DT:51:PHE:HB3 | 41:DT:53:VAL:HG23 | 1.96 | 0.47 |
| 42:DU:38:ILE:HG13 | 42:DU:39:ASN:N | 2.29 | 0.47 |
| 42:DU:51:LEU:HD22 | 42:DU:52:ASN:OD1 | 2.14 | 0.47 |
| 24:DV:30:ILE:O | 24:DV:37:PRO:HA | 2.13 | 0.47 |
| 24:DV:80:HIS:HA | 24:DV:87:GLN:OE1 | 2.14 | 0.47 |
| 43:DW:46:ALA:HB2 | 43:DW:78:PHE:HD1 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DW:58:LEU:HG | 43:DW:79:ILE:HD12 | 1.95 | 0.47 |
| 46:DZ:7:VAL:HG11 | 46:DZ:51:VAL:HG13 | 1.95 | 0.47 |
| 1:AA:109:A:H4' | 1:AA:110:C:OP2 | 2.14 | 0.47 |
| 1:AA:366:A:O2' | 1:AA:394:G:N2 | 2.48 | 0.47 |
| 1:AA:443:C:H2' | 1:AA:444:G:H8 | 1.78 | 0.47 |
| 1:AA:591:U:H2' | 1:AA:592:G:H8 | 1.77 | 0.47 |
| 1:AA:805:C:O2' | 1:AA:806:C:H5' | 2.13 | 0.47 |
| 1:AA:814:A:H2' | 1:AA:816:A:O5' | 2.14 | 0.47 |
| 1:AA:82:G:H1' | 1:AA:89:U:H1' | 1.96 | 0.47 |
| 20:AB:53:LEU:HD13 | 20:AB:216:VAL:HG12 | 1.96 | 0.47 |
| 8:AI:22:PRO:HA | 8:AI:60:LEU:CB | 2.44 | 0.47 |
| 9:AJ:41:PRO:HA | 9:AJ:72:ARG:HD3 | 1.96 | 0.47 |
| 13:AN:64:ARG:HB2 | 13:AN:77:GLY:O | 2.13 | 0.47 |
| 16:AQ:11:VAL:HG13 | 16:AQ:20:ILE:HG23 | 1.95 | 0.47 |
| 16:AQ:59:GLU:HG3 | 16:AQ:78:VAL:HG21 | 1.95 | 0.47 |
| 21:AU:3:ILE:HB | 21:AU:19:LYS:HD2 | 1.96 | 0.47 |
| 21:AU:20:ARG:HG3 | 21:AU:24:LYS:HG3 | 1.97 | 0.47 |
| 50:B3:54:LEU:CG | 50:B3:58:ILE:HD11 | 2.43 | 0.47 |
| 22:BA:11:C:H5' | 43:BW:71:LYS:CG | 2.44 | 0.47 |
| 22:BA:71:C:H2' | 22:BA:72:G:O4' | 2.14 | 0.47 |
| 22:BA:91:C:O2' | 22:BA:92:C:H5' | 2.14 | 0.47 |
| 23:BB:1100:C:H2' | 23:BB:1101:U:C6 | 2.48 | 0.47 |
| 23:BB:1405:U:H2' | 23:BB:1406:U:C6 | 2.49 | 0.47 |
| 23:BB:1593:A:H2' | 23:BB:1594:U:H6 | 1.75 | 0.47 |
| 23:BB:1640:A:H2' | 23:BB:1641:A:H8 | 1.79 | 0.47 |
| 23:BB:758:C:O2 | 23:BB:1981:A:H2 | 1.96 | 0.47 |
| 23:BB:2101:A:C2' | 23:BB:2102:G:H5'' | 2.44 | 0.47 |
| 23:BB:2709:G:H2' | 23:BB:2710:C:C6 | 2.49 | 0.47 |
| 23:BB:297:G:OP1 | 42:BU:91:LYS:HD3 | 2.14 | 0.47 |
| 23:BB:648:G:O2' | 23:BB:649:G:H5' | 2.15 | 0.47 |
| 23:BB:696:G:O2' | 23:BB:697:G:H5' | 2.14 | 0.47 |
| 25:BC:144:GLU:CA | 25:BC:151:GLY:HA2 | 2.42 | 0.47 |
| 23:BB:2444:G:OP2 | 27:BE:63:LYS:HD2 | 2.13 | 0.47 |
| 28:BF:87:LYS:CG | 28:BF:88:VAL:H | 2.25 | 0.47 |
| 30:BH:40:THR:O | 30:BH:42:LYS:N | 2.40 | 0.47 |
| 23:BB:558:U:OP1 | 31:BJ:114:LEU:HB2 | 2.14 | 0.47 |
| 35:BN:73:ASN:O | 35:BN:76:VAL:HG22 | 2.14 | 0.47 |
| 38:BQ:23:TYR:N | 38:BQ:23:TYR:CD2 | 2.81 | 0.47 |
| 38:BQ:80:ASN:O | 38:BQ:116:LEU:HD11 | 2.14 | 0.47 |
| 40:BS:47:VAL:HG23 | 40:BS:48:LYS:N | 2.28 | 0.47 |
| 44:BX:26:PHE:HD1 | 44:BX:27:ASN:ND2 | 2.10 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1035:A:H2' | 1:CA:1036:A:C8 | 2.49 | 0.47 |
| 1:CA:1510:C:H2' | 1:CA:1511:G:H8 | 1.79 | 0.47 |
| 1:CA:242:G:H2' | 1:CA:243:A:H5'' | 1.96 | 0.47 |
| 1:CA:269:C:H2' | 1:CA:270:A:H8 | 1.74 | 0.47 |
| 1:CA:309:A:O2' | 1:CA:310:G:H5' | 2.14 | 0.47 |
| 1:CA:411:A:N6 | 1:CA:413:G:H21 | 2.10 | 0.47 |
| 3:CD:44:LYS:HD2 | 3:CD:46:ARG:CG | 2.44 | 0.47 |
| 3:CD:94:GLU:HG3 | 3:CD:99:ASN:ND2 | 2.29 | 0.47 |
| 13:CN:79:SER:HG | 13:CN:82:LYS:HG2 | 1.79 | 0.47 |
| 14:CO:88:ARG:CA | 14:CO:88:ARG:HH11 | 2.20 | 0.47 |
| 22:DA:55:U:H2' | 22:DA:56:G:C8 | 2.48 | 0.47 |
| 23:DB:1162:G:H1' | 39:DR:23:GLU:OE2 | 2.14 | 0.47 |
| 23:DB:53:A:H61 | 23:DB:117:G:H1' | 1.79 | 0.47 |
| 23:DB:1222:U:P | 39:DR:90:ARG:HH22 | 2.38 | 0.47 |
| 23:DB:1266:G:N2 | 23:DB:2012:G:H2' | 2.29 | 0.47 |
| 23:DB:1416:G:HO2' | 23:DB:1417:C:H6 | 1.60 | 0.47 |
| 23:DB:1970:A:H1' | 23:DB:1972:G:C8 | 2.48 | 0.47 |
| 23:DB:2065:C:H1' | 23:DB:2449:U:O2 | 2.13 | 0.47 |
| 23:DB:2520:C:O2' | 23:DB:2521:C:H5' | 2.14 | 0.47 |
| 23:DB:2553:G:H2' | 23:DB:2554:U:H4' | 1.96 | 0.47 |
| 23:DB:2814:A:H2' | 23:DB:2815:C:H6 | 1.78 | 0.47 |
| 23:DB:335:C:H5'' | 42:DU:81:ARG:NH1 | 2.29 | 0.47 |
| 23:DB:335:C:O2' | 23:DB:336:C:H5' | 2.14 | 0.47 |
| 23:DB:337:C:H2' | 23:DB:338:G:O4' | 2.13 | 0.47 |
| 23:DB:247:G:H4' | 23:DB:386:G:C5 | 2.50 | 0.47 |
| 23:DB:754:U:H2' | 23:DB:755:U:C6 | 2.48 | 0.47 |
| 23:DB:934:U:H2' | 23:DB:935:C:H6 | 1.80 | 0.47 |
| 25:DC:68:ARG:HB3 | 25:DC:128:THR:OG1 | 2.14 | 0.47 |
| 25:DC:141:HIS:O | 25:DC:143:VAL:HG23 | 2.14 | 0.47 |
| 23:DB:659:G:H4' | 27:DE:95:LYS:HD3 | 1.96 | 0.47 |
| 30:DH:53:GLU:CB | 30:DH:57:LYS:HB3 | 2.44 | 0.47 |
| 31:DJ:88:THR:HG22 | 31:DJ:91:GLU:OE1 | 2.14 | 0.47 |
| 35:DN:54:LEU:HD11 | 35:DN:62:ASN:HB3 | 1.96 | 0.47 |
| 35:DN:99:LYS:O | 47:D0:42:ILE:HG12 | 2.14 | 0.47 |
| 36:DO:9:ARG:HA | 36:DO:12:THR:OG1 | 2.13 | 0.47 |
| 37:DP:50:ARG:CB | 37:DP:56:SER:HB3 | 2.43 | 0.47 |
| 32:DK:120:PRO:HA | 37:DP:65:ASN:HD21 | 1.80 | 0.47 |
| 38:DQ:85:ALA:HB2 | 38:DQ:115:ALA:HB1 | 1.95 | 0.47 |
| 38:DQ:96:ASP:C | 38:DQ:98:ALA:H | 2.18 | 0.47 |
| 39:DR:21:ARG:C | 39:DR:22:LEU:HD23 | 2.35 | 0.47 |
| 41:DT:2:ILE:HG13 | 41:DT:3:ARG:CZ | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:DT:43:ILE:O | 41:DT:46:ALA:HB3 | 2.13 | 0.47 |
| 43:DW:23:LYS:CG | 43:DW:24:ARG:N | 2.76 | 0.47 |
| 46:DZ:36:HIS:O | 46:DZ:48:THR:HA | 2.15 | 0.47 |
| 1:AA:1300:G:H1' | 1:AA:1301:U:C5 | 2.49 | 0.47 |
| 1:AA:1499:A:O2' | 1:AA:1500:A:H5' | 2.14 | 0.47 |
| 1:AA:251:G:H1 | 1:AA:271:C:N4 | 2.12 | 0.47 |
| 1:AA:366:A:H1' | 1:AA:395:C:O2 | 2.14 | 0.47 |
| 1:AA:454:G:H2' | 1:AA:455:G:H8 | 1.78 | 0.47 |
| 1:AA:562:U:H4' | 1:AA:563:A:O5' | 2.15 | 0.47 |
| 20:AB:163:ILE:HD12 | 20:AB:185:ILE:HD12 | 1.97 | 0.47 |
| 20:AB:19:THR:HG23 | 20:AB:20:ARG:N | 2.23 | 0.47 |
| 20:AB:83:ALA:HA | 20:AB:88:GLN:NE2 | 2.29 | 0.47 |
| 3:AD:22:SER:N | 3:AD:109:THR:HG22 | 2.29 | 0.47 |
| 6:AG:144:ALA:O | 6:AG:145:GLU:HB3 | 2.15 | 0.47 |
| 9:AJ:80:THR:HB | 9:AJ:83:THR:OG1 | 2.15 | 0.47 |
| 13:AN:27:LYS:HG3 | 13:AN:28:ALA:H | 1.79 | 0.47 |
| 23:BB:771:G:OP1 | 49:B2:14:ARG:HD2 | 2.14 | 0.47 |
| 22:BA:30:C:H2' | 22:BA:31:C:H5' | 1.97 | 0.47 |
| 23:BB:1038:G:H2' | 23:BB:1039:A:H8 | 1.76 | 0.47 |
| 23:BB:1126:A:H4' | 23:BB:1127:A:O5' | 2.14 | 0.47 |
| 23:BB:1130:U:O2 | 23:BB:2025:C:H5'' | 2.15 | 0.47 |
| 23:BB:1197:G:O2' | 23:BB:1198:U:H5' | 2.14 | 0.47 |
| 23:BB:1222:U:O2' | 23:BB:1223:G:H5' | 2.14 | 0.47 |
| 23:BB:1717:A:H2' | 23:BB:1718:G:O4' | 2.15 | 0.47 |
| 23:BB:2070:A:C2 | 23:BB:2442:C:C2 | 3.01 | 0.47 |
| 23:BB:2602:A:H3' | 23:BB:2602:A:OP1 | 2.14 | 0.47 |
| 23:BB:2811:G:OP1 | 26:BD:62:LYS:HD2 | 2.14 | 0.47 |
| 23:BB:2818:U:H4' | 23:BB:2837:A:O4' | 2.15 | 0.47 |
| 23:BB:533:G:H5' | 38:BQ:23:TYR:CD2 | 2.49 | 0.47 |
| 23:BB:859:G:HO2' | 23:BB:916:G:H1 | 1.61 | 0.47 |
| 27:BE:146:VAL:HA | 27:BE:185:LYS:O | 2.14 | 0.47 |
| 30:BH:110:VAL:HB | 30:BH:132:PHE:CE1 | 2.49 | 0.47 |
| 30:BH:49:ALA:HB3 | 30:BH:50:ARG:NH1 | 2.29 | 0.47 |
| 31:BJ:43:GLU:O | 31:BJ:45:THR:HG22 | 2.15 | 0.47 |
| 31:BJ:55:ILE:CG2 | 31:BJ:123:LYS:HB2 | 2.44 | 0.47 |
| 34:BM:30:SER:HA | 34:BM:133:LYS:HB2 | 1.96 | 0.47 |
| 34:BM:19:GLY:N | 34:BM:38:ARG:HH12 | 2.03 | 0.47 |
| 40:BS:66:ILE:HD13 | 40:BS:66:ILE:N | 2.26 | 0.47 |
| 42:BU:53:GLN:CD | 42:BU:53:GLN:H | 2.18 | 0.47 |
| 42:BU:60:LYS:HA | 42:BU:60:LYS:HE2 | 1.95 | 0.47 |
| 46:BZ:33:LEU:HD23 | 46:BZ:52:SER:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1060:U:H2' | 1:CA:1061:G:H8 | 1.78 | 0.47 |
| 1:CA:1086:U:H3 | 1:CA:1099:G:N2 | 1.94 | 0.47 |
| 1:CA:1125:U:O2' | 1:CA:1126:U:H2' | 2.15 | 0.47 |
| 1:CA:1363:A:H2' | 1:CA:1363:A:N3 | 2.30 | 0.47 |
| 1:CA:208:U:O2' | 1:CA:209:U:H3' | 2.13 | 0.47 |
| 1:CA:65:A:C6 | 1:CA:381:C:N3 | 2.83 | 0.47 |
| 1:CA:702:A:C8 | 23:DB:1848:A:H1' | 2.50 | 0.47 |
| 20:CB:130:LYS:HA | 20:CB:130:LYS:NZ | 2.29 | 0.47 |
| 3:CD:33:ILE:HD12 | 3:CD:34:GLU:H | 1.79 | 0.47 |
| 3:CD:47:LEU:HD13 | 3:CD:52:VAL:HG22 | 1.96 | 0.47 |
| 8:CI:18:VAL:HA | 8:CI:64:ILE:HA | 1.96 | 0.47 |
| 13:CN:26:LEU:HD12 | 13:CN:44:VAL:HG13 | 1.96 | 0.47 |
| 14:CO:67:ASP:O | 14:CO:71:ARG:HG3 | 2.14 | 0.47 |
| 23:DB:1138:G:H2' | 23:DB:1139:G:O4' | 2.14 | 0.47 |
| 23:DB:140:C:H4' | 23:DB:141:G:C6 | 2.50 | 0.47 |
| 23:DB:1444:G:H2' | 23:DB:1445:G:C8 | 2.49 | 0.47 |
| 23:DB:2840:C:O2' | 23:DB:2841:C:H5' | 2.14 | 0.47 |
| 25:DC:183:VAL:HG22 | 25:DC:187:CYS:SG | 2.54 | 0.47 |
| 27:DE:172:ALA:HB2 | 27:DE:195:GLN:NE2 | 2.30 | 0.47 |
| 28:DF:141:ASP:O | 28:DF:144:LYS:N | 2.47 | 0.47 |
| 52:DI:76:ALA:HA | 52:DI:135:MET:SD | 2.54 | 0.47 |
| 52:DI:35:MET:HE3 | 52:DI:39:LYS:HG2 | 1.96 | 0.47 |
| 31:DJ:30:THR:O | 31:DJ:33:ALA:HB3 | 2.15 | 0.47 |
| 32:DK:98:ARG:C | 32:DK:99:ILE:HD12 | 2.35 | 0.47 |
| 34:DM:69:PRO:HA | 34:DM:94:ALA:HA | 1.95 | 0.47 |
| 34:DM:69:PRO:HG2 | 34:DM:70:ASP:H | 1.79 | 0.47 |
| 35:DN:7:GLY:HA2 | 35:DN:46:ARG:HH12 | 1.79 | 0.47 |
| 35:DN:58:ASP:O | 35:DN:59:SER:HB3 | 2.15 | 0.47 |
| 35:DN:83:LEU:HA | 35:DN:86:ARG:CG | 2.44 | 0.47 |
| 39:DR:5:PHE:HB2 | 39:DR:37:GLU:OE1 | 2.14 | 0.47 |
| 1:AA:1339:A:H2' | 1:AA:1340:A:O4' | 2.14 | 0.47 |
| 1:AA:386:C:C2' | 1:AA:387:U:H5' | 2.45 | 0.47 |
| 1:AA:86:G:H1' | 1:AA:87:C:H5 | 1.77 | 0.47 |
| 1:AA:916:U:O2' | 1:AA:917:G:H5' | 2.14 | 0.47 |
| 20:AB:35:ASN:HD22 | 20:AB:35:ASN:HA | 1.54 | 0.47 |
| 2:AC:111:ASP:HB3 | 2:AC:114:LEU:HD12 | 1.97 | 0.47 |
| 3:AD:162:GLU:HA | 3:AD:166:LYS:NZ | 2.29 | 0.47 |
| 3:AD:33:ILE:O | 3:AD:35:GLN:HG3 | 2.15 | 0.47 |
| 6:AG:78:ARG:NH1 | 6:AG:80:GLY:H | 2.13 | 0.47 |
| 9:AJ:44:THR:HG23 | 9:AJ:69:THR:O | 2.13 | 0.47 |
| 12:AM:86:ARG:CG | 12:AM:96:VAL:HG11 | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:AR:35:SER:O | 17:AR:70:THR:HA | 2.15 | 0.47 |
| 22:BA:82:U:O2' | 22:BA:83:G:H5' | 2.14 | 0.47 |
| 23:BB:1027:A:N6 | 23:BB:1126:A:H1' | 2.29 | 0.47 |
| 23:BB:1193:G:H2' | 23:BB:1194:A:O4' | 2.13 | 0.47 |
| 23:BB:1445:G:H2' | 23:BB:1446:C:O4' | 2.15 | 0.47 |
| 23:BB:1496:A:H2' | 23:BB:1498:C:C5 | 2.49 | 0.47 |
| 23:BB:1790:C:H2' | 23:BB:1791:A:C8 | 2.49 | 0.47 |
| 23:BB:2230:G:H2' | 23:BB:2231:U:C6 | 2.50 | 0.47 |
| 23:BB:2061:G:H5'' | 23:BB:2503:A:C2 | 2.50 | 0.47 |
| 23:BB:2515:C:H2' | 23:BB:2516:A:H8 | 1.80 | 0.47 |
| 23:BB:2553:G:H2' | 23:BB:2554:U:C4' | 2.44 | 0.47 |
| 23:BB:303:G:H2' | 23:BB:304:U:C6 | 2.50 | 0.47 |
| 23:BB:324:A:H2' | 23:BB:325:G:O4' | 2.14 | 0.47 |
| 23:BB:431:U:O2' | 23:BB:432:A:H5' | 2.14 | 0.47 |
| 23:BB:519:U:H2' | 23:BB:520:G:C8 | 2.50 | 0.47 |
| 25:BC:179:GLU:CD | 25:BC:266:ILE:HD11 | 2.35 | 0.47 |
| 23:BB:2052:A:O4' | 26:BD:147:GLY:HA3 | 2.14 | 0.47 |
| 28:BF:134:GLN:HB3 | 28:BF:149:ARG:HB3 | 1.96 | 0.47 |
| 29:BG:10:VAL:CG2 | 29:BG:48:THR:HA | 2.45 | 0.47 |
| 30:BH:65:ALA:C | 30:BH:67:ALA:H | 2.16 | 0.47 |
| 32:BK:119:ALA:O | 32:BK:120:PRO:O | 2.33 | 0.47 |
| 33:BL:118:THR:O | 33:BL:120:VAL:HG23 | 2.14 | 0.47 |
| 33:BL:81:ASP:O | 33:BL:83:ALA:N | 2.48 | 0.47 |
| 23:BB:2880:C:H1' | 35:BN:93:GLY:H | 1.79 | 0.47 |
| 37:BP:6:GLN:O | 37:BP:10:GLU:HG2 | 2.13 | 0.47 |
| 38:BQ:18:LYS:C | 38:BQ:20:ALA:H | 2.17 | 0.47 |
| 23:BB:996:A:C4' | 38:BQ:91:ARG:HD2 | 2.41 | 0.47 |
| 40:BS:4:ILE:CG2 | 40:BS:106:VAL:HG13 | 2.44 | 0.47 |
| 23:BB:138:U:H1' | 41:BT:1:MET:H2 | 1.78 | 0.47 |
| 41:BT:38:ALA:HB3 | 41:BT:81:LYS:HZ3 | 1.79 | 0.47 |
| 1:CA:1414:U:H2' | 1:CA:1415:G:C8 | 2.44 | 0.47 |
| 1:CA:286:C:H2' | 1:CA:287:U:C6 | 2.50 | 0.47 |
| 1:CA:382:A:H2' | 1:CA:383:A:C8 | 2.49 | 0.47 |
| 1:CA:502:A:H2' | 1:CA:503:C:C6 | 2.49 | 0.47 |
| 1:CA:512:U:H2' | 1:CA:513:C:H6 | 1.75 | 0.47 |
| 1:CA:545:C:O2' | 1:CA:546:A:H5' | 2.15 | 0.47 |
| 1:CA:904:U:H2' | 1:CA:905:U:C6 | 2.50 | 0.47 |
| 20:CB:46:VAL:HA | 20:CB:49:PHE:CD2 | 2.50 | 0.47 |
| 2:CC:119:ILE:CG2 | 2:CC:120:THR:N | 2.76 | 0.47 |
| 5:CF:85:ILE:HG22 | 5:CF:86:ARG:H | 1.80 | 0.47 |
| 8:CI:30:ASN:HD22 | 8:CI:65:THR:HA | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1057:A:H62 | 23:DB:1086:A:H2' | 1.80 | 0.47 |
| 23:DB:1064:C:H2' | 23:DB:1065:U:O4' | 2.14 | 0.47 |
| 23:DB:1551:A:C3' | 23:DB:1552:A:H5'' | 2.44 | 0.47 |
| 23:DB:1557:C:H3' | 23:DB:1558:C:C5' | 2.45 | 0.47 |
| 23:DB:1590:A:H2' | 23:DB:1591:A:C8 | 2.49 | 0.47 |
| 23:DB:1672:A:C6 | 23:DB:1673:G:C6 | 3.02 | 0.47 |
| 23:DB:1682:G:H2' | 23:DB:1683:U:C6 | 2.49 | 0.47 |
| 23:DB:2197:U:O2' | 23:DB:2198:A:H2' | 2.14 | 0.47 |
| 23:DB:2247:A:H2' | 23:DB:2248:C:C6 | 2.50 | 0.47 |
| 23:DB:2700:A:H2' | 23:DB:2701:U:C6 | 2.48 | 0.47 |
| 23:DB:288:U:H2' | 23:DB:289:G:H5' | 1.96 | 0.47 |
| 23:DB:512:G:H4' | 23:DB:512:G:OP1 | 2.15 | 0.47 |
| 23:DB:572:A:OP2 | 39:DR:80:ARG:NH2 | 2.47 | 0.47 |
| 23:DB:776:G:H4' | 23:DB:777:G:O5' | 2.14 | 0.47 |
| 25:DC:140:VAL:CG2 | 25:DC:163:ILE:HG12 | 2.45 | 0.47 |
| 23:DB:2822:G:H5'' | 26:DD:164:GLN:HE22 | 1.78 | 0.47 |
| 26:DD:174:SER:O | 26:DD:175:LEU:HB2 | 2.14 | 0.47 |
| 26:DD:187:LEU:HD12 | 26:DD:188:LEU:H | 1.79 | 0.47 |
| 52:DI:10:LEU:O | 52:DI:10:LEU:HD12 | 2.13 | 0.47 |
| 52:DI:129:GLU:HB3 | 52:DI:133:ARG:NH1 | 2.29 | 0.47 |
| 31:DJ:58:ASN:CA | 31:DJ:127:GLY:HA2 | 2.29 | 0.47 |
| 33:DL:51:GLU:O | 33:DL:53:GLY:N | 2.47 | 0.47 |
| 34:DM:63:ILE:N | 34:DM:63:ILE:HD12 | 2.28 | 0.47 |
| 42:DU:90:LYS:O | 42:DU:92:VAL:HG23 | 2.14 | 0.47 |
| 23:DB:929:U:H1' | 45:DY:25:GLY:O | 2.14 | 0.47 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C5 | 2.50 | 0.47 |
| 1:AA:394:G:O2' | 1:AA:395:C:H5' | 2.15 | 0.47 |
| 1:AA:811:C:O2' | 1:AA:901:A:N1 | 2.46 | 0.47 |
| 2:AC:156:LEU:CD1 | 2:AC:165:GLU:HB2 | 2.44 | 0.47 |
| 4:AE:45:VAL:HG11 | 4:AE:117:ALA:HB2 | 1.97 | 0.47 |
| 4:AE:87:VAL:HG23 | 4:AE:92:ARG:HA | 1.96 | 0.47 |
| 5:AF:32:ALA:O | 5:AF:33:GLU:HB2 | 2.15 | 0.47 |
| 5:AF:4:TYR:CE2 | 5:AF:71:ILE:HD13 | 2.50 | 0.47 |
| 7:AH:94:VAL:HG21 | 7:AH:100:ILE:O | 2.14 | 0.47 |
| 7:AH:77:VAL:HG23 | 7:AH:126:CYS:HA | 1.96 | 0.47 |
| 8:AI:56:MET:SD | 8:AI:57:VAL:N | 2.87 | 0.47 |
| 11:AL:66:ILE:N | 11:AL:66:ILE:HD12 | 2.30 | 0.47 |
| 18:AS:40:PHE:O | 18:AS:43:MET:HG3 | 2.15 | 0.47 |
| 23:BB:1381:G:H1' | 23:BB:1571:A:N1 | 2.29 | 0.47 |
| 23:BB:2233:U:H2' | 23:BB:2234:G:H8 | 1.80 | 0.47 |
| 23:BB:2544:G:O2' | 23:BB:2545:G:H5' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2679:A:O2' | 23:BB:2680:U:H5' | 2.14 | 0.47 |
| 23:BB:2697:G:H2' | 23:BB:2698:U:O4' | 2.15 | 0.47 |
| 23:BB:2708:G:O2' | 23:BB:2709:G:H5' | 2.14 | 0.47 |
| 23:BB:499:U:H2' | 23:BB:500:G:O4' | 2.14 | 0.47 |
| 23:BB:531:C:O2' | 23:BB:563:A:H5'' | 2.14 | 0.47 |
| 25:BC:259:ASN:C | 25:BC:261:ARG:H | 2.18 | 0.47 |
| 27:BE:115:GLN:O | 27:BE:117:ARG:HG3 | 2.14 | 0.47 |
| 27:BE:157:LEU:O | 27:BE:160:ALA:HB3 | 2.15 | 0.47 |
| 27:BE:48:THR:HG23 | 27:BE:51:GLU:OE2 | 2.15 | 0.47 |
| 28:BF:137:PHE:CD2 | 28:BF:137:PHE:N | 2.83 | 0.47 |
| 28:BF:155:ILE:HG22 | 28:BF:156:THR:N | 2.30 | 0.47 |
| 29:BG:106:LEU:O | 29:BG:108:PHE:HD1 | 1.97 | 0.47 |
| 29:BG:94:ARG:HA | 29:BG:128:THR:HG22 | 1.97 | 0.47 |
| 30:BH:81:ALA:HB2 | 30:BH:147:VAL:HG23 | 1.95 | 0.47 |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:N | 2.23 | 0.47 |
| 32:BK:104:THR:H | 32:BK:107:LEU:CD1 | 2.26 | 0.47 |
| 32:BK:112:PHE:O | 32:BK:113:MET:C | 2.53 | 0.47 |
| 42:BU:85:ARG:HH11 | 42:BU:86:PHE:N | 2.13 | 0.47 |
| 1:CA:1120:C:H2' | 1:CA:1121:U:C6 | 2.49 | 0.47 |
| 1:CA:1406:U:H2' | 1:CA:1407:C:H5' | 1.96 | 0.47 |
| 1:CA:142:G:N3 | 1:CA:196:A:H2 | 2.12 | 0.47 |
| 1:CA:197:A:H4' | 1:CA:198:G:O5' | 2.13 | 0.47 |
| 1:CA:358:U:H2' | 1:CA:359:G:C8 | 2.50 | 0.47 |
| 1:CA:435:A:H2' | 1:CA:435:A:N3 | 2.30 | 0.47 |
| 1:CA:44:A:O2' | 1:CA:45:G:H5' | 2.14 | 0.47 |
| 1:CA:659:U:O2' | 1:CA:660:C:H5' | 2.15 | 0.47 |
| 1:CA:844:G:OP2 | 1:CA:844:G:H3' | 2.14 | 0.47 |
| 20:CB:80:LYS:HG3 | 20:CB:81:ASP:N | 2.29 | 0.47 |
| 2:CC:190:THR:HG22 | 2:CC:191:THR:H | 1.78 | 0.47 |
| 6:CG:144:ALA:O | 6:CG:145:GLU:HB3 | 2.14 | 0.47 |
| 7:CH:10:LEU:CD2 | 7:CH:74:ILE:HD11 | 2.44 | 0.47 |
| 1:CA:967:C:H4' | 8:CI:129:ARG:HG2 | 1.96 | 0.47 |
| 8:CI:19:PHE:HB2 | 8:CI:63:TYR:HB3 | 1.97 | 0.47 |
| 17:CR:63:TYR:HD2 | 17:CR:63:TYR:N | 2.11 | 0.47 |
| 18:CS:48:ILE:O | 18:CS:58:PRO:HA | 2.14 | 0.47 |
| 23:DB:1203:U:H3' | 23:DB:1204:A:C5' | 2.44 | 0.47 |
| 23:DB:1729:U:C2' | 23:DB:1730:C:H4' | 2.39 | 0.47 |
| 23:DB:184:C:H2' | 23:DB:185:G:C8 | 2.49 | 0.47 |
| 23:DB:241:A:H8 | 23:DB:241:A:OP1 | 1.97 | 0.47 |
| 23:DB:2589:A:H2' | 23:DB:2590:A:C8 | 2.49 | 0.47 |
| 23:DB:269:C:H2' | 23:DB:270:A:H8 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:335:C:H2' | 23:DB:336:C:H6 | 1.79 | 0.47 |
| 23:DB:37:C:O2' | 23:DB:38:A:H5' | 2.15 | 0.47 |
| 23:DB:28:A:O2' | 23:DB:583:G:H5' | 2.15 | 0.47 |
| 23:DB:615:U:O4 | 27:DE:39:ALA:HB2 | 2.14 | 0.47 |
| 23:DB:692:C:H2' | 23:DB:693:A:C8 | 2.49 | 0.47 |
| 23:DB:784:G:HO2' | 23:DB:785:G:H5'' | 1.79 | 0.47 |
| 26:DD:123:LYS:HD3 | 26:DD:165:MET:SD | 2.54 | 0.47 |
| 23:DB:2635:A:H4' | 26:DD:79:LEU:HB2 | 1.96 | 0.47 |
| 29:DG:95:ALA:HA | 29:DG:104:LEU:HD23 | 1.96 | 0.47 |
| 29:DG:148:ARG:HB2 | 29:DG:152:ARG:HH11 | 1.79 | 0.47 |
| 30:DH:21:VAL:HG22 | 30:DH:22:LYS:N | 2.29 | 0.47 |
| 30:DH:9:VAL:CG1 | 30:DH:12:LEU:HG | 2.45 | 0.47 |
| 52:DI:18:ASN:HB2 | 52:DI:38:CYS:SG | 2.54 | 0.47 |
| 52:DI:18:ASN:N | 52:DI:19:PRO:CD | 2.77 | 0.47 |
| 32:DK:59:LYS:HD2 | 32:DK:89:ASN:O | 2.15 | 0.47 |
| 33:DL:89:VAL:HG13 | 33:DL:89:VAL:O | 2.15 | 0.47 |
| 36:DO:93:ASP:C | 36:DO:95:SER:H | 2.16 | 0.47 |
| 37:DP:4:ILE:C | 37:DP:6:GLN:N | 2.66 | 0.47 |
| 40:DS:52:GLU:HA | 40:DS:55:ILE:CG2 | 2.43 | 0.47 |
| 41:DT:54:GLU:HB3 | 41:DT:88:LYS:HB2 | 1.95 | 0.47 |
| 42:DU:60:LYS:HA | 42:DU:60:LYS:HE2 | 1.97 | 0.47 |
| 1:AA:1071:C:O2' | 1:AA:1072:G:H5' | 2.15 | 0.47 |
| 1:AA:222:C:H2' | 1:AA:223:A:H8 | 1.79 | 0.47 |
| 1:AA:246:A:C2 | 1:AA:282:A:C5 | 3.03 | 0.47 |
| 1:AA:462:G:H5' | 1:AA:463:U:P | 2.55 | 0.47 |
| 20:AB:120:SER:HA | 20:AB:125:PHE:CD1 | 2.49 | 0.47 |
| 20:AB:46:VAL:HA | 20:AB:49:PHE:CD2 | 2.49 | 0.47 |
| 2:AC:71:ARG:O | 2:AC:75:VAL:HG23 | 2.14 | 0.47 |
| 2:AC:87:ARG:HD3 | 2:AC:88:LYS:N | 2.30 | 0.47 |
| 3:AD:44:LYS:HD2 | 3:AD:46:ARG:CG | 2.44 | 0.47 |
| 11:AL:51:VAL:HG12 | 11:AL:63:THR:HG22 | 1.96 | 0.47 |
| 13:AN:60:ARG:HE | 13:AN:62:ARG:HG2 | 1.79 | 0.47 |
| 23:BB:115:C:O2' | 23:BB:116:C:H5' | 2.14 | 0.47 |
| 23:BB:1516:G:O2' | 23:BB:1517:G:H5' | 2.14 | 0.47 |
| 23:BB:1438:U:C4 | 23:BB:1552:A:N6 | 2.83 | 0.47 |
| 23:BB:1607:C:N4 | 23:BB:1622:G:OP2 | 2.48 | 0.47 |
| 23:BB:2261:C:O2' | 23:BB:2262:U:H5' | 2.14 | 0.47 |
| 23:BB:2586:U:H2' | 23:BB:2587:A:C8 | 2.50 | 0.47 |
| 23:BB:2895:G:O2' | 23:BB:2896:C:H5' | 2.15 | 0.47 |
| 23:BB:538:A:N6 | 23:BB:555:G:O2' | 2.46 | 0.47 |
| 23:BB:656:G:O2' | 23:BB:657:U:H5' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:97:C:H2' | 23:BB:98:G:O4' | 2.15 | 0.47 |
| 26:BD:55:LYS:HZ1 | 26:BD:59:ARG:HD2 | 1.78 | 0.47 |
| 27:BE:97:ASN:N | 27:BE:97:ASN:OD1 | 2.48 | 0.47 |
| 28:BF:79:ARG:HB2 | 28:BF:82:TYR:CE2 | 2.50 | 0.47 |
| 33:BL:17:LYS:O | 33:BL:18:ARG:HG2 | 2.13 | 0.47 |
| 37:BP:19:PHE:CE2 | 37:BP:83:ILE:HD11 | 2.50 | 0.47 |
| 38:BQ:49:ARG:HG2 | 38:BQ:49:ARG:HH11 | 1.79 | 0.47 |
| 39:BR:31:GLU:O | 39:BR:63:VAL:HG22 | 2.14 | 0.47 |
| 40:BS:20:VAL:C | 40:BS:22:ASP:H | 2.18 | 0.47 |
| 40:BS:25:ARG:HE | 40:BS:74:ILE:CG2 | 2.27 | 0.47 |
| 1:CA:1073:U:H2' | 1:CA:1074:G:H8 | 1.78 | 0.47 |
| 1:CA:119:A:H4' | 1:CA:120:A:O4' | 2.15 | 0.47 |
| 1:CA:1216:A:H2' | 1:CA:1217:C:H6 | 1.80 | 0.47 |
| 1:CA:213:G:H3' | 1:CA:214:C:H6 | 1.79 | 0.47 |
| 1:CA:692:U:H2' | 1:CA:694:A:OP2 | 2.15 | 0.47 |
| 1:CA:92:U:H2' | 1:CA:93:U:C6 | 2.49 | 0.47 |
| 3:CD:188:SER:C | 3:CD:190:LEU:H | 2.18 | 0.47 |
| 5:CF:36:ILE:N | 5:CF:36:ILE:HD12 | 2.30 | 0.47 |
| 5:CF:54:LEU:HD22 | 5:CF:54:LEU:N | 2.28 | 0.47 |
| 6:CG:30:MET:HA | 6:CG:38:ALA:CB | 2.45 | 0.47 |
| 8:CI:123:ARG:HB3 | 8:CI:123:ARG:CZ | 2.44 | 0.47 |
| 8:CI:16:ALA:HA | 8:CI:66:VAL:HA | 1.96 | 0.47 |
| 1:CA:36:C:H4' | 11:CL:118:VAL:O | 2.15 | 0.47 |
| 12:CM:77:LYS:O | 12:CM:80:MET:HG2 | 2.13 | 0.47 |
| 13:CN:63:CYS:HB3 | 13:CN:68:ARG:H | 1.80 | 0.47 |
| 15:CP:21:VAL:HG12 | 15:CP:33:ILE:HD12 | 1.97 | 0.47 |
| 19:CT:2:ASN:CG | 19:CT:3:ILE:N | 2.67 | 0.47 |
| 48:D1:39:ASP:OD1 | 48:D1:41:VAL:HB | 2.13 | 0.47 |
| 22:DA:73:A:H2' | 22:DA:73:A:N3 | 2.29 | 0.47 |
| 22:DA:95:U:H2' | 22:DA:96:G:H8 | 1.78 | 0.47 |
| 23:DB:1376:C:H3' | 56:DB:3279:HOH:O | 2.14 | 0.47 |
| 23:DB:1845:G:O2' | 23:DB:1846:G:H5' | 2.15 | 0.47 |
| 23:DB:20:C:H2' | 23:DB:21:A:H8 | 1.80 | 0.47 |
| 23:DB:235:U:H2' | 23:DB:236:C:C6 | 2.50 | 0.47 |
| 23:DB:2655:G:O2' | 23:DB:2656:U:P | 2.72 | 0.47 |
| 23:DB:2683:C:O2' | 23:DB:2684:U:H5' | 2.14 | 0.47 |
| 23:DB:2848:G:H1 | 23:DB:2867:G:N2 | 2.13 | 0.47 |
| 23:DB:2892:G:H5'' | 23:DB:2894:G:N2 | 2.30 | 0.47 |
| 23:DB:657:U:H2' | 23:DB:658:U:C6 | 2.50 | 0.47 |
| 25:DC:123:ILE:O | 25:DC:123:ILE:HG13 | 2.15 | 0.47 |
| 26:DD:116:LYS:HG3 | 26:DD:165:MET:SD | 2.54 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DE:97:ASN:OD1 | 27:DE:97:ASN:N | 2.47 | 0.47 |
| 52:DI:129:GLU:CB | 52:DI:133:ARG:HH12 | 2.27 | 0.47 |
| 52:DI:17:ALA:O | 52:DI:18:ASN:HB3 | 2.13 | 0.47 |
| 52:DI:37:PHE:HB2 | 52:DI:66:PHE:CE2 | 2.50 | 0.47 |
| 32:DK:85:VAL:HG21 | 32:DK:115:ILE:HD11 | 1.97 | 0.47 |
| 33:DL:100:ILE:O | 33:DL:100:ILE:HG12 | 2.15 | 0.47 |
| 33:DL:57:LEU:C | 33:DL:59:ARG:H | 2.16 | 0.47 |
| 34:DM:42:THR:O | 34:DM:45:GLN:HB2 | 2.14 | 0.47 |
| 35:DN:11:ASN:HA | 35:DN:11:ASN:HD22 | 1.55 | 0.47 |
| 35:DN:8:ARG:HB3 | 35:DN:43:GLU:OE2 | 2.14 | 0.47 |
| 36:DO:4:LYS:O | 36:DO:8:ILE:HG13 | 2.15 | 0.47 |
| 38:DQ:109:VAL:HG12 | 38:DQ:113:LYS:HE3 | 1.97 | 0.47 |
| 39:DR:31:GLU:H | 39:DR:63:VAL:HG22 | 1.80 | 0.47 |
| 40:DS:46:LEU:O | 40:DS:50:VAL:HG23 | 2.15 | 0.47 |
| 40:DS:60:HIS:O | 40:DS:61:ASN:CB | 2.62 | 0.47 |
| 40:DS:71:VAL:O | 40:DS:71:VAL:HG22 | 2.13 | 0.47 |
| 41:DT:85:VAL:C | 41:DT:86:THR:HG23 | 2.35 | 0.47 |
| 24:DV:51:GLN:HB2 | 24:DV:57:TYR:OH | 2.13 | 0.47 |
| 43:DW:18:LYS:HE3 | 43:DW:19:ARG:NH2 | 2.29 | 0.47 |
| 1:AA:1009:U:H1' | 1:AA:1021:A:C2 | 2.49 | 0.47 |
| 1:AA:1024:G:H2' | 1:AA:1025:U:C6 | 2.50 | 0.47 |
| 1:AA:1097:C:H2' | 1:AA:1098:C:H6 | 1.79 | 0.47 |
| 1:AA:1169:A:H2' | 1:AA:1170:A:C8 | 2.50 | 0.47 |
| 1:AA:1486:G:C2' | 1:AA:1487:G:O4' | 2.63 | 0.47 |
| 1:AA:377:G:H2' | 1:AA:378:G:H8 | 1.80 | 0.47 |
| 1:AA:57:G:H2' | 1:AA:58:C:C6 | 2.49 | 0.47 |
| 1:AA:900:A:H2' | 1:AA:901:A:C8 | 2.50 | 0.47 |
| 1:AA:889:A:N1 | 1:AA:907:A:H5'' | 2.29 | 0.47 |
| 1:AA:953:G:H2' | 1:AA:954:G:O4' | 2.15 | 0.47 |
| 20:AB:116:LEU:HA | 20:AB:119:GLN:CG | 2.45 | 0.47 |
| 4:AE:88:HIS:CE1 | 4:AE:137:ARG:HD2 | 2.49 | 0.47 |
| 5:AF:1:MET:HG2 | 5:AF:67:PRO:HD3 | 1.97 | 0.47 |
| 6:AG:110:ARG:HD3 | 6:AG:118:ARG:HA | 1.96 | 0.47 |
| 6:AG:30:MET:HA | 6:AG:38:ALA:CB | 2.44 | 0.47 |
| 7:AH:58:LEU:HD22 | 7:AH:60:LEU:HB2 | 1.96 | 0.47 |
| 8:AI:117:LEU:HD22 | 8:AI:123:ARG:HG2 | 1.96 | 0.47 |
| 10:AK:37:GLN:HB2 | 10:AK:39:ASN:ND2 | 2.29 | 0.47 |
| 10:AK:83:VAL:CG2 | 10:AK:106:ILE:HD11 | 2.45 | 0.47 |
| 19:AT:3:ILE:HG13 | 19:AT:3:ILE:H | 1.46 | 0.47 |
| 50:B3:32:LEU:HA | 50:B3:35:LYS:HD2 | 1.97 | 0.47 |
| 23:BB:1010:A:N3 | 23:BB:1153:C:H1' | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:131:A:O2' | 23:BB:132:G:H5' | 2.15 | 0.47 |
| 23:BB:1324:G:N1 | 23:BB:1331:G:C6 | 2.83 | 0.47 |
| 23:BB:1374:G:O2' | 23:BB:1375:U:H5' | 2.15 | 0.47 |
| 23:BB:1419:A:H2' | 23:BB:1421:G:C8 | 2.50 | 0.47 |
| 23:BB:2179:C:H2' | 23:BB:2180:U:H6 | 1.79 | 0.47 |
| 23:BB:2897:U:H2' | 23:BB:2898:U:H6 | 1.79 | 0.47 |
| 23:BB:510:C:O2' | 23:BB:1236:G:H5' | 2.15 | 0.47 |
| 23:BB:589:U:H2' | 23:BB:590:A:C8 | 2.49 | 0.47 |
| 23:BB:63:A:H2' | 23:BB:63:A:OP2 | 2.15 | 0.47 |
| 23:BB:920:A:H2' | 23:BB:921:C:H6 | 1.79 | 0.47 |
| 25:BC:115:ILE:HA | 25:BC:124:LYS:HZ1 | 1.77 | 0.47 |
| 25:BC:129:LEU:CD2 | 25:BC:133:ASN:HB2 | 2.45 | 0.47 |
| 25:BC:75:ALA:HB1 | 25:BC:93:VAL:HG22 | 1.97 | 0.47 |
| 29:BG:104:LEU:HB3 | 29:BG:106:LEU:HD21 | 1.96 | 0.47 |
| 29:BG:95:ALA:HA | 29:BG:104:LEU:HD23 | 1.95 | 0.47 |
| 31:BJ:16:TYR:N | 31:BJ:137:PRO:HB3 | 2.29 | 0.47 |
| 32:BK:119:ALA:HB3 | 32:BK:120:PRO:HD3 | 1.97 | 0.47 |
| 34:BM:55:ARG:HH22 | 34:BM:58:LYS:HA | 1.80 | 0.47 |
| 34:BM:69:PRO:HG2 | 34:BM:70:ASP:H | 1.79 | 0.47 |
| 36:BO:28:VAL:HG12 | 36:BO:93:ASP:O | 2.15 | 0.47 |
| 37:BP:3:ILE:HD13 | 37:BP:3:ILE:C | 2.35 | 0.47 |
| 39:BR:7:SER:HB2 | 39:BR:22:LEU:CB | 2.42 | 0.47 |
| 46:BZ:64:ILE:HG22 | 46:BZ:68:LEU:CD1 | 2.44 | 0.47 |
| 1:CA:284:C:H2' | 1:CA:285:C:C6 | 2.49 | 0.47 |
| 1:CA:342:C:O2' | 1:CA:343:U:H5' | 2.15 | 0.47 |
| 1:CA:429:U:H3' | 3:CD:8:LEU:CD2 | 2.45 | 0.47 |
| 1:CA:762:U:H2' | 1:CA:763:G:H8 | 1.79 | 0.47 |
| 2:CC:110:LEU:HD21 | 2:CC:140:ALA:O | 2.14 | 0.47 |
| 2:CC:110:LEU:HD22 | 2:CC:145:ALA:HB2 | 1.97 | 0.47 |
| 2:CC:21:TRP:CH2 | 2:CC:31:ASN:HB3 | 2.50 | 0.47 |
| 3:CD:192:ALA:C | 3:CD:194:ILE:H | 2.18 | 0.47 |
| 4:CE:92:ARG:HB3 | 4:CE:92:ARG:NH1 | 2.29 | 0.47 |
| 5:CF:11:HIS:CG | 5:CF:12:PRO:HD2 | 2.49 | 0.47 |
| 5:CF:2:ARG:HB3 | 5:CF:92:THR:OG1 | 2.14 | 0.47 |
| 9:CJ:41:PRO:O | 9:CJ:42:LEU:HB2 | 2.15 | 0.47 |
| 10:CK:61:ALA:O | 10:CK:64:VAL:HG13 | 2.13 | 0.47 |
| 15:CP:3:THR:CG2 | 15:CP:66:THR:HB | 2.41 | 0.47 |
| 22:DA:78:A:H2' | 22:DA:79:G:O4' | 2.13 | 0.47 |
| 22:DA:82:U:O2' | 22:DA:83:G:H5' | 2.14 | 0.47 |
| 23:DB:1253:A:H4' | 23:DB:1254:A:OP2 | 2.14 | 0.47 |
| 23:DB:1299:G:H5' | 23:DB:1300:G:OP1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1324:G:H1' | 23:DB:1616:A:C6 | 2.49 | 0.47 |
| 23:DB:1439:A:N7 | 23:DB:1440:U:C2 | 2.83 | 0.47 |
| 23:DB:758:C:O2 | 23:DB:1981:A:H2 | 1.98 | 0.47 |
| 23:DB:2085:U:O2' | 23:DB:2086:U:H5' | 2.15 | 0.47 |
| 23:DB:2094:A:H2' | 23:DB:2095:A:H8 | 1.79 | 0.47 |
| 23:DB:2138:G:H2' | 23:DB:2139:U:O4' | 2.14 | 0.47 |
| 23:DB:2281:A:O2' | 23:DB:2282:G:H5' | 2.15 | 0.47 |
| 23:DB:2331:G:O2' | 23:DB:2332:C:H5' | 2.15 | 0.47 |
| 23:DB:2362:C:OP2 | 50:D3:43:LEU:HD21 | 2.15 | 0.47 |
| 23:DB:2583:G:H2' | 23:DB:2584:U:O4' | 2.15 | 0.47 |
| 23:DB:392:U:O2' | 23:DB:393:C:H5' | 2.14 | 0.47 |
| 23:DB:437:U:H2' | 23:DB:438:G:C8 | 2.50 | 0.47 |
| 23:DB:547:A:H3' | 23:DB:547:A:OP1 | 2.13 | 0.47 |
| 23:DB:580:U:O3' | 38:DQ:30:VAL:HG13 | 2.15 | 0.47 |
| 23:DB:632:A:H2' | 23:DB:633:A:C8 | 2.49 | 0.47 |
| 23:DB:648:G:O2' | 23:DB:649:G:H5' | 2.15 | 0.47 |
| 23:DB:718:A:H5' | 23:DB:719:C:C5 | 2.50 | 0.47 |
| 23:DB:728:G:O2' | 23:DB:730:A:H8 | 1.97 | 0.47 |
| 23:DB:816:C:O2' | 23:DB:817:C:H5' | 2.15 | 0.47 |
| 23:DB:97:C:H2' | 23:DB:98:G:O4' | 2.15 | 0.47 |
| 23:DB:993:G:H5'' | 38:DQ:49:ARG:NH1 | 2.29 | 0.47 |
| 25:DC:102:TYR:O | 25:DC:103:ILE:HG13 | 2.15 | 0.47 |
| 23:DB:1998:A:OP2 | 26:DD:141:ARG:NH2 | 2.48 | 0.47 |
| 27:DE:137:LYS:O | 27:DE:141:MET:HG3 | 2.15 | 0.47 |
| 28:DF:74:ALA:HB3 | 28:DF:77:LYS:O | 2.15 | 0.47 |
| 52:DI:2:LYS:O | 52:DI:3:LYS:HG3 | 2.14 | 0.47 |
| 23:DB:956:G:C4' | 34:DM:82:MET:HE1 | 2.45 | 0.47 |
| 35:DN:114:GLU:CD | 35:DN:118:ARG:HH11 | 2.18 | 0.47 |
| 38:DQ:80:ASN:C | 38:DQ:82:LEU:H | 2.18 | 0.47 |
| 40:DS:47:VAL:HG12 | 40:DS:103:ILE:HG21 | 1.97 | 0.47 |
| 41:DT:68:LYS:HD3 | 41:DT:68:LYS:N | 2.29 | 0.47 |
| 42:DU:10:VAL:HB | 42:DU:69:VAL:HB | 1.95 | 0.47 |
| 45:DY:23:LEU:CD1 | 45:DY:28:LEU:HB2 | 2.43 | 0.47 |
| 45:DY:50:VAL:O | 45:DY:54:VAL:HG22 | 2.15 | 0.47 |
| 46:DZ:76:GLU:HG3 | 46:DZ:77:LYS:H | 1.79 | 0.47 |
| 1:AA:1222:G:C2' | 1:AA:1223:C:H5' | 2.44 | 0.47 |
| 1:AA:323:U:H2' | 1:AA:324:G:O4' | 2.14 | 0.47 |
| 1:AA:468:A:H3' | 1:AA:469:C:C6 | 2.50 | 0.47 |
| 1:AA:373:A:C1' | 1:AA:481:G:H1' | 2.45 | 0.47 |
| 1:AA:586:C:C2' | 1:AA:587:G:H5' | 2.45 | 0.47 |
| 1:AA:981:U:H2' | 1:AA:982:U:C5 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AB:93:HIS:HA | 20:AB:94:ARG:NH2 | 2.30 | 0.47 |
| 15:AP:20:VAL:HG21 | 15:AP:32:PHE:CG | 2.50 | 0.47 |
| 1:AA:1320:C:OP2 | 18:AS:69:LYS:HE3 | 2.14 | 0.47 |
| 22:BA:16:G:O2' | 22:BA:17:C:H5' | 2.15 | 0.47 |
| 22:BA:32:U:H2' | 22:BA:33:G:O4' | 2.14 | 0.47 |
| 23:BB:1396:U:H5' | 23:BB:1396:U:O2 | 2.15 | 0.47 |
| 23:BB:2305:U:H2' | 23:BB:2306:C:O4' | 2.15 | 0.47 |
| 23:BB:2553:G:H2' | 23:BB:2554:U:H4' | 1.97 | 0.47 |
| 23:BB:2675:A:N1 | 23:BB:2732:G:O6 | 2.47 | 0.47 |
| 23:BB:352:A:H3' | 23:BB:353:C:H6 | 1.80 | 0.47 |
| 23:BB:425:G:O2' | 23:BB:426:C:H5' | 2.13 | 0.47 |
| 23:BB:68:G:H2' | 23:BB:69:C:C6 | 2.49 | 0.47 |
| 23:BB:971:G:OP2 | 23:BB:974:G:N2 | 2.47 | 0.47 |
| 23:BB:98:G:H1 | 42:BU:6:ARG:NH1 | 2.11 | 0.47 |
| 23:BB:993:G:H5'' | 38:BQ:49:ARG:NH1 | 2.29 | 0.47 |
| 25:BC:229:HIS:ND1 | 25:BC:230:PRO:HD2 | 2.29 | 0.47 |
| 27:BE:179:SER:HA | 27:BE:182:ALA:HB3 | 1.96 | 0.47 |
| 28:BF:33:ILE:HG12 | 28:BF:155:ILE:HG13 | 1.97 | 0.47 |
| 33:BL:123:ARG:HD2 | 33:BL:124:GLY:N | 2.30 | 0.47 |
| 35:BN:83:LEU:O | 35:BN:86:ARG:HB2 | 2.15 | 0.47 |
| 36:BO:4:LYS:O | 36:BO:8:ILE:HG13 | 2.14 | 0.47 |
| 37:BP:4:ILE:C | 37:BP:6:GLN:N | 2.67 | 0.47 |
| 38:BQ:85:ALA:HB2 | 38:BQ:115:ALA:HB1 | 1.96 | 0.47 |
| 39:BR:75:VAL:O | 39:BR:76:LYS:HD2 | 2.15 | 0.47 |
| 24:BV:19:ARG:O | 24:BV:22:ALA:HB3 | 2.15 | 0.47 |
| 24:BV:30:ILE:HG23 | 24:BV:72:VAL:HG11 | 1.97 | 0.47 |
| 43:BW:51:GLY:N | 43:BW:59:PHE:HB2 | 2.29 | 0.47 |
| 1:CA:1016:A:H4' | 1:CA:1218:C:H4' | 1.96 | 0.47 |
| 1:CA:1222:G:C2' | 1:CA:1223:C:H5' | 2.45 | 0.47 |
| 1:CA:202:G:H2' | 1:CA:203:G:H8 | 1.80 | 0.47 |
| 1:CA:224:U:H2' | 1:CA:225:C:H6 | 1.80 | 0.47 |
| 1:CA:429:U:H1' | 1:CA:430:A:H5'' | 1.96 | 0.47 |
| 1:CA:811:C:O2' | 1:CA:901:A:N1 | 2.48 | 0.47 |
| 20:CB:116:LEU:HA | 20:CB:119:GLN:HG3 | 1.97 | 0.47 |
| 20:CB:186:VAL:O | 20:CB:200:PRO:HA | 2.14 | 0.47 |
| 10:CK:88:PRO:HD3 | 21:CU:28:LEU:CD1 | 2.34 | 0.47 |
| 11:CL:33:CYS:HA | 11:CL:54:VAL:HA | 1.97 | 0.47 |
| 13:CN:53:ASP:HA | 13:CN:58:ARG:NE | 2.30 | 0.47 |
| 22:DA:55:U:H2' | 22:DA:56:G:H8 | 1.79 | 0.47 |
| 23:DB:1287:A:P | 35:DN:104:ALA:HB3 | 2.55 | 0.47 |
| 23:DB:1336:A:H3' | 23:DB:1337:G:H8 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1599:U:H2' | 23:DB:1600:C:C6 | 2.49 | 0.47 |
| 23:DB:2258:C:O2' | 23:DB:2427:C:OP2 | 2.32 | 0.47 |
| 23:DB:292:U:O2' | 23:DB:293:U:H5' | 2.14 | 0.47 |
| 23:DB:406:G:O2' | 23:DB:407:G:H5' | 2.15 | 0.47 |
| 23:DB:4:U:H2' | 23:DB:5:A:H8 | 1.80 | 0.47 |
| 23:DB:693:A:H2' | 23:DB:694:U:H6 | 1.80 | 0.47 |
| 25:DC:78:GLU:HB2 | 25:DC:92:LEU:HD23 | 1.96 | 0.47 |
| 28:DF:65:LEU:CD2 | 28:DF:87:LYS:HD2 | 2.42 | 0.47 |
| 29:DG:140:ILE:HA | 29:DG:143:VAL:CG2 | 2.44 | 0.47 |
| 29:DG:71:LEU:HD13 | 29:DG:74:MET:SD | 2.55 | 0.47 |
| 30:DH:92:GLY:O | 30:DH:93:SER:HB2 | 2.15 | 0.47 |
| 31:DJ:98:GLU:HB3 | 31:DJ:124:VAL:HG21 | 1.96 | 0.47 |
| 32:DK:104:THR:H | 32:DK:107:LEU:CD1 | 2.28 | 0.47 |
| 33:DL:132:ARG:O | 33:DL:135:ILE:HG22 | 2.14 | 0.47 |
| 34:DM:38:ARG:HG2 | 34:DM:38:ARG:HH11 | 1.79 | 0.47 |
| 35:DN:2:ARG:NE | 35:DN:2:ARG:O | 2.45 | 0.47 |
| 36:DO:68:LYS:H | 36:DO:102:ARG:HD3 | 1.79 | 0.47 |
| 38:DQ:57:ARG:HA | 38:DQ:60:TRP:CE3 | 2.50 | 0.47 |
| 41:DT:50:LEU:O | 41:DT:52:GLU:N | 2.47 | 0.47 |
| 42:DU:53:GLN:H | 42:DU:53:GLN:CD | 2.18 | 0.47 |
| 1:AA:1510:C:H2' | 1:AA:1511:G:C8 | 2.49 | 0.47 |
| 1:AA:475:C:H2' | 1:AA:476:U:H6 | 1.76 | 0.47 |
| 1:AA:76:G:H8 | 1:AA:76:G:OP2 | 1.97 | 0.47 |
| 20:AB:118:THR:HA | 20:AB:121:GLN:HB2 | 1.95 | 0.47 |
| 20:AB:172:ILE:HD12 | 20:AB:172:ILE:N | 2.30 | 0.47 |
| 2:AC:110:LEU:HD22 | 2:AC:145:ALA:HB2 | 1.96 | 0.47 |
| 7:AH:87:ARG:HD3 | 7:AH:90:GLU:OE1 | 2.15 | 0.47 |
| 1:AA:1187:G:OP1 | 8:AI:114:LYS:HE3 | 2.15 | 0.47 |
| 8:AI:123:ARG:CZ | 8:AI:123:ARG:HB3 | 2.45 | 0.47 |
| 10:AK:75:GLU:N | 10:AK:75:GLU:CD | 2.68 | 0.47 |
| 12:AM:38:ILE:HD12 | 12:AM:47:LEU:HD11 | 1.95 | 0.47 |
| 12:AM:84:CYS:O | 12:AM:88:LEU:HG | 2.15 | 0.47 |
| 18:AS:2:ARG:HD3 | 18:AS:3:SER:N | 2.29 | 0.47 |
| 22:BA:73:A:H2' | 22:BA:73:A:N3 | 2.30 | 0.47 |
| 23:BB:1439:A:N7 | 23:BB:1440:U:C2 | 2.82 | 0.47 |
| 23:BB:1478:G:O2' | 23:BB:1479:G:H5' | 2.14 | 0.47 |
| 23:BB:1670:C:H2' | 23:BB:1671:U:O4' | 2.15 | 0.47 |
| 23:BB:1998:A:H2' | 23:BB:1999:C:H6 | 1.80 | 0.47 |
| 23:BB:2153:C:O5' | 23:BB:2153:C:H6 | 1.97 | 0.47 |
| 23:BB:2271:G:H2' | 23:BB:2272:U:H6 | 1.79 | 0.47 |
| 23:BB:2634:A:H2' | 23:BB:2635:A:H8 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2729:G:H2' | 23:BB:2730:C:C6 | 2.49 | 0.47 |
| 25:BC:188:ARG:HH21 | 25:BC:188:ARG:HG2 | 1.80 | 0.47 |
| 25:BC:36:ASN:ND2 | 25:BC:61:TYR:HB2 | 2.30 | 0.47 |
| 26:BD:114:LYS:HG3 | 26:BD:116:LYS:HG2 | 1.97 | 0.47 |
| 28:BF:121:PHE:HB3 | 28:BF:127:TYR:CD2 | 2.50 | 0.47 |
| 28:BF:168:LEU:O | 28:BF:170:ALA:N | 2.48 | 0.47 |
| 32:BK:47:ILE:CG1 | 32:BK:48:PRO:HD2 | 2.35 | 0.47 |
| 33:BL:93:ASN:O | 33:BL:95:LEU:HD12 | 2.14 | 0.47 |
| 23:BB:2847:U:OP1 | 37:BP:95:LYS:HD3 | 2.15 | 0.47 |
| 41:BT:23:ALA:C | 41:BT:25:GLU:H | 2.17 | 0.47 |
| 23:BB:922:C:H1' | 43:BW:22:VAL:CG2 | 2.44 | 0.47 |
| 23:BB:1000:A:H4' | 45:BY:10:ARG:HH22 | 1.80 | 0.47 |
| 46:BZ:70:GLU:C | 46:BZ:72:ARG:N | 2.67 | 0.47 |
| 1:CA:960:U:H6 | 1:CA:1222:G:O2' | 1.98 | 0.47 |
| 1:CA:1242:G:H2' | 1:CA:1243:C:O4' | 2.14 | 0.47 |
| 1:CA:364:A:H2' | 1:CA:365:U:O2 | 2.14 | 0.47 |
| 20:CB:27:LYS:C | 20:CB:29:PHE:H | 2.18 | 0.47 |
| 2:CC:91:ALA:HB2 | 2:CC:98:ALA:H | 1.80 | 0.47 |
| 8:CI:11:ARG:HH21 | 8:CI:12:LYS:HD2 | 1.80 | 0.47 |
| 9:CJ:6:ILE:O | 9:CJ:75:ASP:HA | 2.15 | 0.47 |
| 10:CK:83:VAL:HG22 | 10:CK:106:ILE:HD11 | 1.95 | 0.47 |
| 12:CM:90:HIS:CE1 | 12:CM:96:VAL:HG21 | 2.49 | 0.47 |
| 15:CP:26:ASN:HD22 | 15:CP:26:ASN:HA | 1.59 | 0.47 |
| 12:CM:92:ARG:NH1 | 18:CS:79:TYR:HD2 | 2.12 | 0.47 |
| 19:CT:56:ILE:O | 19:CT:60:GLN:HG2 | 2.15 | 0.47 |
| 50:D3:58:ILE:H | 50:D3:58:ILE:HG13 | 1.41 | 0.47 |
| 51:D4:8:LYS:HG2 | 51:D4:9:LYS:HD3 | 1.97 | 0.47 |
| 22:DA:48:U:O2' | 36:DO:100:HIS:HE1 | 1.98 | 0.47 |
| 22:DA:83:G:H4' | 45:DY:52:PHE:CD2 | 2.50 | 0.47 |
| 23:DB:1324:G:C6 | 23:DB:1331:G:C6 | 3.03 | 0.47 |
| 23:DB:1419:A:H2' | 23:DB:1421:G:C8 | 2.49 | 0.47 |
| 23:DB:1541:C:H2' | 23:DB:1542:U:C6 | 2.50 | 0.47 |
| 23:DB:1744:A:H2' | 23:DB:1745:A:C8 | 2.49 | 0.47 |
| 23:DB:1893:C:H2' | 23:DB:1894:C:O4' | 2.15 | 0.47 |
| 23:DB:1969:A:O2' | 23:DB:1972:G:N3 | 2.40 | 0.47 |
| 23:DB:2261:C:N4 | 43:DW:10:ARG:HB3 | 2.30 | 0.47 |
| 23:DB:2526:G:H5' | 23:DB:2742:G:O2' | 2.15 | 0.47 |
| 23:DB:2526:G:H2' | 23:DB:2527:C:H6 | 1.80 | 0.47 |
| 23:DB:2569:G:O2' | 23:DB:2570:G:H5' | 2.15 | 0.47 |
| 23:DB:2716:C:H2' | 23:DB:2717:C:C6 | 2.49 | 0.47 |
| 23:DB:277:G:H4' | 23:DB:278:A:N7 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:418:C:H2' | 23:DB:419:U:H6 | 1.80 | 0.47 |
| 23:DB:532:A:H2' | 38:DQ:27:ARG:NH2 | 2.21 | 0.47 |
| 23:DB:753:A:O2' | 23:DB:754:U:H5' | 2.13 | 0.47 |
| 23:DB:770:G:O2' | 23:DB:771:G:H5' | 2.13 | 0.47 |
| 25:DC:129:LEU:CD2 | 25:DC:133:ASN:HB2 | 2.45 | 0.47 |
| 26:DD:104:VAL:HA | 26:DD:106:LYS:HZ1 | 1.80 | 0.47 |
| 27:DE:179:SER:HA | 27:DE:182:ALA:HB3 | 1.95 | 0.47 |
| 27:DE:73:ILE:HG12 | 27:DE:73:ILE:O | 2.15 | 0.47 |
| 28:DF:103:ILE:HD11 | 28:DF:174:PHE:CG | 2.50 | 0.47 |
| 28:DF:76:PHE:HD2 | 28:DF:78:ILE:HD13 | 1.78 | 0.47 |
| 29:DG:14:VAL:O | 29:DG:16:VAL:HG23 | 2.14 | 0.47 |
| 30:DH:12:LEU:HG | 30:DH:12:LEU:O | 2.15 | 0.47 |
| 52:DI:49:GLU:HB3 | 52:DI:52:LEU:HD12 | 1.97 | 0.47 |
| 52:DI:52:LEU:HD13 | 52:DI:81:LYS:HZ3 | 1.79 | 0.47 |
| 31:DJ:35:ARG:HA | 31:DJ:40:HIS:CD2 | 2.50 | 0.47 |
| 32:DK:119:ALA:HB3 | 32:DK:120:PRO:HD3 | 1.97 | 0.47 |
| 23:DB:663:G:OP1 | 33:DL:17:LYS:HG2 | 2.15 | 0.47 |
| 33:DL:81:ASP:O | 33:DL:83:ALA:N | 2.48 | 0.47 |
| 37:DP:83:ILE:O | 37:DP:83:ILE:HD13 | 2.15 | 0.47 |
| 41:DT:15:HIS:O | 41:DT:16:VAL:C | 2.51 | 0.47 |
| 1:AA:1072:G:H2' | 1:AA:1073:U:C6 | 2.51 | 0.47 |
| 1:AA:1118:U:H1' | 1:AA:1179:A:C5 | 2.49 | 0.47 |
| 1:AA:1302:C:H5' | 1:AA:1302:C:H6 | 1.80 | 0.47 |
| 1:AA:1238:A:C8 | 1:AA:1303:C:H1' | 2.50 | 0.47 |
| 1:AA:130:A:H1' | 1:AA:263:A:O2' | 2.14 | 0.47 |
| 1:AA:279:A:C5' | 1:AA:280:C:H3' | 2.43 | 0.47 |
| 1:AA:332:G:H2' | 1:AA:333:U:H6 | 1.80 | 0.47 |
| 1:AA:5:U:H1' | 1:AA:6:G:C2 | 2.50 | 0.47 |
| 20:AB:80:LYS:HG3 | 20:AB:81:ASP:N | 2.30 | 0.47 |
| 3:AD:123:MET:CB | 3:AD:128:VAL:HA | 2.45 | 0.47 |
| 1:AA:429:U:OP2 | 3:AD:31:CYS:HB2 | 2.15 | 0.47 |
| 6:AG:101:ARG:HG2 | 6:AG:105:GLU:OE2 | 2.15 | 0.47 |
| 6:AG:125:ASP:HB3 | 6:AG:131:GLY:H | 1.78 | 0.47 |
| 7:AH:83:ARG:HB3 | 7:AH:85:TYR:CE1 | 2.50 | 0.47 |
| 8:AI:87:MET:HA | 8:AI:90:ASP:O | 2.15 | 0.47 |
| 10:AK:37:GLN:HB2 | 10:AK:39:ASN:HD22 | 1.80 | 0.47 |
| 12:AM:37:GLY:O | 12:AM:38:ILE:HD13 | 2.15 | 0.47 |
| 18:AS:51:HIS:HB2 | 18:AS:56:HIS:CE1 | 2.49 | 0.47 |
| 51:B4:2:LYS:HD3 | 51:B4:4:ARG:HE | 1.80 | 0.47 |
| 23:BB:1082:U:C2 | 23:BB:1086:A:N1 | 2.83 | 0.47 |
| 23:BB:1140:C:H2' | 23:BB:1141:U:H5' | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1172:C:H2' | 23:BB:1173:U:O5' | 2.15 | 0.47 |
| 23:BB:126:A:H5' | 49:B2:19:ARG:CG | 2.45 | 0.47 |
| 23:BB:129:C:H4' | 23:BB:1348:C:O2' | 2.15 | 0.47 |
| 23:BB:1403:A:H2' | 23:BB:1404:C:H6 | 1.80 | 0.47 |
| 23:BB:1433:A:H2' | 23:BB:1434:A:O4' | 2.15 | 0.47 |
| 23:BB:1506:U:H2' | 23:BB:1507:C:C6 | 2.50 | 0.47 |
| 23:BB:1672:A:C6 | 23:BB:1673:G:C6 | 3.03 | 0.47 |
| 23:BB:1922:G:H2' | 23:BB:1923:U:O4' | 2.15 | 0.47 |
| 23:BB:2756:U:H1' | 23:BB:2757:A:H5'' | 1.96 | 0.47 |
| 23:BB:512:G:H4' | 23:BB:512:G:OP1 | 2.14 | 0.47 |
| 23:BB:720:U:H2' | 23:BB:721:A:H8 | 1.77 | 0.47 |
| 23:BB:754:U:H2' | 23:BB:755:U:C6 | 2.50 | 0.47 |
| 23:BB:924:G:H2' | 23:BB:925:A:H8 | 1.80 | 0.47 |
| 28:BF:102:LEU:HA | 28:BF:106:ALA:HB2 | 1.97 | 0.47 |
| 28:BF:33:ILE:HG23 | 28:BF:155:ILE:HD12 | 1.97 | 0.47 |
| 28:BF:65:LEU:CD2 | 28:BF:87:LYS:HD2 | 2.40 | 0.47 |
| 29:BG:33:THR:HG21 | 29:BG:74:MET:HB3 | 1.96 | 0.47 |
| 31:BJ:45:THR:HG23 | 31:BJ:45:THR:O | 2.15 | 0.47 |
| 33:BL:23:ILE:N | 33:BL:23:ILE:HD12 | 2.30 | 0.47 |
| 37:BP:83:ILE:HD13 | 37:BP:83:ILE:O | 2.15 | 0.47 |
| 38:BQ:108:LEU:N | 39:BR:48:LYS:HD3 | 2.30 | 0.47 |
| 38:BQ:16:ILE:O | 38:BQ:18:LYS:N | 2.43 | 0.47 |
| 38:BQ:45:ALA:O | 38:BQ:49:ARG:N | 2.46 | 0.47 |
| 40:BS:84:ARG:HB3 | 40:BS:96:ILE:HG23 | 1.96 | 0.47 |
| 23:BB:2355:G:H4' | 43:BW:20:LEU:CD1 | 2.44 | 0.47 |
| 23:BB:2386:A:C2 | 43:BW:38:ARG:HB3 | 2.49 | 0.47 |
| 1:CA:1081:A:OP1 | 4:CE:21:SER:O | 2.33 | 0.47 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:C5' | 2.44 | 0.47 |
| 1:CA:193:C:H2' | 1:CA:194:C:C5 | 2.49 | 0.47 |
| 1:CA:586:C:C2' | 1:CA:587:G:H5' | 2.44 | 0.47 |
| 1:CA:861:G:H2' | 1:CA:862:C:H6 | 1.80 | 0.47 |
| 1:CA:908:A:H2' | 1:CA:909:A:C8 | 2.50 | 0.47 |
| 1:CA:571:U:O2 | 1:CA:918:A:H5' | 2.14 | 0.47 |
| 20:CB:131:LYS:HG3 | 20:CB:132:GLU:N | 2.30 | 0.47 |
| 2:CC:72:PRO:O | 2:CC:76:ILE:HG12 | 2.13 | 0.47 |
| 3:CD:123:MET:HG3 | 3:CD:143:SER:OG | 2.15 | 0.47 |
| 8:CI:78:ILE:HG22 | 8:CI:82:ILE:CD1 | 2.45 | 0.47 |
| 8:CI:9:GLY:HA3 | 8:CI:81:GLY:N | 2.30 | 0.47 |
| 1:CA:716:A:N3 | 10:CK:118:ASN:O | 2.48 | 0.47 |
| 11:CL:106:VAL:CG2 | 11:CL:116:TYR:HB3 | 2.44 | 0.47 |
| 12:CM:68:LEU:O | 12:CM:72:ILE:HG22 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:CU:11:PHE:CE1 | 21:CU:13:VAL:HG12 | 2.50 | 0.47 |
| 47:D0:26:SER:HB3 | 47:D0:39:ARG:NH2 | 2.29 | 0.47 |
| 49:D2:10:LEU:HD11 | 49:D2:14:ARG:CZ | 2.46 | 0.47 |
| 23:DB:121:G:H2' | 23:DB:122:G:C8 | 2.49 | 0.47 |
| 23:DB:1294:U:C2' | 23:DB:1295:C:H5' | 2.44 | 0.47 |
| 23:DB:218:A:O2' | 23:DB:219:A:H5' | 2.15 | 0.47 |
| 23:DB:2562:U:H2' | 23:DB:2563:U:H5' | 1.97 | 0.47 |
| 23:DB:2628:C:O2' | 23:DB:2781:A:H2' | 2.15 | 0.47 |
| 23:DB:392:U:H2' | 23:DB:393:C:H6 | 1.80 | 0.47 |
| 23:DB:540:C:O2' | 23:DB:541:A:H5' | 2.15 | 0.47 |
| 23:DB:862:G:H2' | 23:DB:863:A:O4' | 2.15 | 0.47 |
| 23:DB:974:G:H1' | 23:DB:975:A:C8 | 2.50 | 0.47 |
| 25:DC:41:GLY:O | 25:DC:48:ILE:HA | 2.15 | 0.47 |
| 26:DD:125:TRP:CE3 | 26:DD:125:TRP:HA | 2.50 | 0.47 |
| 28:DF:3:LEU:HD11 | 28:DF:172:PHE:CD1 | 2.50 | 0.47 |
| 28:DF:31:GLU:HB3 | 28:DF:156:THR:O | 2.14 | 0.47 |
| 29:DG:106:LEU:O | 29:DG:108:PHE:HD1 | 1.98 | 0.47 |
| 30:DH:125:THR:HA | 30:DH:146:VAL:CB | 2.45 | 0.47 |
| 30:DH:25:TYR:CD1 | 30:DH:30:LEU:HG | 2.50 | 0.47 |
| 30:DH:89:LYS:HD2 | 30:DH:89:LYS:N | 2.30 | 0.47 |
| 32:DK:112:PHE:O | 32:DK:113:MET:C | 2.53 | 0.47 |
| 35:DN:116:VAL:O | 35:DN:117:ASP:CB | 2.60 | 0.47 |
| 37:DP:31:VAL:O | 37:DP:32:VAL:HG12 | 2.14 | 0.47 |
| 38:DQ:7:VAL:HG23 | 38:DQ:8:ILE:N | 2.30 | 0.47 |
| 38:DQ:108:LEU:N | 39:DR:48:LYS:HD3 | 2.29 | 0.47 |
| 1:AA:1040:U:H2' | 1:AA:1041:G:C8 | 2.50 | 0.46 |
| 1:AA:1225:A:H3' | 1:AA:1226:C:C6 | 2.50 | 0.46 |
| 1:AA:220:G:O2' | 1:AA:221:C:H5' | 2.16 | 0.46 |
| 1:AA:286:C:H2' | 1:AA:287:U:C6 | 2.51 | 0.46 |
| 1:AA:556:C:O2' | 1:AA:557:G:H5' | 2.14 | 0.46 |
| 20:AB:27:LYS:C | 20:AB:29:PHE:H | 2.17 | 0.46 |
| 3:AD:90:LEU:HD11 | 3:AD:194:ILE:HD11 | 1.95 | 0.46 |
| 4:AE:156:ARG:HB3 | 7:AH:43:GLY:O | 2.15 | 0.46 |
| 5:AF:11:HIS:CG | 5:AF:12:PRO:HD2 | 2.51 | 0.46 |
| 5:AF:6:ILE:O | 5:AF:6:ILE:HG13 | 2.15 | 0.46 |
| 8:AI:50:PRO:HD3 | 8:AI:79:ARG:CG | 2.45 | 0.46 |
| 9:AJ:13:PHE:CD2 | 9:AJ:69:THR:HG23 | 2.50 | 0.46 |
| 14:AO:68:TYR:HA | 14:AO:71:ARG:HE | 1.79 | 0.46 |
| 47:B0:9:ARG:HB2 | 47:B0:12:ARG:NH2 | 2.30 | 0.46 |
| 48:B1:18:HIS:NE2 | 48:B1:40:PRO:HD2 | 2.30 | 0.46 |
| 48:B1:6:GLU:HB2 | 48:B1:52:LYS:CE | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:B4:8:LYS:HG2 | 51:B4:9:LYS:HD3 | 1.98 | 0.46 |
| 22:BA:3:C:H2' | 22:BA:4:C:H6 | 1.79 | 0.46 |
| 23:BB:1169:A:O5' | 23:BB:1169:A:H8 | 1.98 | 0.46 |
| 23:BB:1429:G:H2' | 23:BB:1430:G:C8 | 2.49 | 0.46 |
| 23:BB:1477:A:H2' | 23:BB:1478:G:O4' | 2.15 | 0.46 |
| 23:BB:1485:U:O2' | 23:BB:1486:U:H5' | 2.15 | 0.46 |
| 23:BB:1687:G:O2' | 23:BB:1688:U:H5' | 2.14 | 0.46 |
| 23:BB:2023:C:H4' | 23:BB:2617:U:O3' | 2.14 | 0.46 |
| 23:BB:2249:U:H4' | 23:BB:2275:C:C5 | 2.50 | 0.46 |
| 23:BB:2628:C:O2' | 23:BB:2781:A:H2' | 2.14 | 0.46 |
| 23:BB:2889:C:O2' | 23:BB:2890:G:H5' | 2.15 | 0.46 |
| 23:BB:950:G:H2' | 23:BB:951:C:C6 | 2.50 | 0.46 |
| 23:BB:1812:U:O2' | 25:BC:43:ASN:ND2 | 2.48 | 0.46 |
| 25:BC:57:HIS:CG | 25:BC:58:LYS:H | 2.32 | 0.46 |
| 26:BD:107:VAL:HG12 | 26:BD:109:VAL:HG23 | 1.97 | 0.46 |
| 26:BD:51:THR:HG23 | 26:BD:78:GLY:O | 2.15 | 0.46 |
| 27:BE:73:ILE:O | 27:BE:73:ILE:HG12 | 2.15 | 0.46 |
| 30:BH:96:THR:C | 30:BH:98:ASP:H | 2.17 | 0.46 |
| 52:BI:122:GLU:CD | 52:BI:122:GLU:H | 2.18 | 0.46 |
| 32:BK:61:VAL:HG11 | 32:BK:112:PHE:CZ | 2.50 | 0.46 |
| 32:BK:64:ARG:NH2 | 37:BP:67:GLU:HG3 | 2.29 | 0.46 |
| 33:BL:78:ARG:NH2 | 33:BL:113:ALA:HB1 | 2.29 | 0.46 |
| 34:BM:28:PHE:HB3 | 34:BM:64:TRP:CE2 | 2.50 | 0.46 |
| 34:BM:56:ALA:C | 34:BM:58:LYS:H | 2.18 | 0.46 |
| 35:BN:83:LEU:HA | 35:BN:86:ARG:CG | 2.43 | 0.46 |
| 36:BO:67:ASN:O | 36:BO:69:ASP:N | 2.47 | 0.46 |
| 40:BS:52:GLU:HA | 40:BS:55:ILE:CG2 | 2.44 | 0.46 |
| 41:BT:40:LYS:HA | 41:BT:43:ILE:HB | 1.96 | 0.46 |
| 42:BU:86:PHE:CD2 | 42:BU:92:VAL:HG21 | 2.50 | 0.46 |
| 1:CA:1147:C:H2' | 1:CA:1148:U:H6 | 1.80 | 0.46 |
| 1:CA:1169:A:H2' | 1:CA:1170:A:C8 | 2.50 | 0.46 |
| 1:CA:1245:C:H2' | 1:CA:1246:A:H8 | 1.80 | 0.46 |
| 1:CA:1266:G:N2 | 1:CA:1268:G:H3' | 2.29 | 0.46 |
| 1:CA:1360:A:H2' | 1:CA:1361:G:O4' | 2.16 | 0.46 |
| 1:CA:1465:A:H2' | 1:CA:1466:C:C6 | 2.50 | 0.46 |
| 1:CA:201:G:O2' | 1:CA:469:C:H4' | 2.15 | 0.46 |
| 1:CA:373:A:C1' | 1:CA:481:G:H1' | 2.45 | 0.46 |
| 1:CA:664:G:P | 17:CR:52:ARG:HH21 | 2.38 | 0.46 |
| 1:CA:697:U:H2' | 1:CA:698:G:H5' | 1.98 | 0.46 |
| 1:CA:787:A:O2' | 1:CA:788:U:H5' | 2.15 | 0.46 |
| 10:CK:112:VAL:HA | 17:CR:72:ARG:HH21 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:CL:60:PHE:O | 11:CL:62:VAL:N | 2.48 | 0.46 |
| 15:CP:43:ALA:CA | 15:CP:46:LYS:HE3 | 2.45 | 0.46 |
| 48:D1:33:LEU:HD12 | 48:D1:34:GLU:N | 2.30 | 0.46 |
| 23:DB:1062:G:H2' | 23:DB:1063:G:H8 | 1.79 | 0.46 |
| 23:DB:1176:U:H2' | 23:DB:1177:G:C8 | 2.50 | 0.46 |
| 23:DB:1477:A:H2' | 23:DB:1478:G:O4' | 2.15 | 0.46 |
| 23:DB:1936:A:H2 | 23:DB:1943:U:C5 | 2.33 | 0.46 |
| 23:DB:2386:A:H2' | 23:DB:2387:U:C6 | 2.51 | 0.46 |
| 23:DB:2462:C:H2' | 23:DB:2463:C:H6 | 1.80 | 0.46 |
| 23:DB:499:U:H2' | 23:DB:500:G:O4' | 2.15 | 0.46 |
| 23:DB:643:A:C5 | 23:DB:644:A:N7 | 2.83 | 0.46 |
| 23:DB:705:A:N6 | 23:DB:726:G:H1' | 2.30 | 0.46 |
| 23:DB:1354:A:OP1 | 25:DC:35:LYS:HE2 | 2.14 | 0.46 |
| 29:DG:148:ARG:HD3 | 29:DG:152:ARG:NH1 | 2.29 | 0.46 |
| 29:DG:91:VAL:HG23 | 29:DG:92:GLY:H | 1.80 | 0.46 |
| 36:DO:88:LYS:HE3 | 36:DO:88:LYS:HB3 | 1.66 | 0.46 |
| 32:DK:79:PHE:CD2 | 37:DP:69:VAL:HG12 | 2.49 | 0.46 |
| 38:DQ:64:ILE:HD12 | 38:DQ:95:ALA:CB | 2.45 | 0.46 |
| 24:DV:1:MET:HG3 | 24:DV:2:PHE:CD2 | 2.50 | 0.46 |
| 24:DV:21:ARG:HE | 24:DV:87:GLN:CB | 2.24 | 0.46 |
| 46:DZ:35:SER:HA | 46:DZ:49:LEU:O | 2.14 | 0.46 |
| 1:AA:193:C:H2' | 1:AA:194:C:C5 | 2.51 | 0.46 |
| 1:AA:202:G:H2' | 1:AA:203:G:H8 | 1.79 | 0.46 |
| 20:AB:23:ASN:O | 20:AB:25:LYS:N | 2.48 | 0.46 |
| 2:AC:146:LYS:HB2 | 2:AC:202:PHE:CD2 | 2.49 | 0.46 |
| 2:AC:129:PHE:CE2 | 2:AC:156:LEU:HD13 | 2.50 | 0.46 |
| 4:AE:136:VAL:HG13 | 4:AE:137:ARG:H | 1.79 | 0.46 |
| 6:AG:71:THR:H | 6:AG:141:HIS:CE1 | 2.33 | 0.46 |
| 8:AI:83:THR:OG1 | 8:AI:97:LEU:HD22 | 2.15 | 0.46 |
| 16:AQ:64:ARG:HG2 | 16:AQ:65:PRO:HD2 | 1.95 | 0.46 |
| 19:AT:64:GLY:O | 19:AT:66:ILE:N | 2.47 | 0.46 |
| 21:AU:44:ARG:HG3 | 21:AU:44:ARG:HH11 | 1.81 | 0.46 |
| 47:B0:9:ARG:O | 47:B0:12:ARG:HB3 | 2.16 | 0.46 |
| 49:B2:30:VAL:HG22 | 49:B2:33:ARG:NH2 | 2.20 | 0.46 |
| 51:B4:17:VAL:HG11 | 51:B4:19:ARG:HE | 1.80 | 0.46 |
| 22:BA:54:G:O2' | 22:BA:55:U:H5' | 2.15 | 0.46 |
| 23:BB:1210:G:H5' | 23:BB:1212:G:O4' | 2.15 | 0.46 |
| 23:BB:1596:A:O2' | 23:BB:1597:A:H5' | 2.16 | 0.46 |
| 23:BB:1749:A:H2' | 23:BB:1750:G:C8 | 2.50 | 0.46 |
| 23:BB:1885:A:H2' | 23:BB:1886:U:O4' | 2.14 | 0.46 |
| 23:BB:2230:G:H5'' | 46:BZ:30:LEU:HD11 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:242:G:N7 | 50:B3:4:LYS:HG2 | 2.30 | 0.46 |
| 23:BB:2636:C:H2' | 23:BB:2637:U:C6 | 2.51 | 0.46 |
| 23:BB:2845:U:O2' | 23:BB:2846:G:H5' | 2.14 | 0.46 |
| 23:BB:329:G:C6 | 42:BU:16:LYS:HG2 | 2.50 | 0.46 |
| 23:BB:455:C:N3 | 23:BB:472:A:H2' | 2.31 | 0.46 |
| 23:BB:785:G:H2' | 23:BB:786:C:H6 | 1.80 | 0.46 |
| 25:BC:119:VAL:HG13 | 25:BC:133:ASN:ND2 | 2.30 | 0.46 |
| 27:BE:106:LYS:CE | 27:BE:200:LEU:HB3 | 2.45 | 0.46 |
| 27:BE:176:ASP:O | 27:BE:180:LEU:HG | 2.15 | 0.46 |
| 23:BB:2307:G:O6 | 28:BF:40:GLY:HA3 | 2.16 | 0.46 |
| 29:BG:88:LEU:HD13 | 29:BG:93:TYR:HB3 | 1.96 | 0.46 |
| 30:BH:133:GLN:O | 30:BH:133:GLN:HG2 | 2.11 | 0.46 |
| 52:BI:19:PRO:HB2 | 52:BI:22:PRO:HD2 | 1.97 | 0.46 |
| 31:BJ:128:ASN:O | 31:BJ:129:GLU:HB3 | 2.16 | 0.46 |
| 33:BL:132:ARG:O | 33:BL:135:ILE:HG22 | 2.14 | 0.46 |
| 34:BM:68:PHE:CG | 34:BM:69:PRO:HD2 | 2.51 | 0.46 |
| 35:BN:58:ASP:O | 35:BN:59:SER:HB3 | 2.15 | 0.46 |
| 39:BR:34:GLU:HB3 | 39:BR:58:VAL:HG21 | 1.95 | 0.46 |
| 41:BT:50:LEU:O | 41:BT:52:GLU:N | 2.49 | 0.46 |
| 41:BT:55:VAL:HG22 | 41:BT:87:LEU:CD2 | 2.45 | 0.46 |
| 43:BW:43:LYS:HB3 | 43:BW:79:ILE:HD11 | 1.97 | 0.46 |
| 23:BB:988:A:H3' | 45:BY:13:ILE:CD1 | 2.44 | 0.46 |
| 46:BZ:27:ARG:HD2 | 46:BZ:29:PHE:CE1 | 2.50 | 0.46 |
| 1:CA:1175:G:O2' | 1:CA:1176:A:H5' | 2.14 | 0.46 |
| 1:CA:1241:G:O2' | 1:CA:1242:G:H5' | 2.15 | 0.46 |
| 1:CA:1300:G:H1' | 1:CA:1301:U:C5 | 2.49 | 0.46 |
| 1:CA:1302:C:H6 | 1:CA:1302:C:H5' | 1.80 | 0.46 |
| 1:CA:1390:U:O2' | 1:CA:1391:U:H5' | 2.15 | 0.46 |
| 1:CA:687:A:C2 | 1:CA:704:A:C5 | 3.04 | 0.46 |
| 1:CA:805:C:O2' | 1:CA:806:C:H5' | 2.15 | 0.46 |
| 1:CA:817:C:C2 | 1:CA:819:A:O4' | 2.68 | 0.46 |
| 1:CA:953:G:H2' | 1:CA:954:G:O4' | 2.16 | 0.46 |
| 21:AU:10:PRO:CB | 2:CC:71:ARG:HE | 2.22 | 0.46 |
| 3:CD:187:ARG:CZ | 3:CD:191:SER:HB3 | 2.46 | 0.46 |
| 7:CH:83:ARG:HB3 | 7:CH:85:TYR:CE1 | 2.49 | 0.46 |
| 9:CJ:18:ILE:HG13 | 9:CJ:72:ARG:HG2 | 1.97 | 0.46 |
| 10:CK:65:ALA:O | 10:CK:68:ARG:HB3 | 2.15 | 0.46 |
| 19:CT:61:ALA:HB1 | 19:CT:67:HIS:HA | 1.98 | 0.46 |
| 23:DB:150:U:H2' | 23:DB:151:C:H6 | 1.78 | 0.46 |
| 23:DB:1439:A:H1' | 23:DB:1553:A:N6 | 2.30 | 0.46 |
| 23:DB:1640:A:H2' | 23:DB:1641:A:H8 | 1.77 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:962:G:N2 | 23:DB:2250:G:H22 | 1.95 | 0.46 |
| 23:DB:2339:C:H2' | 23:DB:2340:A:H8 | 1.79 | 0.46 |
| 23:DB:962:G:H2' | 23:DB:963:U:H6 | 1.80 | 0.46 |
| 25:DC:165:ALA:HB3 | 25:DC:172:THR:HG23 | 1.96 | 0.46 |
| 25:DC:221:GLY:O | 25:DC:224:MET:HG3 | 2.15 | 0.46 |
| 26:DD:114:LYS:HG3 | 26:DD:116:LYS:HG2 | 1.96 | 0.46 |
| 26:DD:125:TRP:HE1 | 26:DD:161:MET:H | 1.63 | 0.46 |
| 26:DD:33:ARG:NH1 | 26:DD:53:GLY:O | 2.48 | 0.46 |
| 27:DE:134:LEU:HD21 | 27:DE:161:ALA:HB2 | 1.97 | 0.46 |
| 27:DE:176:ASP:O | 27:DE:180:LEU:HG | 2.15 | 0.46 |
| 28:DF:105:ILE:C | 28:DF:108:PRO:HD2 | 2.34 | 0.46 |
| 28:DF:29:ARG:HB2 | 28:DF:158:THR:HG21 | 1.97 | 0.46 |
| 30:DH:147:VAL:HG12 | 30:DH:148:ALA:N | 2.29 | 0.46 |
| 30:DH:44:ILE:O | 30:DH:48:GLU:HB3 | 2.16 | 0.46 |
| 34:DM:90:GLU:HA | 34:DM:90:GLU:OE1 | 2.14 | 0.46 |
| 35:DN:61:ALA:C | 35:DN:63:ARG:N | 2.68 | 0.46 |
| 36:DO:100:HIS:HA | 36:DO:104:GLN:NE2 | 2.29 | 0.46 |
| 36:DO:30:ARG:HG3 | 36:DO:30:ARG:NH1 | 2.30 | 0.46 |
| 36:DO:74:VAL:O | 36:DO:77:ALA:HB3 | 2.15 | 0.46 |
| 39:DR:43:ASN:ND2 | 39:DR:44:GLY:N | 2.63 | 0.46 |
| 41:DT:67:VAL:HG22 | 41:DT:74:ILE:HD11 | 1.97 | 0.46 |
| 42:DU:62:ALA:O | 42:DU:63:ALA:HB3 | 2.15 | 0.46 |
| 1:AA:1465:A:H2' | 1:AA:1466:C:C6 | 2.51 | 0.46 |
| 1:AA:429:U:H1' | 1:AA:430:A:H5'' | 1.98 | 0.46 |
| 1:AA:521:G:O2' | 1:AA:522:C:H5' | 2.16 | 0.46 |
| 1:AA:549:C:H2' | 1:AA:550:G:C8 | 2.51 | 0.46 |
| 1:AA:599:C:O2' | 1:AA:600:A:H5' | 2.15 | 0.46 |
| 20:AB:116:LEU:O | 20:AB:119:GLN:HB2 | 2.15 | 0.46 |
| 2:AC:149:LYS:HG3 | 2:AC:168:ARG:HB2 | 1.97 | 0.46 |
| 3:AD:160:LEU:HA | 3:AD:163:GLN:CG | 2.44 | 0.46 |
| 3:AD:61:ARG:HG3 | 3:AD:71:PHE:CD2 | 2.50 | 0.46 |
| 5:AF:36:ILE:N | 5:AF:36:ILE:HD12 | 2.30 | 0.46 |
| 5:AF:9:MET:HB3 | 5:AF:59:TYR:CD2 | 2.50 | 0.46 |
| 6:AG:137:ARG:HB3 | 6:AG:137:ARG:HE | 1.52 | 0.46 |
| 6:AG:75:LYS:HD3 | 6:AG:76:SER:N | 2.30 | 0.46 |
| 7:AH:12:ARG:HH11 | 7:AH:12:ARG:HG3 | 1.80 | 0.46 |
| 11:AL:17:LYS:NZ | 11:AL:17:LYS:N | 2.64 | 0.46 |
| 12:AM:3:ILE:HA | 12:AM:56:ARG:HB2 | 1.97 | 0.46 |
| 12:AM:3:ILE:H | 12:AM:56:ARG:NH2 | 2.13 | 0.46 |
| 14:AO:23:SER:HB3 | 14:AO:26:VAL:CG2 | 2.45 | 0.46 |
| 15:AP:22:ALA:HA | 15:AP:33:ILE:HG13 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:102:G:O2' | 22:BA:103:U:H5' | 2.15 | 0.46 |
| 23:BB:1253:A:H4' | 23:BB:1254:A:OP2 | 2.15 | 0.46 |
| 23:BB:159:G:O2' | 23:BB:160:A:H5'' | 2.15 | 0.46 |
| 23:BB:1759:A:H2' | 23:BB:1759:A:N3 | 2.30 | 0.46 |
| 23:BB:1854:A:H2 | 23:BB:2087:G:N3 | 2.13 | 0.46 |
| 23:BB:1912:A:HO2' | 23:BB:1913:A:C5' | 2.28 | 0.46 |
| 23:BB:2149:U:H2' | 23:BB:2150:C:C6 | 2.49 | 0.46 |
| 23:BB:2212:A:C8 | 23:BB:2214:C:N4 | 2.83 | 0.46 |
| 23:BB:2256:G:O2' | 23:BB:2257:U:H5' | 2.15 | 0.46 |
| 23:BB:2355:G:H4' | 43:BW:20:LEU:HD13 | 1.98 | 0.46 |
| 23:BB:826:U:H5'' | 23:BB:2428:G:O3' | 2.14 | 0.46 |
| 23:BB:2514:U:H2' | 23:BB:2515:C:C6 | 2.50 | 0.46 |
| 23:BB:945:A:H4' | 23:BB:945:A:OP2 | 2.15 | 0.46 |
| 25:BC:107:LYS:O | 25:BC:109:LEU:HD22 | 2.15 | 0.46 |
| 25:BC:45:ASN:H | 25:BC:45:ASN:ND2 | 2.12 | 0.46 |
| 26:BD:101:PHE:CZ | 26:BD:204:LYS:HA | 2.49 | 0.46 |
| 27:BE:34:ALA:HA | 27:BE:94:GLN:NE2 | 2.31 | 0.46 |
| 28:BF:135:ILE:HG13 | 28:BF:137:PHE:H | 1.80 | 0.46 |
| 29:BG:1:SER:O | 29:BG:3:VAL:N | 2.49 | 0.46 |
| 30:BH:128:HIS:CB | 30:BH:144:VAL:HB | 2.34 | 0.46 |
| 33:BL:47:ARG:HH21 | 33:BL:47:ARG:CB | 2.28 | 0.46 |
| 37:BP:75:THR:O | 37:BP:80:VAL:HG11 | 2.15 | 0.46 |
| 39:BR:20:VAL:HG12 | 39:BR:21:ARG:N | 2.28 | 0.46 |
| 41:BT:69:ARG:NH1 | 41:BT:69:ARG:HA | 2.31 | 0.46 |
| 42:BU:32:LYS:HG3 | 42:BU:65:GLN:HA | 1.97 | 0.46 |
| 1:CA:1040:U:H2' | 1:CA:1041:G:O4' | 2.16 | 0.46 |
| 1:CA:1291:U:H2' | 1:CA:1292:G:H8 | 1.79 | 0.46 |
| 1:CA:1343:G:H2' | 1:CA:1344:C:H6 | 1.80 | 0.46 |
| 1:CA:220:G:O2' | 1:CA:221:C:H5' | 2.15 | 0.46 |
| 1:CA:270:A:H2' | 1:CA:271:C:O4' | 2.16 | 0.46 |
| 1:CA:308:C:H2' | 1:CA:309:A:C8 | 2.51 | 0.46 |
| 1:CA:814:A:H2' | 1:CA:816:A:O5' | 2.14 | 0.46 |
| 1:CA:86:G:O2' | 1:CA:87:C:O5' | 2.27 | 0.46 |
| 1:CA:945:G:H21 | 1:CA:1334:G:H4' | 1.80 | 0.46 |
| 1:CA:984:C:H2' | 1:CA:985:C:C6 | 2.51 | 0.46 |
| 20:CB:134:LEU:HD12 | 20:CB:134:LEU:HA | 1.82 | 0.46 |
| 20:CB:172:ILE:HD12 | 20:CB:172:ILE:N | 2.30 | 0.46 |
| 20:CB:59:ILE:HG21 | 20:CB:158:ASP:HB3 | 1.97 | 0.46 |
| 8:CI:82:ILE:O | 8:CI:86:LEU:HB2 | 2.16 | 0.46 |
| 11:CL:78:VAL:O | 11:CL:102:ASP:HB2 | 2.16 | 0.46 |
| 10:CK:108:ASN:HD21 | 21:CU:6:ARG:HD2 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:D0:18:HIS:C | 47:D0:20:ALA:H | 2.19 | 0.46 |
| 22:DA:91:C:O2' | 22:DA:92:C:H5' | 2.15 | 0.46 |
| 23:DB:1098:A:H2' | 52:DI:4:VAL:C | 2.36 | 0.46 |
| 23:DB:1173:U:H2' | 23:DB:1174:U:C5 | 2.50 | 0.46 |
| 23:DB:1174:U:H1' | 23:DB:1176:U:O2 | 2.15 | 0.46 |
| 23:DB:1214:A:H2' | 23:DB:1215:G:H8 | 1.81 | 0.46 |
| 23:DB:1854:A:H2 | 23:DB:2087:G:N3 | 2.13 | 0.46 |
| 23:DB:19:A:O2' | 23:DB:20:C:H5' | 2.15 | 0.46 |
| 23:DB:2630:G:H2' | 23:DB:2631:G:H8 | 1.81 | 0.46 |
| 23:DB:311:A:H3' | 23:DB:312:G:C8 | 2.50 | 0.46 |
| 23:DB:431:U:O2' | 23:DB:432:A:H5' | 2.15 | 0.46 |
| 23:DB:510:C:O2' | 23:DB:1236:G:H5' | 2.16 | 0.46 |
| 26:DD:116:LYS:HD2 | 26:DD:123:LYS:HE2 | 1.97 | 0.46 |
| 23:DB:1245:G:H4' | 27:DE:33:VAL:HG13 | 1.96 | 0.46 |
| 28:DF:147:ARG:HD2 | 28:DF:148:VAL:HG22 | 1.96 | 0.46 |
| 52:DI:2:LYS:N | 52:DI:2:LYS:HD2 | 2.31 | 0.46 |
| 52:DI:89:SER:HA | 52:DI:97:VAL:HG11 | 1.98 | 0.46 |
| 31:DJ:4:PHE:HB3 | 31:DJ:44:TYR:CD1 | 2.51 | 0.46 |
| 31:DJ:45:THR:HG23 | 31:DJ:45:THR:O | 2.15 | 0.46 |
| 32:DK:41:ILE:HG13 | 32:DK:42:THR:H | 1.80 | 0.46 |
| 34:DM:101:VAL:HG22 | 34:DM:101:VAL:O | 2.15 | 0.46 |
| 36:DO:84:GLU:C | 36:DO:86:GLY:N | 2.69 | 0.46 |
| 37:DP:100:ARG:HB3 | 37:DP:101:GLU:OE2 | 2.15 | 0.46 |
| 38:DQ:35:PHE:O | 38:DQ:39:ILE:HG12 | 2.16 | 0.46 |
| 41:DT:48:GLN:HA | 41:DT:48:GLN:NE2 | 2.30 | 0.46 |
| 41:DT:54:GLU:CB | 41:DT:88:LYS:HB2 | 2.45 | 0.46 |
| 1:AA:1242:G:H2' | 1:AA:1243:C:O4' | 2.14 | 0.46 |
| 1:AA:1278:G:H4' | 1:AA:1279:G:O4' | 2.16 | 0.46 |
| 1:AA:1369:C:H2' | 1:AA:1370:G:C8 | 2.51 | 0.46 |
| 1:AA:451:A:H4' | 1:AA:452:A:O4' | 2.16 | 0.46 |
| 1:AA:669:G:H2' | 1:AA:670:G:C8 | 2.50 | 0.46 |
| 1:AA:707:U:H2' | 1:AA:708:C:H6 | 1.79 | 0.46 |
| 1:AA:984:C:O2' | 1:AA:985:C:H5' | 2.15 | 0.46 |
| 3:AD:75:TYR:CE1 | 3:AD:200:VAL:HA | 2.50 | 0.46 |
| 7:AH:46:GLU:N | 7:AH:63:LYS:HB2 | 2.31 | 0.46 |
| 8:AI:129:ARG:HB2 | 8:AI:129:ARG:CZ | 2.45 | 0.46 |
| 13:AN:97:LYS:HB3 | 13:AN:97:LYS:NZ | 2.31 | 0.46 |
| 19:AT:70:LYS:O | 19:AT:74:HIS:HB2 | 2.14 | 0.46 |
| 48:B1:33:LEU:HD12 | 48:B1:34:GLU:N | 2.31 | 0.46 |
| 22:BA:52:A:OP1 | 22:BA:52:A:H4' | 2.15 | 0.46 |
| 23:BB:1439:A:N7 | 23:BB:1440:U:C6 | 2.83 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1441:G:H2' | 23:BB:1442:U:H6 | 1.80 | 0.46 |
| 23:BB:1669:A:H2' | 23:BB:1669:A:N3 | 2.30 | 0.46 |
| 23:BB:2074:U:O2' | 23:BB:2075:U:H5' | 2.16 | 0.46 |
| 23:BB:2240:U:O2' | 23:BB:2241:A:H5' | 2.15 | 0.46 |
| 23:BB:2537:U:H2' | 23:BB:2538:C:H6 | 1.79 | 0.46 |
| 23:BB:2626:C:H2' | 23:BB:2627:G:C8 | 2.50 | 0.46 |
| 25:BC:43:ASN:ND2 | 25:BC:44:ASN:N | 2.60 | 0.46 |
| 27:BE:67:ARG:HD2 | 27:BE:68:ALA:O | 2.15 | 0.46 |
| 29:BG:33:THR:C | 29:BG:34:ARG:HD3 | 2.35 | 0.46 |
| 30:BH:47:PHE:CA | 30:BH:50:ARG:HH21 | 2.28 | 0.46 |
| 30:BH:78:VAL:HB | 30:BH:143:ILE:CG1 | 2.44 | 0.46 |
| 31:BJ:30:THR:O | 31:BJ:33:ALA:HB3 | 2.16 | 0.46 |
| 33:BL:51:GLU:O | 33:BL:53:GLY:N | 2.48 | 0.46 |
| 34:BM:53:MET:O | 34:BM:57:VAL:HG23 | 2.16 | 0.46 |
| 36:BO:52:SER:C | 36:BO:54:VAL:H | 2.19 | 0.46 |
| 37:BP:52:ARG:HG2 | 37:BP:52:ARG:NH1 | 2.29 | 0.46 |
| 24:BV:21:ARG:HE | 24:BV:87:GLN:CB | 2.24 | 0.46 |
| 23:BB:923:G:N3 | 43:BW:23:LYS:HE3 | 2.31 | 0.46 |
| 1:CA:1130:A:H2' | 1:CA:1131:G:C8 | 2.50 | 0.46 |
| 1:CA:1212:U:H4' | 1:CA:1213:A:C8 | 2.50 | 0.46 |
| 1:CA:1476:A:H2' | 1:CA:1477:U:O4' | 2.14 | 0.46 |
| 1:CA:425:G:H2' | 1:CA:426:U:C6 | 2.50 | 0.46 |
| 1:CA:984:C:H2' | 1:CA:985:C:H6 | 1.80 | 0.46 |
| 3:CD:40:HIS:O | 3:CD:43:ARG:HG2 | 2.15 | 0.46 |
| 4:CE:45:VAL:HG11 | 4:CE:117:ALA:HB2 | 1.97 | 0.46 |
| 8:CI:16:ALA:HA | 8:CI:66:VAL:HG23 | 1.97 | 0.46 |
| 11:CL:17:LYS:NZ | 11:CL:17:LYS:N | 2.64 | 0.46 |
| 12:CM:13:HIS:O | 12:CM:17:ALA:HB2 | 2.15 | 0.46 |
| 12:CM:44:ILE:O | 12:CM:47:LEU:HB2 | 2.15 | 0.46 |
| 14:CO:69:LEU:HD11 | 14:CO:76:ARG:CB | 2.46 | 0.46 |
| 15:CP:42:ILE:HG22 | 15:CP:43:ALA:N | 2.31 | 0.46 |
| 22:DA:75:G:H2' | 22:DA:76:G:C8 | 2.51 | 0.46 |
| 23:DB:1126:A:H4' | 23:DB:1127:A:O5' | 2.16 | 0.46 |
| 23:DB:1749:A:H2' | 23:DB:1750:G:C8 | 2.50 | 0.46 |
| 23:DB:1823:G:O2' | 23:DB:1824:G:H5' | 2.15 | 0.46 |
| 23:DB:1945:G:H2' | 23:DB:1946:U:C6 | 2.50 | 0.46 |
| 23:DB:1958:C:H2' | 23:DB:1959:G:H8 | 1.81 | 0.46 |
| 23:DB:2075:U:H2' | 23:DB:2238:G:N2 | 2.29 | 0.46 |
| 23:DB:211:C:O2' | 23:DB:212:G:H5' | 2.16 | 0.46 |
| 23:DB:233:A:N6 | 23:DB:428:A:N6 | 2.62 | 0.46 |
| 23:DB:2579:C:H1' | 26:DD:130:GLN:HE22 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:2720:U:H2' | 23:DB:2721:A:H8 | 1.80 | 0.46 |
| 23:DB:39:G:H2' | 23:DB:40:U:C6 | 2.50 | 0.46 |
| 23:DB:454:A:H3' | 23:DB:455:C:H5' | 1.97 | 0.46 |
| 23:DB:566:U:H5'' | 33:DL:29:LYS:HZ2 | 1.79 | 0.46 |
| 23:DB:839:U:H1' | 23:DB:1191:G:H1' | 1.97 | 0.46 |
| 25:DC:119:VAL:HG13 | 25:DC:133:ASN:ND2 | 2.29 | 0.46 |
| 25:DC:71:ASP:O | 25:DC:73:ILE:HG12 | 2.15 | 0.46 |
| 28:DF:19:PHE:HE1 | 28:DF:167:ALA:HB2 | 1.80 | 0.46 |
| 29:DG:122:ALA:HA | 29:DG:131:VAL:O | 2.15 | 0.46 |
| 30:DH:70:GLU:CD | 30:DH:71:LYS:N | 2.69 | 0.46 |
| 32:DK:105:ARG:H | 32:DK:105:ARG:CD | 2.28 | 0.46 |
| 34:DM:29:GLY:HA2 | 34:DM:106:ASP:HB2 | 1.97 | 0.46 |
| 38:DQ:92:LYS:O | 38:DQ:95:ALA:HB3 | 2.15 | 0.46 |
| 42:DU:12:VAL:HA | 42:DU:69:VAL:HA | 1.98 | 0.46 |
| 24:DV:9:ARG:NE | 24:DV:20:LEU:HD11 | 2.29 | 0.46 |
| 23:DB:2355:G:H4' | 43:DW:20:LEU:CD1 | 2.45 | 0.46 |
| 1:AA:1147:C:H2' | 1:AA:1148:U:H6 | 1.81 | 0.46 |
| 1:AA:1180:A:OP1 | 8:AI:104:THR:HG22 | 2.16 | 0.46 |
| 1:AA:189:A:O2' | 1:AA:190:A:H5' | 2.16 | 0.46 |
| 1:AA:197:A:H4' | 1:AA:198:G:O5' | 2.16 | 0.46 |
| 1:AA:640:A:O2' | 1:AA:641:U:H5' | 2.16 | 0.46 |
| 1:AA:659:U:O2' | 1:AA:660:C:H5' | 2.16 | 0.46 |
| 1:AA:16:A:N1 | 1:AA:919:A:H2 | 2.13 | 0.46 |
| 1:AA:948:C:O2' | 1:AA:949:A:H5' | 2.16 | 0.46 |
| 2:AC:63:ILE:HD12 | 2:AC:90:VAL:HG12 | 1.96 | 0.46 |
| 8:AI:34:LEU:HD21 | 8:AI:48:ARG:NH2 | 2.18 | 0.46 |
| 13:AN:12:ARG:NE | 13:AN:58:ARG:HH12 | 2.13 | 0.46 |
| 19:AT:72:ALA:HA | 19:AT:75:LYS:HD3 | 1.96 | 0.46 |
| 22:BA:116:G:H4' | 36:BO:54:VAL:CG2 | 2.39 | 0.46 |
| 23:BB:111:A:H2' | 23:BB:112:U:C6 | 2.50 | 0.46 |
| 23:BB:1290:C:O2' | 23:BB:1291:C:H5' | 2.15 | 0.46 |
| 23:BB:1930:G:H2' | 23:BB:1968:G:C6 | 2.51 | 0.46 |
| 23:BB:2248:C:H2' | 23:BB:2249:U:O4' | 2.15 | 0.46 |
| 23:BB:2339:C:H2' | 23:BB:2340:A:H8 | 1.78 | 0.46 |
| 23:BB:236:C:O2' | 23:BB:237:C:H5' | 2.16 | 0.46 |
| 23:BB:2758:A:C2' | 23:BB:2759:G:H5' | 2.45 | 0.46 |
| 23:BB:38:A:N3 | 27:BE:43:THR:HB | 2.31 | 0.46 |
| 23:BB:39:G:H2' | 23:BB:40:U:H6 | 1.80 | 0.46 |
| 23:BB:581:C:OP1 | 38:BQ:32:ARG:HG3 | 2.15 | 0.46 |
| 23:BB:902:C:H2' | 23:BB:903:C:C6 | 2.50 | 0.46 |
| 25:BC:76:VAL:CG1 | 25:BC:114:GLN:HG2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BC:144:GLU:OE2 | 25:BC:188:ARG:HG3 | 2.16 | 0.46 |
| 26:BD:36:GLN:HE21 | 26:BD:36:GLN:HB2 | 1.53 | 0.46 |
| 29:BG:49:LEU:HD23 | 29:BG:51:PHE:CZ | 2.50 | 0.46 |
| 30:BH:90:LEU:CB | 30:BH:123:ARG:HD2 | 2.45 | 0.46 |
| 31:BJ:18:VAL:HG12 | 31:BJ:54:ILE:HD11 | 1.96 | 0.46 |
| 32:BK:8:LEU:H | 32:BK:8:LEU:HD12 | 1.79 | 0.46 |
| 32:BK:95:ILE:O | 32:BK:95:ILE:HG13 | 2.15 | 0.46 |
| 33:BL:122:VAL:HB | 33:BL:143:GLU:OE1 | 2.15 | 0.46 |
| 35:BN:54:LEU:HD11 | 35:BN:62:ASN:HB3 | 1.98 | 0.46 |
| 36:BO:88:LYS:HB3 | 36:BO:88:LYS:HE3 | 1.66 | 0.46 |
| 38:BQ:91:ARG:HB2 | 39:BR:11:GLN:OE1 | 2.16 | 0.46 |
| 40:BS:4:ILE:CG2 | 40:BS:106:VAL:HG22 | 2.45 | 0.46 |
| 41:BT:85:VAL:C | 41:BT:86:THR:HG23 | 2.36 | 0.46 |
| 24:BV:80:HIS:HB2 | 24:BV:85:LYS:HG3 | 1.98 | 0.46 |
| 1:CA:16:A:H2 | 1:CA:1080:A:N3 | 2.14 | 0.46 |
| 1:CA:1095:U:H5'' | 1:CA:1109:C:O2 | 2.16 | 0.46 |
| 1:CA:1125:U:C6 | 9:CJ:40:ILE:HD13 | 2.51 | 0.46 |
| 1:CA:1178:G:H3' | 8:CI:98:ARG:NH2 | 2.29 | 0.46 |
| 1:CA:1181:G:H1' | 1:CA:1182:G:C5 | 2.51 | 0.46 |
| 1:CA:1293:C:O2' | 1:CA:1294:G:H5' | 2.14 | 0.46 |
| 1:CA:204:G:H2' | 1:CA:205:A:H8 | 1.79 | 0.46 |
| 1:CA:333:U:H2' | 1:CA:334:C:C6 | 2.51 | 0.46 |
| 20:CB:129:THR:O | 20:CB:131:LYS:N | 2.48 | 0.46 |
| 20:CB:93:HIS:HA | 20:CB:94:ARG:NH2 | 2.30 | 0.46 |
| 3:CD:75:TYR:CE1 | 3:CD:200:VAL:HA | 2.50 | 0.46 |
| 4:CE:68:ARG:O | 4:CE:69:ASN:HB2 | 2.16 | 0.46 |
| 6:CG:71:THR:H | 6:CG:141:HIS:CE1 | 2.33 | 0.46 |
| 6:CG:59:GLU:O | 6:CG:63:VAL:HG23 | 2.15 | 0.46 |
| 6:CG:74:VAL:HG12 | 6:CG:87:PRO:HB3 | 1.98 | 0.46 |
| 7:CH:68:LYS:HG3 | 7:CH:69:ALA:N | 2.30 | 0.46 |
| 9:CJ:8:ILE:H | 9:CJ:8:ILE:HD12 | 1.80 | 0.46 |
| 1:CA:707:U:H4' | 10:CK:21:HIS:CD2 | 2.50 | 0.46 |
| 16:CQ:3:LYS:HG3 | 16:CQ:4:ILE:H | 1.79 | 0.46 |
| 23:DB:1010:A:N3 | 23:DB:1153:C:H1' | 2.30 | 0.46 |
| 23:DB:1023:U:H2' | 23:DB:1024:G:H5' | 1.98 | 0.46 |
| 23:DB:1092:C:C2' | 23:DB:1093:G:H5' | 2.45 | 0.46 |
| 23:DB:1387:A:H2' | 23:DB:1388:G:C8 | 2.51 | 0.46 |
| 23:DB:1429:G:H2' | 23:DB:1430:G:C8 | 2.49 | 0.46 |
| 23:DB:1458:U:C2' | 23:DB:1459:G:H5'' | 2.45 | 0.46 |
| 23:DB:1848:A:H2' | 23:DB:1849:G:C8 | 2.50 | 0.46 |
| 23:DB:1919:A:N3 | 23:DB:1919:A:H2' | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:2305:U:H2' | 23:DB:2306:C:O4' | 2.16 | 0.46 |
| 23:DB:2674:G:H2' | 23:DB:2675:A:H8 | 1.80 | 0.46 |
| 23:DB:485:C:O2' | 23:DB:486:C:H5' | 2.15 | 0.46 |
| 23:DB:493:G:O2' | 40:DS:7:HIS:HA | 2.15 | 0.46 |
| 23:DB:596:U:O2' | 23:DB:597:G:H5' | 2.15 | 0.46 |
| 23:DB:68:G:H2' | 23:DB:69:C:C6 | 2.51 | 0.46 |
| 23:DB:935:C:H2' | 23:DB:936:A:C8 | 2.50 | 0.46 |
| 26:DD:106:LYS:HD3 | 26:DD:106:LYS:N | 2.30 | 0.46 |
| 27:DE:137:LYS:HG3 | 27:DE:141:MET:SD | 2.56 | 0.46 |
| 29:DG:33:THR:C | 29:DG:34:ARG:HD3 | 2.36 | 0.46 |
| 30:DH:117:LEU:HD22 | 30:DH:130:VAL:CG1 | 2.45 | 0.46 |
| 30:DH:26:ALA:C | 30:DH:28:ASN:N | 2.68 | 0.46 |
| 32:DK:40:LYS:NZ | 32:DK:59:LYS:HE3 | 2.31 | 0.46 |
| 33:DL:123:ARG:HD2 | 33:DL:124:GLY:N | 2.30 | 0.46 |
| 33:DL:132:ARG:O | 33:DL:136:GLU:HG2 | 2.15 | 0.46 |
| 34:DM:35:ALA:HB3 | 34:DM:99:GLY:H | 1.78 | 0.46 |
| 36:DO:18:LEU:HD23 | 36:DO:25:ARG:CD | 2.45 | 0.46 |
| 38:DQ:26:ALA:HA | 38:DQ:29:ARG:CG | 2.45 | 0.46 |
| 41:DT:14:PRO:HA | 41:DT:32:LEU:HB2 | 1.97 | 0.46 |
| 44:DX:56:LEU:O | 44:DX:58:ASN:N | 2.42 | 0.46 |
| 45:DY:50:VAL:HA | 45:DY:52:PHE:CE1 | 2.51 | 0.46 |
| 1:AA:1125:U:C6 | 9:AJ:40:ILE:HD13 | 2.51 | 0.46 |
| 1:AA:119:A:H4' | 1:AA:120:A:O4' | 2.14 | 0.46 |
| 1:AA:1216:A:H2' | 1:AA:1217:C:H6 | 1.81 | 0.46 |
| 1:AA:279:A:H5' | 1:AA:281:G:O4' | 2.15 | 0.46 |
| 1:AA:600:A:OP1 | 7:AH:87:ARG:HB3 | 2.16 | 0.46 |
| 1:AA:669:G:H2' | 1:AA:670:G:H8 | 1.80 | 0.46 |
| 1:AA:697:U:H2' | 1:AA:698:G:H5' | 1.97 | 0.46 |
| 4:AE:132:PRO:HG2 | 4:AE:133:ILE:H | 1.79 | 0.46 |
| 5:AF:7:VAL:O | 5:AF:7:VAL:HG13 | 2.15 | 0.46 |
| 6:AG:13:PRO:O | 6:AG:14:ASP:C | 2.53 | 0.46 |
| 7:AH:40:LYS:HD3 | 7:AH:48:PHE:CE1 | 2.49 | 0.46 |
| 8:AI:99:LYS:HE3 | 9:CJ:80:THR:CA | 2.41 | 0.46 |
| 13:AN:20:PHE:CD1 | 13:AN:24:ALA:HB2 | 2.51 | 0.46 |
| 9:AJ:53:ILE:HG13 | 13:AN:84:ARG:CZ | 2.46 | 0.46 |
| 19:AT:2:ASN:CG | 19:AT:3:ILE:N | 2.69 | 0.46 |
| 21:AU:11:PHE:CE1 | 21:AU:13:VAL:HG12 | 2.50 | 0.46 |
| 48:B1:39:ASP:OD1 | 48:B1:41:VAL:HB | 2.15 | 0.46 |
| 23:BB:643:A:H1' | 48:B1:43:ARG:NH2 | 2.31 | 0.46 |
| 23:BB:1030:C:O2' | 23:BB:1031:G:H5' | 2.15 | 0.46 |
| 23:BB:2559:C:H2' | 23:BB:2560:A:H8 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:2578:G:O2' | 23:BB:2579:C:H5' | 2.15 | 0.46 |
| 23:BB:2617:U:O2' | 23:BB:2618:G:H5' | 2.15 | 0.46 |
| 23:BB:359:G:O2' | 23:BB:360:U:H5' | 2.15 | 0.46 |
| 23:BB:657:U:H2' | 23:BB:658:U:C6 | 2.51 | 0.46 |
| 23:BB:851:C:H2' | 23:BB:852:U:C6 | 2.51 | 0.46 |
| 23:BB:921:C:H2' | 23:BB:922:C:H6 | 1.81 | 0.46 |
| 25:BC:138:SER:O | 25:BC:162:GLN:HA | 2.14 | 0.46 |
| 25:BC:83:ASP:HB3 | 25:BC:86:ARG:HG2 | 1.97 | 0.46 |
| 26:BD:106:LYS:N | 26:BD:106:LYS:HD3 | 2.31 | 0.46 |
| 28:BF:59:ILE:HG12 | 28:BF:137:PHE:CE2 | 2.50 | 0.46 |
| 28:BF:98:PHE:C | 28:BF:100:GLU:N | 2.69 | 0.46 |
| 34:BM:38:ARG:HG2 | 34:BM:38:ARG:HH11 | 1.81 | 0.46 |
| 36:BO:84:GLU:C | 36:BO:86:GLY:N | 2.69 | 0.46 |
| 37:BP:77:SER:O | 37:BP:80:VAL:HG12 | 2.15 | 0.46 |
| 40:BS:41:LYS:O | 40:BS:43:ALA:N | 2.49 | 0.46 |
| 42:BU:11:ILE:HG12 | 42:BU:20:LYS:O | 2.16 | 0.46 |
| 42:BU:23:LYS:HD2 | 42:BU:23:LYS:H | 1.80 | 0.46 |
| 24:BV:9:ARG:NE | 24:BV:20:LEU:HD11 | 2.30 | 0.46 |
| 43:BW:61:LYS:O | 43:BW:62:ALA:O | 2.33 | 0.46 |
| 23:BB:188:G:OP1 | 46:BZ:14:THR:HG23 | 2.15 | 0.46 |
| 46:BZ:36:HIS:O | 46:BZ:48:THR:HA | 2.16 | 0.46 |
| 1:CA:1102:A:H2' | 1:CA:1103:C:C6 | 2.51 | 0.46 |
| 1:CA:251:G:H1 | 1:CA:271:C:N4 | 2.13 | 0.46 |
| 1:CA:373:A:H2' | 1:CA:374:A:C8 | 2.47 | 0.46 |
| 1:CA:36:C:O2' | 1:CA:37:U:H5' | 2.16 | 0.46 |
| 1:CA:586:C:H5'' | 7:CH:81:GLY:HA2 | 1.98 | 0.46 |
| 1:CA:893:C:H2' | 1:CA:894:G:H8 | 1.81 | 0.46 |
| 3:CD:162:GLU:C | 3:CD:164:ARG:H | 2.19 | 0.46 |
| 3:CD:24:VAL:O | 3:CD:27:ILE:HG13 | 2.14 | 0.46 |
| 3:CD:2:ARG:HG3 | 3:CD:114:ARG:NH1 | 2.31 | 0.46 |
| 3:CD:90:LEU:HD13 | 3:CD:93:LEU:HD12 | 1.97 | 0.46 |
| 5:CF:10:VAL:HG12 | 5:CF:11:HIS:N | 2.31 | 0.46 |
| 10:CK:37:GLN:HB2 | 10:CK:39:ASN:ND2 | 2.31 | 0.46 |
| 1:CA:1308:U:H3' | 12:CM:97:ARG:NH1 | 2.31 | 0.46 |
| 16:CQ:64:ARG:HG2 | 16:CQ:65:PRO:HD2 | 1.97 | 0.46 |
| 22:DA:75:G:N1 | 22:DA:102:G:N2 | 2.63 | 0.46 |
| 23:DB:1082:U:C2 | 23:DB:1086:A:N1 | 2.83 | 0.46 |
| 23:DB:1547:C:H2' | 23:DB:1548:A:C8 | 2.50 | 0.46 |
| 23:DB:1872:A:H2' | 23:DB:1873:G:O4' | 2.15 | 0.46 |
| 23:DB:2334:U:O3' | 36:DO:13:ARG:HB2 | 2.14 | 0.46 |
| 23:DB:2379:G:C5' | 36:DO:21:LEU:HD11 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2489:U:O2' | 23:DB:2490:G:H5' | 2.15 | 0.46 |
| 23:DB:2492:U:O2' | 23:DB:2493:U:H5' | 2.15 | 0.46 |
| 23:DB:63:A:H2' | 23:DB:63:A:OP2 | 2.15 | 0.46 |
| 23:DB:5:A:H2' | 23:DB:6:A:H8 | 1.81 | 0.46 |
| 23:DB:754:U:H2' | 23:DB:755:U:H6 | 1.81 | 0.46 |
| 23:DB:771:G:O2' | 23:DB:772:C:H5' | 2.16 | 0.46 |
| 23:DB:899:A:C2 | 23:DB:900:A:H1' | 2.51 | 0.46 |
| 25:DC:64:VAL:O | 25:DC:65:ASP:CB | 2.62 | 0.46 |
| 23:DB:2314:A:O4' | 28:DF:154:THR:HG21 | 2.16 | 0.46 |
| 30:DH:87:GLU:HB2 | 30:DH:89:LYS:HZ2 | 1.81 | 0.46 |
| 31:DJ:58:ASN:C | 31:DJ:60:ASP:H | 2.18 | 0.46 |
| 33:DL:133:ALA:HA | 33:DL:136:GLU:HB2 | 1.98 | 0.46 |
| 34:DM:101:VAL:HG13 | 34:DM:101:VAL:O | 2.16 | 0.46 |
| 23:DB:2820:A:H4' | 35:DN:3:HIS:ND1 | 2.30 | 0.46 |
| 38:DQ:64:ILE:HD12 | 38:DQ:95:ALA:HB3 | 1.97 | 0.46 |
| 40:DS:41:LYS:O | 40:DS:42:LYS:C | 2.54 | 0.46 |
| 40:DS:88:ARG:HG3 | 40:DS:88:ARG:HH21 | 1.81 | 0.46 |
| 42:DU:86:PHE:CD2 | 42:DU:92:VAL:HG21 | 2.50 | 0.46 |
| 24:DV:16:ALA:HA | 24:DV:19:ARG:HH21 | 1.81 | 0.46 |
| 46:DZ:5:CYS:SG | 46:DZ:7:VAL:HG12 | 2.56 | 0.46 |
| 1:AA:106:C:HO2' | 1:AA:107:G:H5' | 1.80 | 0.46 |
| 1:AA:1317:C:H3' | 1:AA:1318:A:C8 | 2.49 | 0.46 |
| 1:AA:1360:A:H2' | 1:AA:1361:G:O4' | 2.15 | 0.46 |
| 1:AA:1392:G:H2' | 1:AA:1393:U:C6 | 2.51 | 0.46 |
| 1:AA:503:C:H2' | 1:AA:504:C:C6 | 2.51 | 0.46 |
| 1:AA:762:U:H2' | 1:AA:763:G:H8 | 1.80 | 0.46 |
| 1:AA:803:G:H2' | 1:AA:804:U:O4' | 2.15 | 0.46 |
| 1:AA:87:C:C2' | 1:AA:88:U:H4' | 2.45 | 0.46 |
| 4:AE:77:ASN:CG | 4:AE:78:GLY:H | 2.17 | 0.46 |
| 9:AJ:6:ILE:O | 9:AJ:8:ILE:HD12 | 2.16 | 0.46 |
| 11:AL:78:VAL:O | 11:AL:102:ASP:HB2 | 2.16 | 0.46 |
| 15:AP:52:LEU:CD2 | 15:AP:75:ILE:HA | 2.45 | 0.46 |
| 22:BA:32:U:H1' | 22:BA:52:A:N7 | 2.31 | 0.46 |
| 23:BB:1460:U:H3' | 23:BB:1461:C:H5' | 1.98 | 0.46 |
| 23:BB:1505:A:H2' | 23:BB:1506:U:C6 | 2.51 | 0.46 |
| 23:BB:1936:A:H2 | 23:BB:1943:U:C5 | 2.34 | 0.46 |
| 23:BB:265:A:O2' | 23:BB:266:G:C4' | 2.64 | 0.46 |
| 23:BB:2756:U:C1' | 23:BB:2757:A:H5'' | 2.45 | 0.46 |
| 23:BB:969:G:H2' | 23:BB:970:U:C6 | 2.50 | 0.46 |
| 5:AF:80:PHE:CE1 | 25:BC:135:PRO:HG2 | 2.51 | 0.46 |
| 26:BD:15:PHE:HD1 | 26:BD:15:PHE:H | 1.64 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:11:VAL:HG21 | 28:BF:172:PHE:HE1 | 1.81 | 0.46 |
| 28:BF:28:PRO:O | 28:BF:168:LEU:HG | 2.16 | 0.46 |
| 28:BF:43:ILE:HG13 | 28:BF:44:ALA:N | 2.31 | 0.46 |
| 28:BF:43:ILE:HA | 28:BF:46:LYS:CE | 2.45 | 0.46 |
| 28:BF:65:LEU:O | 28:BF:86:CYS:HA | 2.15 | 0.46 |
| 31:BJ:16:TYR:CD2 | 31:BJ:140:LEU:HD12 | 2.51 | 0.46 |
| 31:BJ:58:ASN:C | 31:BJ:60:ASP:H | 2.18 | 0.46 |
| 31:BJ:64:VAL:O | 31:BJ:65:THR:HG22 | 2.16 | 0.46 |
| 34:BM:19:GLY:N | 34:BM:38:ARG:NH2 | 2.63 | 0.46 |
| 35:BN:13:ASN:OD1 | 35:BN:16:HIS:HB2 | 2.15 | 0.46 |
| 36:BO:18:LEU:HD23 | 36:BO:25:ARG:CD | 2.44 | 0.46 |
| 37:BP:54:LEU:HD12 | 37:BP:76:HIS:HB2 | 1.98 | 0.46 |
| 38:BQ:86:SER:HB3 | 39:BR:51:VAL:CA | 2.46 | 0.46 |
| 23:BB:572:A:OP2 | 39:BR:80:ARG:NH2 | 2.49 | 0.46 |
| 42:BU:12:VAL:HA | 42:BU:69:VAL:HA | 1.98 | 0.46 |
| 42:BU:71:ILE:HD11 | 42:BU:81:ARG:O | 2.16 | 0.46 |
| 42:BU:85:ARG:NH1 | 42:BU:86:PHE:N | 2.64 | 0.46 |
| 1:CA:1499:A:O2' | 1:CA:1500:A:H5' | 2.16 | 0.46 |
| 1:CA:562:U:H4' | 1:CA:563:A:O5' | 2.15 | 0.46 |
| 1:CA:751:U:O2' | 14:CO:24:THR:HG23 | 2.16 | 0.46 |
| 20:CB:102:ASN:HD21 | 20:CB:105:THR:HB | 1.81 | 0.46 |
| 20:CB:160:LEU:HD22 | 20:CB:182:VAL:HA | 1.97 | 0.46 |
| 2:CC:134:LYS:HA | 2:CC:167:TYR:HE2 | 1.81 | 0.46 |
| 2:CC:50:SER:CB | 2:CC:70:ALA:HB3 | 2.46 | 0.46 |
| 3:CD:33:ILE:HG13 | 3:CD:34:GLU:N | 2.30 | 0.46 |
| 6:CG:136:LYS:O | 6:CG:140:VAL:HG23 | 2.16 | 0.46 |
| 8:CI:49:GLN:HA | 8:CI:52:GLU:HG2 | 1.98 | 0.46 |
| 9:CJ:12:ALA:H | 9:CJ:18:ILE:HD13 | 1.81 | 0.46 |
| 9:CJ:8:ILE:HA | 9:CJ:100:ILE:HG22 | 1.97 | 0.46 |
| 10:CK:28:ASN:ND2 | 10:CK:29:THR:H | 2.14 | 0.46 |
| 21:CU:33:ARG:HG2 | 21:CU:34:ARG:N | 2.28 | 0.46 |
| 49:D2:21:ARG:HG2 | 49:D2:31:LEU:HD21 | 1.98 | 0.46 |
| 23:DB:1099:G:OP2 | 52:DI:2:LYS:O | 2.33 | 0.46 |
| 23:DB:1733:G:H5' | 23:DB:1733:G:H8 | 1.81 | 0.46 |
| 23:DB:1999:C:H2' | 23:DB:2000:C:O4' | 2.16 | 0.46 |
| 23:DB:2148:G:O3' | 23:DB:2149:U:H6 | 1.99 | 0.46 |
| 23:DB:2648:G:H2' | 23:DB:2649:C:H6 | 1.79 | 0.46 |
| 23:DB:2849:U:H4' | 23:DB:2850:A:C5' | 2.44 | 0.46 |
| 23:DB:533:G:H5' | 38:DQ:23:TYR:CD2 | 2.51 | 0.46 |
| 23:DB:796:C:H2' | 23:DB:797:G:H8 | 1.79 | 0.46 |
| 23:DB:877:A:H2' | 23:DB:877:A:N3 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:153:LEU:HD13 | 25:DC:175:LEU:HD21 | 1.97 | 0.46 |
| 28:DF:139:GLU:O | 28:DF:141:ASP:N | 2.49 | 0.46 |
| 28:DF:33:ILE:O | 28:DF:90:LEU:HB2 | 2.15 | 0.46 |
| 29:DG:37:ASN:HD22 | 29:DG:40:VAL:CB | 2.25 | 0.46 |
| 30:DH:60:GLU:C | 30:DH:62:LEU:N | 2.68 | 0.46 |
| 30:DH:95:GLY:O | 30:DH:98:ASP:N | 2.49 | 0.46 |
| 52:DI:23:VAL:HG12 | 52:DI:24:GLY:N | 2.31 | 0.46 |
| 31:DJ:44:TYR:CD2 | 31:DJ:44:TYR:C | 2.89 | 0.46 |
| 32:DK:11:ALA:HB3 | 32:DK:85:VAL:CG2 | 2.46 | 0.46 |
| 33:DL:105:ILE:HG22 | 33:DL:106:GLU:N | 2.31 | 0.46 |
| 34:DM:56:ALA:C | 34:DM:58:LYS:H | 2.18 | 0.46 |
| 23:DB:2009:A:O4' | 35:DN:107:ASN:HB2 | 2.16 | 0.46 |
| 35:DN:11:ASN:O | 35:DN:12:ARG:HB2 | 2.15 | 0.46 |
| 35:DN:48:VAL:O | 35:DN:51:LEU:N | 2.49 | 0.46 |
| 35:DN:61:ALA:C | 35:DN:63:ARG:H | 2.19 | 0.46 |
| 36:DO:3:LYS:HG2 | 36:DO:3:LYS:H | 1.50 | 0.46 |
| 39:DR:54:VAL:HG13 | 39:DR:56:GLY:O | 2.15 | 0.46 |
| 39:DR:59:ILE:HA | 39:DR:100:GLY:HA3 | 1.97 | 0.46 |
| 39:DR:63:VAL:O | 39:DR:63:VAL:HG23 | 2.16 | 0.46 |
| 41:DT:40:LYS:O | 41:DT:43:ILE:HB | 2.15 | 0.46 |
| 41:DT:61:LEU:C | 41:DT:61:LEU:HD12 | 2.36 | 0.46 |
| 42:DU:11:ILE:HB | 42:DU:72:PHE:HD1 | 1.81 | 0.46 |
| 24:DV:80:HIS:HB2 | 24:DV:85:LYS:HG3 | 1.97 | 0.46 |
| 1:AA:313:A:H2' | 1:AA:314:C:H6 | 1.80 | 0.46 |
| 1:AA:502:A:H2' | 1:AA:503:C:C6 | 2.50 | 0.46 |
| 1:AA:545:C:O2' | 1:AA:546:A:H5' | 2.15 | 0.46 |
| 1:AA:861:G:H2' | 1:AA:862:C:H6 | 1.80 | 0.46 |
| 1:AA:918:A:C6 | 1:AA:919:A:C6 | 3.04 | 0.46 |
| 20:AB:117:GLU:HA | 20:AB:140:LEU:CD2 | 2.45 | 0.46 |
| 20:AB:151:LYS:HG3 | 20:AB:152:ASP:N | 2.30 | 0.46 |
| 2:AC:106:ARG:HG2 | 2:AC:106:ARG:HH11 | 1.81 | 0.46 |
| 3:AD:162:GLU:C | 3:AD:164:ARG:H | 2.19 | 0.46 |
| 8:AI:109:GLN:CD | 8:AI:110:VAL:H | 2.19 | 0.46 |
| 8:AI:56:MET:SD | 8:AI:57:VAL:HG23 | 2.55 | 0.46 |
| 8:AI:16:ALA:HA | 8:AI:66:VAL:HG23 | 1.98 | 0.46 |
| 8:AI:78:ILE:HG22 | 8:AI:82:ILE:CD1 | 2.46 | 0.46 |
| 9:AJ:8:ILE:HD12 | 9:AJ:8:ILE:H | 1.81 | 0.46 |
| 12:AM:19:THR:HG22 | 12:AM:29:SER:HB3 | 1.98 | 0.46 |
| 18:AS:40:PHE:HB2 | 18:AS:43:MET:HE2 | 1.97 | 0.46 |
| 22:BA:106:G:H2' | 22:BA:107:G:C8 | 2.51 | 0.46 |
| 23:BB:1482:G:N2 | 23:BB:1508:A:H1' | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:1737:G:H5' | 23:BB:1738:G:OP2 | 2.16 | 0.46 |
| 23:BB:740:C:H5'' | 23:BB:1784:A:OP1 | 2.15 | 0.46 |
| 23:BB:2024:G:O2' | 23:BB:2025:C:H5' | 2.15 | 0.46 |
| 23:BB:2655:G:O2' | 23:BB:2656:U:P | 2.74 | 0.46 |
| 23:BB:2658:C:H2' | 23:BB:2659:G:H5' | 1.97 | 0.46 |
| 23:BB:28:A:N6 | 23:BB:512:G:O2' | 2.48 | 0.46 |
| 23:BB:348:A:H2' | 23:BB:349:U:C6 | 2.51 | 0.46 |
| 23:BB:434:U:H1' | 23:BB:435:C:H5 | 1.81 | 0.46 |
| 23:BB:583:G:H2' | 23:BB:584:C:H6 | 1.79 | 0.46 |
| 23:BB:663:G:OP1 | 33:BL:17:LYS:HG2 | 2.16 | 0.46 |
| 23:BB:942:G:H2' | 23:BB:943:A:O4' | 2.16 | 0.46 |
| 23:BB:974:G:H1' | 23:BB:975:A:C8 | 2.50 | 0.46 |
| 26:BD:125:TRP:HE1 | 26:BD:161:MET:H | 1.63 | 0.46 |
| 23:BB:2635:A:H5' | 26:BD:79:LEU:HD23 | 1.98 | 0.46 |
| 27:BE:148:ILE:HA | 27:BE:187:VAL:CG2 | 2.46 | 0.46 |
| 29:BG:109:SER:O | 29:BG:110:HIS:HB3 | 2.16 | 0.46 |
| 31:BJ:63:ALA:HA | 31:BJ:69:ARG:HH22 | 1.80 | 0.46 |
| 32:BK:59:LYS:HD2 | 32:BK:89:ASN:O | 2.16 | 0.46 |
| 34:BM:63:ILE:N | 34:BM:63:ILE:HD12 | 2.30 | 0.46 |
| 35:BN:8:ARG:HB3 | 35:BN:43:GLU:OE2 | 2.15 | 0.46 |
| 22:BA:48:U:O2' | 36:BO:100:HIS:HE1 | 1.99 | 0.46 |
| 39:BR:70:GLU:O | 39:BR:90:ARG:HD2 | 2.16 | 0.46 |
| 41:BT:14:PRO:HA | 41:BT:32:LEU:CB | 2.46 | 0.46 |
| 23:BB:309:A:H4' | 42:BU:15:GLY:HA2 | 1.97 | 0.46 |
| 1:CA:1252:A:H2' | 1:CA:1253:G:O4' | 2.16 | 0.46 |
| 1:CA:395:C:H2' | 1:CA:396:C:C6 | 2.50 | 0.46 |
| 1:CA:517:G:H22 | 1:CA:533:A:P | 2.39 | 0.46 |
| 1:CA:775:G:H2' | 1:CA:776:G:C8 | 2.51 | 0.46 |
| 1:CA:9:G:H5' | 4:CE:107:GLY:HA3 | 1.98 | 0.46 |
| 2:CC:122:GLN:O | 2:CC:127:VAL:HG13 | 2.16 | 0.46 |
| 2:CC:149:LYS:O | 2:CC:200:TRP:HE3 | 1.98 | 0.46 |
| 6:CG:13:PRO:O | 6:CG:14:ASP:C | 2.53 | 0.46 |
| 8:CI:17:ARG:HB2 | 8:CI:65:THR:HB | 1.96 | 0.46 |
| 9:CJ:35:GLN:HG2 | 9:CJ:78:GLU:OE2 | 2.14 | 0.46 |
| 11:CL:51:VAL:HG12 | 11:CL:52:CYS:N | 2.29 | 0.46 |
| 11:CL:51:VAL:HG12 | 11:CL:63:THR:HG22 | 1.97 | 0.46 |
| 12:CM:3:ILE:H | 12:CM:56:ARG:NH2 | 2.13 | 0.46 |
| 13:CN:20:PHE:CD1 | 13:CN:24:ALA:HB2 | 2.50 | 0.46 |
| 51:D4:2:LYS:HD3 | 51:D4:4:ARG:HE | 1.81 | 0.46 |
| 23:DB:1054:A:H2' | 23:DB:1055:G:C8 | 2.49 | 0.46 |
| 23:DB:1745:A:H2' | 23:DB:1746:A:C8 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2023:C:H4' | 23:DB:2617:U:O3' | 2.16 | 0.46 |
| 23:DB:2223:G:H2' | 23:DB:2224:G:H5' | 1.97 | 0.46 |
| 23:DB:2626:C:H2' | 23:DB:2627:G:C8 | 2.51 | 0.46 |
| 23:DB:2668:G:O2' | 23:DB:2669:G:H5' | 2.16 | 0.46 |
| 23:DB:353:C:O2 | 23:DB:353:C:H2' | 2.15 | 0.46 |
| 23:DB:582:A:H2' | 23:DB:583:G:C8 | 2.50 | 0.46 |
| 23:DB:623:C:H2' | 23:DB:624:C:H6 | 1.81 | 0.46 |
| 23:DB:950:G:H2' | 23:DB:951:C:H6 | 1.81 | 0.46 |
| 26:DD:107:VAL:HG12 | 26:DD:109:VAL:HG23 | 1.98 | 0.46 |
| 28:DF:102:LEU:O | 28:DF:103:ILE:CB | 2.63 | 0.46 |
| 28:DF:33:ILE:H | 28:DF:95:MET:HG3 | 1.81 | 0.46 |
| 29:DG:1:SER:O | 29:DG:3:VAL:N | 2.49 | 0.46 |
| 30:DH:60:GLU:O | 30:DH:62:LEU:HD23 | 2.16 | 0.46 |
| 52:DI:69:VAL:HG23 | 52:DI:69:VAL:O | 2.15 | 0.46 |
| 32:DK:119:ALA:O | 32:DK:120:PRO:O | 2.33 | 0.46 |
| 27:DE:181:ILE:HD13 | 33:DL:3:LEU:HD23 | 1.97 | 0.46 |
| 38:DQ:111:LYS:HZ2 | 38:DQ:111:LYS:HB2 | 1.81 | 0.46 |
| 1:AA:1125:U:HO2' | 1:AA:1126:U:H2' | 1.81 | 0.46 |
| 1:AA:113:G:O2' | 1:AA:354:G:H5' | 2.16 | 0.46 |
| 1:AA:373:A:O2' | 1:AA:374:A:H5' | 2.16 | 0.46 |
| 1:AA:631:C:H3' | 1:AA:632:U:H5' | 1.97 | 0.46 |
| 1:AA:828:U:OP1 | 1:AA:828:U:H4' | 2.14 | 0.46 |
| 2:AC:155:ARG:H | 2:AC:162:ALA:HA | 1.80 | 0.46 |
| 3:AD:148:ALA:O | 3:AD:154:VAL:HG11 | 2.16 | 0.46 |
| 5:AF:93:LYS:O | 5:AF:94:HIS:HB2 | 2.15 | 0.46 |
| 6:AG:2:ARG:HG2 | 6:AG:3:ARG:CD | 2.46 | 0.46 |
| 6:AG:46:LEU:HG | 6:AG:57:GLU:CB | 2.38 | 0.46 |
| 9:AJ:35:GLN:HG2 | 9:AJ:78:GLU:OE2 | 2.16 | 0.46 |
| 14:AO:55:LEU:HD21 | 23:BB:715:A:C2 | 2.51 | 0.46 |
| 16:AQ:60:ILE:HD13 | 16:AQ:60:ILE:H | 1.80 | 0.46 |
| 10:AK:124:LYS:CA | 21:AU:34:ARG:HB3 | 2.39 | 0.46 |
| 23:BB:2392:A:OP1 | 50:B3:30:HIS:HB3 | 2.16 | 0.46 |
| 23:BB:1515:A:H2' | 23:BB:1516:G:O4' | 2.16 | 0.46 |
| 23:BB:2419:U:H2' | 23:BB:2420:C:C6 | 2.51 | 0.46 |
| 23:BB:244:A:H1' | 23:BB:255:A:N6 | 2.31 | 0.46 |
| 23:BB:2733:A:H2' | 23:BB:2734:A:O4' | 2.16 | 0.46 |
| 23:BB:2868:A:H2' | 23:BB:2869:G:H8 | 1.81 | 0.46 |
| 23:BB:544:C:H2' | 23:BB:545:U:C6 | 2.51 | 0.46 |
| 23:BB:655:A:H4' | 23:BB:656:G:H5' | 1.96 | 0.46 |
| 23:BB:730:A:H3' | 56:BB:3593:HOH:O | 2.16 | 0.46 |
| 23:BB:813:U:H2' | 23:BB:814:C:C6 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:839:U:H2' | 23:BB:840:C:H6 | 1.80 | 0.46 |
| 23:BB:90:U:OP2 | 23:BB:91:A:H3' | 2.15 | 0.46 |
| 25:BC:103:ILE:HG22 | 25:BC:105:ALA:N | 2.30 | 0.46 |
| 25:BC:119:VAL:HG13 | 25:BC:133:ASN:HD21 | 1.81 | 0.46 |
| 23:BB:1568:G:H4' | 25:BC:58:LYS:HB3 | 1.97 | 0.46 |
| 26:BD:8:LYS:HZ2 | 26:BD:25:THR:CG2 | 2.29 | 0.46 |
| 27:BE:4:VAL:HG12 | 27:BE:6:LYS:H | 1.80 | 0.46 |
| 37:BP:62:LYS:HB3 | 37:BP:69:VAL:CG2 | 2.45 | 0.46 |
| 23:BB:2019:A:H4' | 38:BQ:33:VAL:HG11 | 1.97 | 0.46 |
| 38:BQ:78:PHE:CZ | 38:BQ:82:LEU:HD11 | 2.51 | 0.46 |
| 40:BS:41:LYS:O | 40:BS:42:LYS:C | 2.54 | 0.46 |
| 42:BU:86:PHE:CG | 42:BU:87:GLU:N | 2.84 | 0.46 |
| 24:BV:48:MET:O | 24:BV:51:GLN:HG3 | 2.16 | 0.46 |
| 24:BV:77:VAL:HG23 | 24:BV:89:ILE:CG2 | 2.45 | 0.46 |
| 1:CA:1276:G:H2' | 1:CA:1277:C:C6 | 2.51 | 0.46 |
| 1:CA:1318:A:H4' | 18:CS:9:PHE:CE1 | 2.50 | 0.46 |
| 1:CA:1369:C:H2' | 1:CA:1370:G:C8 | 2.51 | 0.46 |
| 1:CA:167:A:O2' | 1:CA:168:G:H5' | 2.16 | 0.46 |
| 1:CA:241:G:O2' | 1:CA:242:G:H5' | 2.15 | 0.46 |
| 1:CA:62:U:H5'' | 1:CA:385:C:O2' | 2.15 | 0.46 |
| 1:CA:599:C:O2' | 1:CA:600:A:H5' | 2.15 | 0.46 |
| 1:CA:67:C:H2' | 1:CA:68:G:C8 | 2.51 | 0.46 |
| 1:CA:744:C:H2' | 1:CA:745:G:C8 | 2.50 | 0.46 |
| 1:CA:868:C:H2' | 1:CA:869:G:O4' | 2.16 | 0.46 |
| 20:CB:96:LEU:HB2 | 20:CB:99:MET:HE2 | 1.96 | 0.46 |
| 5:CF:7:VAL:O | 5:CF:7:VAL:HG13 | 2.15 | 0.46 |
| 7:CH:77:VAL:HG23 | 7:CH:126:CYS:HA | 1.98 | 0.46 |
| 7:CH:46:GLU:N | 7:CH:63:LYS:HB2 | 2.31 | 0.46 |
| 14:CO:30:LEU:C | 14:CO:30:LEU:HD23 | 2.36 | 0.46 |
| 19:CT:42:ASP:OD1 | 19:CT:44:ALA:HB3 | 2.16 | 0.46 |
| 47:D0:9:ARG:O | 47:D0:12:ARG:HB3 | 2.15 | 0.46 |
| 49:D2:3:ARG:CZ | 49:D2:3:ARG:HA | 2.46 | 0.46 |
| 22:DA:16:G:O2' | 22:DA:17:C:H5' | 2.16 | 0.46 |
| 23:DB:1093:G:O2' | 23:DB:1094:U:H5' | 2.16 | 0.46 |
| 23:DB:1203:U:H3' | 23:DB:1204:A:H5'' | 1.98 | 0.46 |
| 23:DB:1717:A:H2' | 23:DB:1718:G:O4' | 2.16 | 0.46 |
| 23:DB:1849:G:H2' | 23:DB:1850:G:C8 | 2.50 | 0.46 |
| 23:DB:730:A:H3' | 56:DB:3612:HOH:O | 2.15 | 0.46 |
| 23:DB:60:G:C6 | 23:DB:74:A:N6 | 2.84 | 0.46 |
| 23:DB:852:U:H2' | 23:DB:853:C:C6 | 2.51 | 0.46 |
| 23:DB:878:A:C2' | 23:DB:878:A:N3 | 2.77 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:12:ARG:HA | 25:DC:15:VAL:CG2 | 2.46 | 0.46 |
| 27:DE:146:VAL:HA | 27:DE:185:LYS:O | 2.16 | 0.46 |
| 23:DB:558:U:OP1 | 31:DJ:113:PRO:HB2 | 2.16 | 0.46 |
| 31:DJ:128:ASN:O | 31:DJ:129:GLU:HB3 | 2.16 | 0.46 |
| 33:DL:118:THR:O | 33:DL:120:VAL:HG23 | 2.15 | 0.46 |
| 33:DL:17:LYS:O | 33:DL:18:ARG:HG2 | 2.16 | 0.46 |
| 35:DN:21:PHE:HA | 35:DN:24:MET:HB2 | 1.98 | 0.46 |
| 39:DR:31:GLU:O | 39:DR:63:VAL:HG22 | 2.16 | 0.46 |
| 39:DR:49:ILE:CG2 | 39:DR:54:VAL:HB | 2.45 | 0.46 |
| 40:DS:85:ILE:HD12 | 40:DS:85:ILE:N | 2.31 | 0.46 |
| 42:DU:64:ILE:HG13 | 42:DU:68:ASN:HD22 | 1.81 | 0.46 |
| 1:AA:572:A:N3 | 1:AA:917:G:H1' | 2.31 | 0.46 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.63 | 0.46 |
| 5:AF:43:GLY:HA2 | 5:AF:58:HIS:CD2 | 2.51 | 0.46 |
| 7:AH:82:LEU:O | 7:AH:82:LEU:HD13 | 2.16 | 0.46 |
| 9:AJ:6:ILE:HB | 9:AJ:76:ILE:HD11 | 1.98 | 0.46 |
| 11:AL:113:ARG:NE | 11:AL:120:ARG:HA | 2.30 | 0.46 |
| 14:AO:69:LEU:HD11 | 14:AO:76:ARG:CB | 2.46 | 0.46 |
| 22:BA:52:A:H3' | 22:BA:53:A:C8 | 2.51 | 0.46 |
| 23:BB:1401:G:H2' | 23:BB:1402:U:H6 | 1.80 | 0.46 |
| 23:BB:1417:C:O5' | 23:BB:1588:G:H1' | 2.16 | 0.46 |
| 23:BB:218:A:C2' | 23:BB:219:A:H5' | 2.46 | 0.46 |
| 23:BB:20:C:H2' | 23:BB:21:A:H8 | 1.80 | 0.46 |
| 23:BB:2332:C:H1' | 23:BB:2336:A:C8 | 2.50 | 0.46 |
| 23:BB:233:A:N6 | 23:BB:428:A:N6 | 2.62 | 0.46 |
| 23:BB:2768:U:H2' | 23:BB:2769:U:O4' | 2.16 | 0.46 |
| 23:BB:540:C:O2' | 23:BB:541:A:H5' | 2.16 | 0.46 |
| 23:BB:776:G:H4' | 23:BB:777:G:O5' | 2.16 | 0.46 |
| 26:BD:125:TRP:CE3 | 26:BD:125:TRP:HA | 2.51 | 0.46 |
| 28:BF:34:THR:CG2 | 28:BF:89:THR:HG22 | 2.44 | 0.46 |
| 30:BH:66:ASN:O | 30:BH:134:VAL:HG11 | 2.16 | 0.46 |
| 52:BI:29:GLN:HA | 52:BI:29:GLN:NE2 | 2.31 | 0.46 |
| 31:BJ:111:LYS:CB | 31:BJ:113:PRO:HD2 | 2.46 | 0.46 |
| 33:BL:133:ALA:HA | 33:BL:136:GLU:HB2 | 1.97 | 0.46 |
| 34:BM:108:VAL:HG22 | 34:BM:109:PRO:HD2 | 1.97 | 0.46 |
| 23:BB:534:U:O2' | 38:BQ:45:ALA:HA | 2.15 | 0.46 |
| 39:BR:80:ARG:O | 39:BR:81:LYS:HD3 | 2.15 | 0.46 |
| 40:BS:24:ILE:HD11 | 40:BS:36:LEU:HD21 | 1.97 | 0.46 |
| 1:CA:1096:C:H2' | 1:CA:1097:C:H6 | 1.81 | 0.46 |
| 1:CA:1285:A:HO2' | 1:CA:1286:U:P | 2.39 | 0.46 |
| 1:CA:1250:A:C2 | 1:CA:1370:G:H1' | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1495:U:O2' | 1:CA:1496:C:H5' | 2.16 | 0.46 |
| 1:CA:175:C:H2' | 1:CA:176:C:H6 | 1.78 | 0.46 |
| 1:CA:450:G:N7 | 1:CA:481:G:O6 | 2.49 | 0.46 |
| 1:CA:462:G:H5' | 1:CA:463:U:P | 2.55 | 0.46 |
| 1:CA:593:U:O2' | 1:CA:594:U:H5' | 2.16 | 0.46 |
| 1:CA:627:G:H2' | 1:CA:628:G:H8 | 1.81 | 0.46 |
| 1:CA:865:A:H2' | 1:CA:866:C:C6 | 2.51 | 0.46 |
| 3:CD:25:ARG:HD3 | 3:CD:26:ALA:HB3 | 1.97 | 0.46 |
| 3:CD:61:ARG:HG3 | 3:CD:71:PHE:CD2 | 2.51 | 0.46 |
| 5:CF:32:ALA:O | 5:CF:33:GLU:HB2 | 2.16 | 0.46 |
| 5:CF:3:HIS:CD2 | 5:CF:65:GLU:HG3 | 2.49 | 0.46 |
| 6:CG:129:ASN:HD22 | 6:CG:137:ARG:HH22 | 1.64 | 0.46 |
| 1:CA:642:A:C5 | 7:CH:106:SER:HA | 2.51 | 0.46 |
| 1:CA:970:C:H42 | 8:CI:128:LYS:HG2 | 1.79 | 0.46 |
| 10:CK:70:ALA:C | 10:CK:72:ALA:N | 2.69 | 0.46 |
| 12:CM:106:ARG:HD3 | 12:CM:111:PRO:HA | 1.97 | 0.46 |
| 12:CM:10:ASP:CA | 12:CM:44:ILE:HD13 | 2.42 | 0.46 |
| 13:CN:12:ARG:NE | 13:CN:58:ARG:HH12 | 2.14 | 0.46 |
| 19:CT:64:GLY:O | 19:CT:66:ILE:N | 2.48 | 0.46 |
| 23:DB:129:C:H2' | 23:DB:130:C:H6 | 1.81 | 0.46 |
| 23:DB:1506:U:H2' | 23:DB:1507:C:C6 | 2.51 | 0.46 |
| 23:DB:1523:U:H5'' | 23:DB:1524:G:C8 | 2.51 | 0.46 |
| 23:DB:1541:C:H2' | 23:DB:1542:U:H6 | 1.80 | 0.46 |
| 23:DB:1601:G:O2' | 23:DB:1602:U:H5' | 2.15 | 0.46 |
| 23:DB:1846:G:N2 | 23:DB:1848:A:N6 | 2.64 | 0.46 |
| 23:DB:1940:U:O2 | 23:DB:1940:U:H5'' | 2.16 | 0.46 |
| 23:DB:2386:A:N3 | 43:DW:38:ARG:HB3 | 2.30 | 0.46 |
| 23:DB:418:C:O2' | 23:DB:419:U:H5' | 2.16 | 0.46 |
| 23:DB:560:C:H2' | 23:DB:561:G:O4' | 2.16 | 0.46 |
| 28:DF:165:GLY:O | 28:DF:169:LEU:HD12 | 2.16 | 0.46 |
| 28:DF:1:ALA:O | 28:DF:4:HIS:HB3 | 2.16 | 0.46 |
| 29:DG:9:VAL:HA | 29:DG:48:THR:CG2 | 2.46 | 0.46 |
| 30:DH:119:ASN:ND2 | 30:DH:121:VAL:HG22 | 2.31 | 0.46 |
| 30:DH:9:VAL:HG11 | 30:DH:12:LEU:HG | 1.98 | 0.46 |
| 32:DK:99:ILE:HD13 | 32:DK:118:LEU:HD22 | 1.97 | 0.46 |
| 33:DL:29:LYS:C | 33:DL:31:GLY:H | 2.19 | 0.46 |
| 34:DM:68:PHE:CG | 34:DM:69:PRO:HD2 | 2.51 | 0.46 |
| 37:DP:19:PHE:CE2 | 37:DP:83:ILE:HD11 | 2.50 | 0.46 |
| 41:DT:55:VAL:HG13 | 41:DT:85:VAL:HG12 | 1.97 | 0.46 |
| 24:DV:48:MET:O | 24:DV:51:GLN:HG3 | 2.16 | 0.46 |
| 43:DW:18:LYS:HD2 | 43:DW:18:LYS:HA | 1.71 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:DW:32:ALA:O | 43:DW:34:SER:N | 2.48 | 0.46 |
| 43:DW:65:LYS:N | 43:DW:84:GLU:HB3 | 2.31 | 0.46 |
| 23:DB:1365:A:O3' | 46:DZ:11:ARG:NH1 | 2.49 | 0.46 |
| 46:DZ:70:GLU:C | 46:DZ:72:ARG:N | 2.69 | 0.46 |
| 1:AA:1130:A:H2' | 1:AA:1131:G:C8 | 2.51 | 0.45 |
| 1:AA:1226:C:H3' | 12:AM:101:THR:OG1 | 2.16 | 0.45 |
| 1:AA:1415:G:O2' | 1:AA:1416:G:H5' | 2.16 | 0.45 |
| 1:AA:213:G:H3' | 1:AA:214:C:H6 | 1.81 | 0.45 |
| 1:AA:25:C:H5' | 1:AA:524:G:H1' | 1.98 | 0.45 |
| 1:AA:571:U:O2 | 1:AA:918:A:H5' | 2.15 | 0.45 |
| 1:AA:89:U:H3' | 1:AA:90:C:C6 | 2.50 | 0.45 |
| 1:AA:936:C:H2' | 1:AA:937:A:O4' | 2.16 | 0.45 |
| 1:AA:960:U:H6 | 1:AA:1222:G:O2' | 1.99 | 0.45 |
| 4:AE:106:ALA:HB1 | 4:AE:110:MET:CB | 2.47 | 0.45 |
| 5:AF:12:PRO:C | 5:AF:14:GLN:H | 2.20 | 0.45 |
| 11:AL:24:GLU:HB2 | 11:AL:26:CYS:SG | 2.57 | 0.45 |
| 12:AM:2:ARG:N | 12:AM:2:ARG:HD3 | 2.30 | 0.45 |
| 12:AM:9:PRO:HB2 | 12:AM:17:ALA:HB1 | 1.97 | 0.45 |
| 14:AO:30:LEU:C | 14:AO:30:LEU:HD23 | 2.36 | 0.45 |
| 14:AO:39:GLN:HE22 | 23:BB:716:A:H1' | 1.81 | 0.45 |
| 48:B1:49:LYS:O | 48:B1:50:GLU:HB3 | 2.16 | 0.45 |
| 49:B2:3:ARG:HH21 | 49:B2:3:ARG:HG2 | 1.82 | 0.45 |
| 23:BB:990:A:H1' | 23:BB:1156:A:C2 | 2.51 | 0.45 |
| 23:BB:1258:U:H2' | 23:BB:1259:G:H8 | 1.81 | 0.45 |
| 23:BB:1534:U:H2' | 23:BB:1536:C:C5 | 2.51 | 0.45 |
| 23:BB:1545:A:H2' | 23:BB:1546:G:O4' | 2.15 | 0.45 |
| 23:BB:1845:G:O2' | 23:BB:1846:G:H5' | 2.16 | 0.45 |
| 25:BC:171:VAL:HG23 | 25:BC:185:ALA:HB2 | 1.97 | 0.45 |
| 28:BF:162:ASP:C | 28:BF:166:ARG:HH11 | 2.19 | 0.45 |
| 28:BF:115:GLY:HA3 | 28:BF:177:ARG:HB2 | 1.97 | 0.45 |
| 30:BH:68:ARG:HB2 | 30:BH:134:VAL:HB | 1.97 | 0.45 |
| 32:BK:61:VAL:HG11 | 32:BK:112:PHE:CE2 | 2.50 | 0.45 |
| 32:BK:75:SER:HA | 37:BP:72:VAL:O | 2.16 | 0.45 |
| 33:BL:120:VAL:O | 33:BL:135:ILE:HD11 | 2.16 | 0.45 |
| 35:BN:117:ASP:OD2 | 35:BN:117:ASP:C | 2.55 | 0.45 |
| 35:BN:12:ARG:HD2 | 35:BN:12:ARG:HA | 1.71 | 0.45 |
| 42:BU:40:LEU:HA | 42:BU:60:LYS:O | 2.15 | 0.45 |
| 46:BZ:35:SER:HA | 46:BZ:49:LEU:O | 2.16 | 0.45 |
| 46:BZ:65:ASP:O | 46:BZ:69:ALA:HB2 | 2.16 | 0.45 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:C6 | 2.51 | 0.45 |
| 1:CA:1278:G:H4' | 1:CA:1279:G:O4' | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1456:A:H2' | 1:CA:1457:G:O4' | 2.17 | 0.45 |
| 1:CA:292:G:O2' | 1:CA:609:A:N6 | 2.49 | 0.45 |
| 1:CA:373:A:H1' | 1:CA:481:G:H1' | 1.98 | 0.45 |
| 1:CA:821:G:O2' | 1:CA:822:U:H5' | 2.16 | 0.45 |
| 1:CA:940:C:H2' | 1:CA:941:G:C8 | 2.52 | 0.45 |
| 20:CB:151:LYS:HG3 | 20:CB:152:ASP:N | 2.31 | 0.45 |
| 20:CB:187:ASP:OD1 | 20:CB:203:ASP:HB3 | 2.16 | 0.45 |
| 20:CB:18:GLN:HB2 | 20:CB:188:THR:OG1 | 2.16 | 0.45 |
| 20:CB:71:THR:HG23 | 20:CB:94:ARG:H | 1.78 | 0.45 |
| 2:CC:63:ILE:O | 2:CC:65:VAL:HG23 | 2.16 | 0.45 |
| 4:CE:131:ASN:O | 4:CE:135:VAL:HG23 | 2.16 | 0.45 |
| 5:CF:52:ASN:O | 5:CF:52:ASN:CG | 2.54 | 0.45 |
| 10:CK:122:PRO:HG2 | 21:CU:34:ARG:HA | 1.97 | 0.45 |
| 10:CK:124:LYS:HA | 21:CU:34:ARG:CG | 2.46 | 0.45 |
| 11:CL:82:ARG:HG2 | 11:CL:82:ARG:NH1 | 2.29 | 0.45 |
| 12:CM:30:LYS:HG3 | 12:CM:40:GLU:OE1 | 2.16 | 0.45 |
| 13:CN:26:LEU:HD23 | 13:CN:27:LYS:N | 2.31 | 0.45 |
| 1:CA:255:G:H5' | 16:CQ:17:GLU:O | 2.16 | 0.45 |
| 21:CU:20:ARG:HG3 | 21:CU:24:LYS:HG3 | 1.99 | 0.45 |
| 21:CU:26:GLY:C | 21:CU:28:LEU:H | 2.18 | 0.45 |
| 23:DB:1100:C:H41 | 52:DI:1:ALA:N | 2.13 | 0.45 |
| 23:DB:1197:G:H2' | 23:DB:1198:U:C6 | 2.51 | 0.45 |
| 23:DB:1259:G:O2' | 23:DB:1260:A:H5' | 2.16 | 0.45 |
| 23:DB:2345:G:H4' | 23:DB:2346:A:O5' | 2.16 | 0.45 |
| 23:DB:2500:U:H5' | 23:DB:2501:C:OP2 | 2.16 | 0.45 |
| 23:DB:2547:A:H4' | 32:DK:29:HIS:CE1 | 2.51 | 0.45 |
| 23:DB:2553:G:H2' | 23:DB:2554:U:C4' | 2.46 | 0.45 |
| 23:DB:2580:U:H5' | 26:DD:136:ASN:H | 1.81 | 0.45 |
| 23:DB:2591:C:OP1 | 25:DC:237:ARG:HG3 | 2.16 | 0.45 |
| 23:DB:27:G:HO2' | 23:DB:28:A:H8 | 1.57 | 0.45 |
| 23:DB:571:U:O2' | 23:DB:573:U:O5' | 2.34 | 0.45 |
| 23:DB:935:C:H2' | 23:DB:936:A:H8 | 1.81 | 0.45 |
| 27:DE:141:MET:O | 27:DE:143:LEU:HG | 2.16 | 0.45 |
| 28:DF:31:GLU:HB2 | 28:DF:158:THR:HG22 | 1.98 | 0.45 |
| 28:DF:168:LEU:O | 28:DF:170:ALA:N | 2.49 | 0.45 |
| 28:DF:23:SER:O | 28:DF:26:GLN:HB2 | 2.16 | 0.45 |
| 28:DF:34:THR:OG1 | 28:DF:154:THR:HB | 2.16 | 0.45 |
| 28:DF:83:PRO:O | 28:DF:84:ILE:HD12 | 2.16 | 0.45 |
| 29:DG:102:ILE:HG13 | 29:DG:116:LEU:HD11 | 1.98 | 0.45 |
| 29:DG:10:VAL:CG2 | 29:DG:48:THR:HA | 2.46 | 0.45 |
| 23:DB:1060:U:H5 | 52:DI:131:THR:CG2 | 2.29 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:DI:72:THR:CG2 | 52:DI:112:LYS:HD2 | 2.46 | 0.45 |
| 31:DJ:43:GLU:O | 31:DJ:45:THR:HG22 | 2.16 | 0.45 |
| 32:DK:107:LEU:C | 32:DK:109:SER:H | 2.20 | 0.45 |
| 33:DL:131:ALA:O | 33:DL:134:ALA:HB3 | 2.16 | 0.45 |
| 35:DN:14:SER:O | 35:DN:18:GLN:HB2 | 2.15 | 0.45 |
| 35:DN:24:MET:CE | 35:DN:40:LYS:HB3 | 2.45 | 0.45 |
| 35:DN:29:VAL:HG21 | 35:DN:75:ILE:HB | 1.98 | 0.45 |
| 22:DA:7:G:H5'' | 36:DO:29:HIS:CD2 | 2.51 | 0.45 |
| 36:DO:39:VAL:HB | 36:DO:49:VAL:HG22 | 1.98 | 0.45 |
| 39:DR:60:LYS:H | 39:DR:100:GLY:N | 2.14 | 0.45 |
| 39:DR:43:ASN:CG | 39:DR:45:GLU:H | 2.18 | 0.45 |
| 39:DR:61:ALA:CB | 39:DR:98:ILE:H | 2.29 | 0.45 |
| 41:DT:61:LEU:HG | 41:DT:82:LYS:HB2 | 1.97 | 0.45 |
| 44:DX:39:GLN:HB2 | 44:DX:42:LEU:HD22 | 1.98 | 0.45 |
| 1:AA:1181:G:H1' | 1:AA:1182:G:C5 | 2.50 | 0.45 |
| 1:AA:1206:G:H4' | 2:AC:191:THR:O | 2.15 | 0.45 |
| 1:AA:1299:A:C2' | 1:AA:1301:U:H1' | 2.46 | 0.45 |
| 1:AA:245:U:H2' | 1:AA:246:A:H5' | 1.98 | 0.45 |
| 1:AA:328:C:H4' | 1:AA:329:A:C5' | 2.46 | 0.45 |
| 1:AA:54:C:H2' | 1:AA:352:C:H41 | 1.80 | 0.45 |
| 1:AA:562:U:H5'' | 1:AA:563:A:C4 | 2.51 | 0.45 |
| 1:AA:780:A:O2' | 1:AA:781:A:H5'' | 2.16 | 0.45 |
| 1:AA:833:G:O2' | 1:AA:834:U:H5' | 2.16 | 0.45 |
| 4:AE:19:ARG:O | 4:AE:20:VAL:HB | 2.16 | 0.45 |
| 5:AF:55:HIS:CD2 | 5:AF:56:LYS:HE3 | 2.51 | 0.45 |
| 10:AK:106:ILE:O | 10:AK:107:THR:HG23 | 2.17 | 0.45 |
| 10:AK:72:ALA:O | 10:AK:75:GLU:HG2 | 2.17 | 0.45 |
| 49:B2:4:THR:O | 49:B2:5:PHE:HB2 | 2.17 | 0.45 |
| 22:BA:74:U:H2' | 22:BA:75:G:O4' | 2.16 | 0.45 |
| 23:BB:1056:G:O5' | 23:BB:1056:G:H8 | 2.00 | 0.45 |
| 23:BB:1324:G:H1' | 23:BB:1616:A:C6 | 2.51 | 0.45 |
| 23:BB:1387:A:H2' | 23:BB:1388:G:C8 | 2.51 | 0.45 |
| 23:BB:1465:G:H2' | 23:BB:1466:U:C6 | 2.50 | 0.45 |
| 23:BB:1541:C:H2' | 23:BB:1542:U:C6 | 2.51 | 0.45 |
| 23:BB:1541:C:H2' | 23:BB:1542:U:H6 | 1.81 | 0.45 |
| 23:BB:1970:A:H1' | 23:BB:1972:G:C8 | 2.51 | 0.45 |
| 23:BB:830:G:H1 | 23:BB:2446:G:C4' | 2.29 | 0.45 |
| 23:BB:2892:G:H5'' | 23:BB:2894:G:N2 | 2.31 | 0.45 |
| 23:BB:322:A:H2' | 27:BE:163:ASN:OD1 | 2.15 | 0.45 |
| 23:BB:418:C:O2' | 23:BB:419:U:H5' | 2.16 | 0.45 |
| 23:BB:586:A:H5' | 27:BE:84:THR:OG1 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:83:A:H5'' | 42:BU:1:ALA:H2 | 1.80 | 0.45 |
| 23:BB:862:G:H2' | 23:BB:863:A:O4' | 2.16 | 0.45 |
| 23:BB:2227:A:H5'' | 25:BC:260:LYS:HD2 | 1.98 | 0.45 |
| 26:BD:118:PHE:O | 26:BD:119:ALA:CB | 2.62 | 0.45 |
| 27:BE:141:MET:O | 27:BE:143:LEU:HG | 2.16 | 0.45 |
| 28:BF:147:ARG:HD2 | 28:BF:148:VAL:HG22 | 1.97 | 0.45 |
| 28:BF:19:PHE:HE1 | 28:BF:167:ALA:HB2 | 1.81 | 0.45 |
| 23:BB:1061:U:O4 | 52:BI:10:LEU:HA | 2.16 | 0.45 |
| 31:BJ:11:VAL:HG21 | 31:BJ:13:ARG:NH1 | 2.32 | 0.45 |
| 32:BK:99:ILE:HG12 | 32:BK:115:ILE:HG13 | 1.99 | 0.45 |
| 32:BK:86:LEU:H | 32:BK:86:LEU:CD2 | 2.20 | 0.45 |
| 32:BK:88:ASN:ND2 | 32:BK:89:ASN:N | 2.64 | 0.45 |
| 33:BL:80:SER:HB3 | 33:BL:115:GLU:CD | 2.37 | 0.45 |
| 33:BL:54:GLN:O | 33:BL:56:PRO:HD3 | 2.16 | 0.45 |
| 23:BB:2840:C:H5'' | 35:BN:53:THR:HG21 | 1.97 | 0.45 |
| 36:BO:51:ALA:CB | 36:BO:81:ARG:HH11 | 2.29 | 0.45 |
| 38:BQ:26:ALA:HA | 38:BQ:29:ARG:CG | 2.45 | 0.45 |
| 23:BB:1249:U:C4' | 38:BQ:3:VAL:HG21 | 2.46 | 0.45 |
| 39:BR:49:ILE:CG2 | 39:BR:54:VAL:HB | 2.47 | 0.45 |
| 39:BR:79:ARG:NE | 39:BR:80:ARG:NH2 | 2.64 | 0.45 |
| 40:BS:47:VAL:HG12 | 40:BS:103:ILE:HG21 | 1.98 | 0.45 |
| 42:BU:38:ILE:HG13 | 42:BU:39:ASN:N | 2.31 | 0.45 |
| 24:BV:61:LEU:O | 24:BV:71:LYS:HA | 2.16 | 0.45 |
| 43:BW:9:THR:HG23 | 43:BW:10:ARG:CD | 2.36 | 0.45 |
| 46:BZ:32:ASN:O | 46:BZ:33:LEU:O | 2.34 | 0.45 |
| 1:CA:1163:A:H2' | 1:CA:1164:G:C8 | 2.52 | 0.45 |
| 1:CA:1451:U:O3' | 1:CA:1452:C:H6 | 2.00 | 0.45 |
| 1:CA:545:C:H2' | 1:CA:546:A:C8 | 2.51 | 0.45 |
| 1:CA:677:U:H3 | 1:CA:713:G:H22 | 1.62 | 0.45 |
| 1:CA:79:G:O2' | 1:CA:80:A:H5' | 2.16 | 0.45 |
| 1:CA:81:A:C2' | 1:CA:82:G:H5' | 2.46 | 0.45 |
| 1:CA:847:G:H2' | 1:CA:848:C:H6 | 1.81 | 0.45 |
| 1:CA:574:A:H1' | 1:CA:883:C:O4' | 2.16 | 0.45 |
| 1:CA:922:G:H2' | 1:CA:923:A:C8 | 2.50 | 0.45 |
| 20:CB:172:ILE:CG2 | 20:CB:176:ASN:HD21 | 2.28 | 0.45 |
| 6:CG:120:ALA:O | 6:CG:123:LEU:HB2 | 2.16 | 0.45 |
| 6:CG:137:ARG:HG2 | 6:CG:141:HIS:NE2 | 2.31 | 0.45 |
| 7:CH:23:ALA:CB | 7:CH:61:THR:HA | 2.46 | 0.45 |
| 7:CH:94:VAL:HG12 | 7:CH:99:GLY:HA3 | 1.98 | 0.45 |
| 8:CI:56:MET:HA | 8:CI:59:LYS:HB2 | 1.97 | 0.45 |
| 8:CI:87:MET:HA | 8:CI:90:ASP:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CI:9:GLY:HA2 | 8:CI:80:HIS:CD2 | 2.51 | 0.45 |
| 11:CL:66:ILE:CG2 | 11:CL:71:HIS:HB3 | 2.44 | 0.45 |
| 16:CQ:18:LYS:HG2 | 16:CQ:48:GLU:O | 2.16 | 0.45 |
| 22:DA:42:C:C4 | 28:DF:65:LEU:HD22 | 2.51 | 0.45 |
| 22:DA:60:C:O2' | 22:DA:61:G:H5' | 2.17 | 0.45 |
| 23:DB:1052:C:O2' | 23:DB:1053:C:H5' | 2.16 | 0.45 |
| 23:DB:1283:G:H22 | 23:DB:1286:A:C5' | 2.13 | 0.45 |
| 23:DB:1463:C:H2' | 23:DB:1464:G:C8 | 2.51 | 0.45 |
| 23:DB:1544:A:H2' | 23:DB:1545:A:C8 | 2.51 | 0.45 |
| 23:DB:1547:C:H2' | 23:DB:1548:A:H8 | 1.81 | 0.45 |
| 23:DB:1687:G:O2' | 23:DB:1688:U:H5' | 2.15 | 0.45 |
| 23:DB:1915:U:H2' | 23:DB:1916:A:C8 | 2.52 | 0.45 |
| 23:DB:244:A:H1' | 23:DB:255:A:N6 | 2.31 | 0.45 |
| 23:DB:434:U:H1' | 23:DB:435:C:H5 | 1.81 | 0.45 |
| 23:DB:858:G:H21 | 23:DB:2268:A:C3' | 2.29 | 0.45 |
| 23:DB:988:A:H3' | 45:DY:13:ILE:HD11 | 1.97 | 0.45 |
| 25:DC:107:LYS:O | 25:DC:109:LEU:HD22 | 2.17 | 0.45 |
| 28:DF:98:PHE:C | 28:DF:100:GLU:N | 2.69 | 0.45 |
| 29:DG:33:THR:HG21 | 29:DG:74:MET:HB3 | 1.98 | 0.45 |
| 52:DI:46:ASP:HA | 52:DI:50:LYS:HE2 | 1.97 | 0.45 |
| 31:DJ:20:ALA:CB | 31:DJ:23:LYS:HB2 | 2.45 | 0.45 |
| 32:DK:2:ILE:HD12 | 32:DK:2:ILE:N | 2.31 | 0.45 |
| 33:DL:78:ARG:NH2 | 33:DL:113:ALA:HB1 | 2.30 | 0.45 |
| 35:DN:73:ASN:O | 35:DN:76:VAL:HG22 | 2.17 | 0.45 |
| 41:DT:62:VAL:HG12 | 41:DT:63:VAL:H | 1.82 | 0.45 |
| 42:DU:95:PHE:HE1 | 42:DU:102:ILE:HB | 1.81 | 0.45 |
| 23:DB:98:G:H1 | 42:DU:6:ARG:HH12 | 1.64 | 0.45 |
| 24:DV:77:VAL:HG23 | 24:DV:89:ILE:CG2 | 2.47 | 0.45 |
| 46:DZ:68:LEU:HD22 | 46:DZ:78:TYR:CE1 | 2.52 | 0.45 |
| 1:AA:1004:A:H2' | 1:AA:1005:A:O4' | 2.16 | 0.45 |
| 1:AA:1261:A:H1' | 1:AA:1275:A:N1 | 2.31 | 0.45 |
| 1:AA:14:U:H5'' | 56:AA:2180:HOH:O | 2.16 | 0.45 |
| 1:AA:254:G:O2' | 1:AA:255:G:H5' | 2.15 | 0.45 |
| 1:AA:754:C:H3' | 1:AA:754:C:O2 | 2.16 | 0.45 |
| 1:AA:908:A:H2' | 1:AA:909:A:C8 | 2.51 | 0.45 |
| 20:AB:209:VAL:HG23 | 20:AB:210:THR:N | 2.28 | 0.45 |
| 1:AA:9:G:H5' | 4:AE:107:GLY:HA3 | 1.98 | 0.45 |
| 5:AF:97:THR:HG22 | 5:AF:98:GLU:N | 2.31 | 0.45 |
| 7:AH:12:ARG:NH1 | 7:AH:26:MET:HB3 | 2.31 | 0.45 |
| 8:AI:52:GLU:O | 8:AI:53:LEU:HD13 | 2.16 | 0.45 |
| 10:AK:19:VAL:HG22 | 10:AK:34:THR:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:AQ:18:LYS:HG2 | 16:AQ:48:GLU:O | 2.17 | 0.45 |
| 19:AT:35:TYR:CG | 19:AT:36:ALA:N | 2.84 | 0.45 |
| 49:B2:34:ARG:NE | 49:B2:39:ARG:HG2 | 2.30 | 0.45 |
| 22:BA:30:C:H1' | 22:BA:58:A:N1 | 2.32 | 0.45 |
| 22:BA:95:U:H2' | 22:BA:96:G:H8 | 1.79 | 0.45 |
| 23:BB:1025:G:H8 | 23:BB:1025:G:OP1 | 1.98 | 0.45 |
| 23:BB:1252:G:O3' | 38:BQ:32:ARG:NH1 | 2.50 | 0.45 |
| 23:BB:1488:C:O2' | 23:BB:1489:C:H5' | 2.17 | 0.45 |
| 23:BB:1601:G:O2' | 23:BB:1602:U:H5' | 2.17 | 0.45 |
| 23:BB:2199:A:H3' | 23:BB:2200:C:C6 | 2.51 | 0.45 |
| 23:BB:2221:G:O2' | 23:BB:2222:C:H5' | 2.15 | 0.45 |
| 23:BB:2411:A:H2' | 23:BB:2412:A:H8 | 1.81 | 0.45 |
| 23:BB:2674:G:H2' | 23:BB:2675:A:H8 | 1.81 | 0.45 |
| 23:BB:2729:G:H1' | 26:BD:192:ALA:HB3 | 1.98 | 0.45 |
| 23:BB:2751:G:N3 | 23:BB:2751:G:C2' | 2.76 | 0.45 |
| 23:BB:275:C:C2' | 23:BB:276:U:H5' | 2.46 | 0.45 |
| 23:BB:345:A:H1' | 23:BB:346:A:H2 | 1.80 | 0.45 |
| 23:BB:545:U:H6 | 23:BB:545:U:O5' | 2.00 | 0.45 |
| 23:BB:545:U:H2' | 23:BB:547:A:P | 2.57 | 0.45 |
| 23:BB:584:C:N4 | 23:BB:585:G:C6 | 2.84 | 0.45 |
| 23:BB:643:A:C4 | 48:B1:43:ARG:HD2 | 2.50 | 0.45 |
| 23:BB:921:C:H2' | 23:BB:922:C:C6 | 2.51 | 0.45 |
| 25:BC:140:VAL:CG2 | 25:BC:163:ILE:HG12 | 2.46 | 0.45 |
| 25:BC:165:ALA:HB3 | 25:BC:172:THR:HG23 | 1.99 | 0.45 |
| 26:BD:26:VAL:HG13 | 26:BD:188:LEU:CD2 | 2.46 | 0.45 |
| 27:BE:150:THR:O | 27:BE:192:ALA:HB2 | 2.17 | 0.45 |
| 27:BE:91:ASP:C | 27:BE:93:SER:H | 2.19 | 0.45 |
| 28:BF:103:ILE:HD11 | 28:BF:174:PHE:CD1 | 2.51 | 0.45 |
| 28:BF:34:THR:OG1 | 28:BF:154:THR:HB | 2.15 | 0.45 |
| 30:BH:127:GLU:HG3 | 30:BH:143:ILE:CB | 2.39 | 0.45 |
| 52:BI:135:MET:HG3 | 52:BI:137:LEU:HG | 1.98 | 0.45 |
| 52:BI:62:ALA:C | 52:BI:64:ARG:H | 2.20 | 0.45 |
| 36:BO:111:ARG:HG2 | 36:BO:117:PHE:CE2 | 2.50 | 0.45 |
| 37:BP:56:SER:HB2 | 37:BP:75:THR:HB | 1.98 | 0.45 |
| 39:BR:21:ARG:C | 39:BR:22:LEU:HD23 | 2.36 | 0.45 |
| 39:BR:95:ASP:O | 39:BR:96:VAL:HG13 | 2.16 | 0.45 |
| 42:BU:26:ASN:ND2 | 42:BU:34:ILE:HD12 | 2.23 | 0.45 |
| 42:BU:90:LYS:O | 42:BU:92:VAL:HG23 | 2.16 | 0.45 |
| 24:BV:16:ALA:HA | 24:BV:19:ARG:HH21 | 1.82 | 0.45 |
| 23:BB:855:G:N3 | 43:BW:23:LYS:HE3 | 2.31 | 0.45 |
| 1:CA:1024:G:H2' | 1:CA:1025:U:C6 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1305:G:H22 | 1:CA:1331:G:H2' | 1.81 | 0.45 |
| 1:CA:1480:A:O2' | 1:CA:1481:U:H5' | 2.17 | 0.45 |
| 1:CA:889:A:N1 | 1:CA:907:A:H5'' | 2.32 | 0.45 |
| 3:CD:7:LYS:HB3 | 3:CD:20:LEU:HB3 | 1.97 | 0.45 |
| 5:CF:18:VAL:N | 5:CF:19:PRO:HD2 | 2.31 | 0.45 |
| 8:CI:20:ILE:HD13 | 8:CI:85:ALA:HB3 | 1.99 | 0.45 |
| 11:CL:15:VAL:O | 11:CL:16:ALA:C | 2.54 | 0.45 |
| 18:CS:42:ASN:N | 18:CS:42:ASN:ND2 | 2.62 | 0.45 |
| 18:CS:4:LEU:HD11 | 18:CS:9:PHE:HB3 | 1.97 | 0.45 |
| 21:CU:25:ALA:O | 21:CU:27:VAL:N | 2.49 | 0.45 |
| 51:D4:3:VAL:HB | 51:D4:37:GLN:HE22 | 1.81 | 0.45 |
| 22:DA:76:G:H1 | 22:DA:101:A:N6 | 2.15 | 0.45 |
| 22:DA:27:C:C2' | 22:DA:28:C:H5' | 2.46 | 0.45 |
| 22:DA:32:U:H2' | 22:DA:33:G:C8 | 2.51 | 0.45 |
| 23:DB:1596:A:O2' | 23:DB:1597:A:H5' | 2.17 | 0.45 |
| 23:DB:160:A:H1' | 23:DB:2208:C:O2' | 2.17 | 0.45 |
| 23:DB:1708:C:O2' | 23:DB:1709:U:H5' | 2.17 | 0.45 |
| 23:DB:2256:G:O2' | 23:DB:2257:U:H5' | 2.16 | 0.45 |
| 23:DB:2452:C:C4 | 23:DB:2453:A:C6 | 3.04 | 0.45 |
| 23:DB:2496:C:H2' | 23:DB:2497:A:H5' | 1.98 | 0.45 |
| 23:DB:2548:U:H1' | 32:DK:23:LYS:HZ2 | 1.80 | 0.45 |
| 23:DB:256:A:H2' | 23:DB:257:C:H6 | 1.81 | 0.45 |
| 23:DB:55:G:H2' | 23:DB:56:A:H8 | 1.81 | 0.45 |
| 23:DB:717:C:C3' | 23:DB:718:A:H5'' | 2.46 | 0.45 |
| 23:DB:765:C:H2' | 23:DB:766:U:C6 | 2.51 | 0.45 |
| 23:DB:769:U:H2' | 23:DB:770:G:C8 | 2.51 | 0.45 |
| 26:DD:3:GLY:HA2 | 26:DD:101:PHE:CZ | 2.52 | 0.45 |
| 26:DD:51:THR:HG22 | 26:DD:52:THR:N | 2.27 | 0.45 |
| 28:DF:135:ILE:HG13 | 28:DF:137:PHE:H | 1.81 | 0.45 |
| 29:DG:88:LEU:HD13 | 29:DG:93:TYR:HB3 | 1.97 | 0.45 |
| 52:DI:138:VAL:HG12 | 52:DI:139:VAL:N | 2.32 | 0.45 |
| 52:DI:52:LEU:HD13 | 52:DI:81:LYS:NZ | 2.31 | 0.45 |
| 31:DJ:35:ARG:HA | 31:DJ:40:HIS:NE2 | 2.32 | 0.45 |
| 35:DN:114:GLU:HG2 | 35:DN:115:LEU:N | 2.32 | 0.45 |
| 36:DO:68:LYS:H | 36:DO:102:ARG:CD | 2.30 | 0.45 |
| 36:DO:51:ALA:HB3 | 36:DO:78:VAL:HG13 | 1.97 | 0.45 |
| 39:DR:22:LEU:HD12 | 39:DR:25:LEU:HD23 | 1.97 | 0.45 |
| 39:DR:43:ASN:HD21 | 39:DR:45:GLU:HG2 | 1.81 | 0.45 |
| 46:DZ:77:LYS:HG3 | 46:DZ:78:TYR:H | 1.81 | 0.45 |
| 46:DZ:68:LEU:HD22 | 46:DZ:78:TYR:HE1 | 1.80 | 0.45 |
| 1:AA:1007:U:H2' | 1:AA:1008:U:H6 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1060:U:H2' | 1:AA:1061:G:C8 | 2.51 | 0.45 |
| 1:AA:1096:C:H2' | 1:AA:1097:C:H6 | 1.81 | 0.45 |
| 1:AA:1122:U:H2' | 1:AA:1123:U:C6 | 2.51 | 0.45 |
| 1:AA:1127:G:C2' | 1:AA:1128:C:H5' | 2.46 | 0.45 |
| 1:AA:202:G:H2' | 1:AA:203:G:C8 | 2.51 | 0.45 |
| 1:AA:255:G:H5' | 16:AQ:17:GLU:O | 2.16 | 0.45 |
| 1:AA:373:A:H1' | 1:AA:481:G:H1' | 1.98 | 0.45 |
| 1:AA:634:C:H2' | 1:AA:635:A:C8 | 2.51 | 0.45 |
| 1:AA:85:U:H4' | 1:AA:86:G:OP1 | 2.16 | 0.45 |
| 1:AA:993:G:H21 | 1:AA:996:A:N6 | 2.14 | 0.45 |
| 2:AC:134:LYS:HA | 2:AC:167:TYR:HE2 | 1.82 | 0.45 |
| 2:AC:6:PRO:HB3 | 2:AC:174:LEU:HD21 | 1.99 | 0.45 |
| 6:AG:59:GLU:O | 6:AG:63:VAL:HG23 | 2.17 | 0.45 |
| 7:AH:11:THR:HG22 | 7:AH:14:ARG:NH2 | 2.30 | 0.45 |
| 7:AH:23:ALA:CB | 7:AH:61:THR:HA | 2.46 | 0.45 |
| 8:AI:29:ILE:HG23 | 8:AI:64:ILE:HB | 1.98 | 0.45 |
| 8:AI:30:ASN:HD22 | 8:AI:65:THR:HA | 1.82 | 0.45 |
| 13:AN:5:MET:SD | 13:AN:8:ARG:HD3 | 2.56 | 0.45 |
| 50:B3:15:LYS:HA | 50:B3:21:PHE:HA | 1.97 | 0.45 |
| 23:BB:137:U:H3' | 23:BB:138:U:C6 | 2.51 | 0.45 |
| 23:BB:1432:G:H2' | 23:BB:1433:A:C8 | 2.52 | 0.45 |
| 23:BB:1475:G:OP1 | 23:BB:1475:G:H3' | 2.17 | 0.45 |
| 23:BB:1484:U:H2' | 23:BB:1485:U:H6 | 1.80 | 0.45 |
| 23:BB:1734:G:O2' | 23:BB:1735:A:H5' | 2.16 | 0.45 |
| 23:BB:1846:G:N2 | 23:BB:1848:A:N6 | 2.63 | 0.45 |
| 23:BB:437:U:H2' | 23:BB:438:G:C8 | 2.51 | 0.45 |
| 23:BB:643:A:H1' | 48:B1:43:ARG:HH21 | 1.82 | 0.45 |
| 23:BB:1657:U:O2' | 26:BD:138:LEU:HD12 | 2.16 | 0.45 |
| 30:BH:112:LYS:HE3 | 30:BH:112:LYS:O | 2.16 | 0.45 |
| 37:BP:54:LEU:HA | 37:BP:76:HIS:HD2 | 1.81 | 0.45 |
| 38:BQ:89:ILE:C | 38:BQ:91:ARG:H | 2.19 | 0.45 |
| 41:BT:2:ILE:HG13 | 41:BT:3:ARG:CZ | 2.47 | 0.45 |
| 41:BT:67:VAL:HG22 | 41:BT:74:ILE:HD11 | 1.99 | 0.45 |
| 1:CA:1122:U:H2' | 1:CA:1123:U:C6 | 2.52 | 0.45 |
| 1:CA:1296:C:H4' | 1:CA:1302:C:H42 | 1.82 | 0.45 |
| 1:CA:174:A:O2' | 1:CA:175:C:H5' | 2.17 | 0.45 |
| 1:CA:189:A:O2' | 1:CA:190:A:H5' | 2.16 | 0.45 |
| 1:CA:255:G:P | 16:CQ:70:LYS:HZ3 | 2.40 | 0.45 |
| 1:CA:833:G:O2' | 1:CA:834:U:H5' | 2.17 | 0.45 |
| 4:CE:21:SER:CB | 4:CE:28:ARG:HE | 2.20 | 0.45 |
| 5:CF:18:VAL:O | 5:CF:22:ILE:HG13 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CF:45:ARG:NH2 | 17:CR:25:ILE:HD13 | 2.31 | 0.45 |
| 8:CI:10:ARG:CB | 8:CI:15:ALA:HA | 2.46 | 0.45 |
| 11:CL:31:GLY:HA3 | 11:CL:54:VAL:HG11 | 1.97 | 0.45 |
| 18:CS:52:ASN:HB2 | 18:CS:76:THR:HG22 | 1.98 | 0.45 |
| 51:D4:17:VAL:HG11 | 51:D4:19:ARG:HE | 1.80 | 0.45 |
| 23:DB:2236:U:O2' | 23:DB:2237:G:H5' | 2.16 | 0.45 |
| 23:DB:2725:A:HO2' | 23:DB:2726:A:P | 2.39 | 0.45 |
| 23:DB:465:G:H4' | 49:D2:16:HIS:CD2 | 2.51 | 0.45 |
| 23:DB:566:U:H2' | 23:DB:567:U:O4' | 2.17 | 0.45 |
| 23:DB:56:A:H2' | 23:DB:57:C:C6 | 2.50 | 0.45 |
| 23:DB:813:U:H2' | 23:DB:814:C:C6 | 2.52 | 0.45 |
| 23:DB:902:C:H2' | 23:DB:903:C:C6 | 2.51 | 0.45 |
| 25:DC:264:LYS:HG3 | 25:DC:265:PHE:HD2 | 1.81 | 0.45 |
| 26:DD:10:GLY:HA3 | 26:DD:26:VAL:H | 1.82 | 0.45 |
| 27:DE:187:VAL:HG12 | 27:DE:188:MET:N | 2.31 | 0.45 |
| 28:DF:65:LEU:O | 28:DF:86:CYS:HA | 2.16 | 0.45 |
| 29:DG:132:LEU:HD12 | 29:DG:140:ILE:HG22 | 1.98 | 0.45 |
| 29:DG:23:ILE:HG22 | 29:DG:25:ILE:HD11 | 1.99 | 0.45 |
| 29:DG:66:THR:O | 29:DG:70:LEU:HB2 | 2.16 | 0.45 |
| 30:DH:116:ARG:HB2 | 30:DH:131:SER:OG | 2.16 | 0.45 |
| 23:DB:1059:G:N2 | 52:DI:130:GLY:HA3 | 2.31 | 0.45 |
| 31:DJ:74:TYR:HE2 | 31:DJ:103:ILE:HD11 | 1.81 | 0.45 |
| 33:DL:99:ASN:HA | 56:DL:201:HOH:O | 2.15 | 0.45 |
| 23:DB:2820:A:OP1 | 35:DN:4:ARG:HA | 2.16 | 0.45 |
| 35:DN:83:LEU:O | 35:DN:86:ARG:HB2 | 2.17 | 0.45 |
| 41:DT:12:ARG:HG2 | 44:DX:29:ARG:HH12 | 1.81 | 0.45 |
| 24:DV:19:ARG:O | 24:DV:22:ALA:HB3 | 2.15 | 0.45 |
| 44:DX:23:ARG:HD2 | 44:DX:27:ASN:ND2 | 2.28 | 0.45 |
| 1:AA:1040:U:H2' | 1:AA:1041:G:O4' | 2.16 | 0.45 |
| 1:AA:1085:U:H3' | 1:AA:1086:U:C6 | 2.52 | 0.45 |
| 1:AA:1096:C:H2' | 1:AA:1097:C:C6 | 2.51 | 0.45 |
| 1:AA:175:C:H2' | 1:AA:176:C:C6 | 2.51 | 0.45 |
| 1:AA:227:G:H2' | 1:AA:228:A:C8 | 2.51 | 0.45 |
| 20:AB:120:SER:HA | 20:AB:125:PHE:CB | 2.47 | 0.45 |
| 1:AA:1057:G:H5'' | 2:AC:153:SER:CB | 2.46 | 0.45 |
| 5:AF:52:ASN:O | 5:AF:52:ASN:CG | 2.55 | 0.45 |
| 5:AF:8:PHE:O | 5:AF:60:VAL:HG23 | 2.16 | 0.45 |
| 10:AK:65:ALA:O | 10:AK:68:ARG:HB3 | 2.16 | 0.45 |
| 11:AL:105:GLY:HA3 | 11:AL:117:GLY:O | 2.17 | 0.45 |
| 12:AM:100:ARG:HD3 | 12:AM:103:THR:OG1 | 2.16 | 0.45 |
| 47:B0:41:HIS:N | 47:B0:41:HIS:CD2 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1072:C:N3 | 23:BB:1092:C:N4 | 2.64 | 0.45 |
| 23:BB:1171:G:H2' | 23:BB:1172:C:H6 | 1.80 | 0.45 |
| 23:BB:1173:U:H1' | 23:BB:1177:G:C2 | 2.52 | 0.45 |
| 23:BB:1472:C:H2' | 23:BB:1473:G:C8 | 2.52 | 0.45 |
| 23:BB:1668:A:N3 | 23:BB:1670:C:C4 | 2.85 | 0.45 |
| 23:BB:1877:A:H2' | 23:BB:1878:G:C8 | 2.51 | 0.45 |
| 23:BB:2148:G:H3' | 23:BB:2149:U:C6 | 2.51 | 0.45 |
| 23:BB:2236:U:O2' | 23:BB:2237:G:H5' | 2.16 | 0.45 |
| 23:BB:2284:A:OP2 | 48:B1:5:ARG:HG3 | 2.15 | 0.45 |
| 23:BB:2594:C:O2' | 23:BB:2595:G:H5' | 2.17 | 0.45 |
| 23:BB:2648:G:H2' | 23:BB:2649:C:H6 | 1.81 | 0.45 |
| 23:BB:279:A:H2' | 23:BB:280:U:C5' | 2.46 | 0.45 |
| 23:BB:43:G:H2' | 23:BB:44:A:O4' | 2.16 | 0.45 |
| 23:BB:592:A:H2' | 23:BB:593:U:H6 | 1.81 | 0.45 |
| 23:BB:611:C:H2' | 23:BB:612:G:O4' | 2.17 | 0.45 |
| 23:BB:77:G:O2' | 23:BB:78:U:H5' | 2.16 | 0.45 |
| 25:BC:264:LYS:HG3 | 25:BC:265:PHE:CD2 | 2.52 | 0.45 |
| 26:BD:33:ARG:NH1 | 26:BD:53:GLY:O | 2.49 | 0.45 |
| 27:BE:116:ASP:O | 27:BE:119:ILE:HD11 | 2.16 | 0.45 |
| 27:BE:4:VAL:HA | 27:BE:11:ALA:HA | 1.99 | 0.45 |
| 28:BF:111:ARG:N | 28:BF:111:ARG:CD | 2.80 | 0.45 |
| 28:BF:109:ARG:HB3 | 28:BF:135:ILE:HD12 | 1.99 | 0.45 |
| 29:BG:11:PRO:O | 29:BG:14:VAL:HG22 | 2.16 | 0.45 |
| 30:BH:14:SER:C | 30:BH:16:GLY:H | 2.20 | 0.45 |
| 30:BH:68:ARG:C | 30:BH:134:VAL:HB | 2.36 | 0.45 |
| 32:BK:107:LEU:C | 32:BK:109:SER:H | 2.20 | 0.45 |
| 32:BK:87:LEU:HB2 | 32:BK:93:GLN:C | 2.35 | 0.45 |
| 33:BL:135:ILE:HG12 | 33:BL:140:GLY:HA2 | 1.99 | 0.45 |
| 34:BM:26:VAL:HG22 | 34:BM:133:LYS:HA | 1.98 | 0.45 |
| 36:BO:51:ALA:HB3 | 36:BO:78:VAL:HG13 | 1.98 | 0.45 |
| 37:BP:50:ARG:CB | 37:BP:56:SER:HB3 | 2.45 | 0.45 |
| 38:BQ:33:VAL:HG23 | 38:BQ:34:ALA:N | 2.31 | 0.45 |
| 41:BT:48:GLN:NE2 | 41:BT:48:GLN:HA | 2.30 | 0.45 |
| 42:BU:89:GLY:O | 42:BU:90:LYS:HG3 | 2.16 | 0.45 |
| 43:BW:19:ARG:CD | 43:BW:19:ARG:H | 2.30 | 0.45 |
| 43:BW:45:HIS:N | 43:BW:45:HIS:ND1 | 2.64 | 0.45 |
| 1:CA:109:A:H4' | 1:CA:110:C:OP2 | 2.16 | 0.45 |
| 1:CA:112:G:O2' | 1:CA:113:G:H5' | 2.17 | 0.45 |
| 1:CA:1225:A:H3' | 1:CA:1226:C:C6 | 2.52 | 0.45 |
| 1:CA:1260:G:OP1 | 1:CA:1284:C:H4' | 2.17 | 0.45 |
| 1:CA:1392:G:H2' | 1:CA:1393:U:C6 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1432:G:H5' | 37:DP:105:LYS:CG | 2.45 | 0.45 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C6 | 2.52 | 0.45 |
| 1:CA:323:U:H2' | 1:CA:324:G:O4' | 2.16 | 0.45 |
| 1:CA:53:A:C2 | 1:CA:54:C:H1' | 2.50 | 0.45 |
| 3:CD:97:LEU:HD13 | 3:CD:136:VAL:HG11 | 1.98 | 0.45 |
| 4:CE:19:ARG:O | 4:CE:20:VAL:HB | 2.16 | 0.45 |
| 8:CI:29:ILE:HG23 | 8:CI:64:ILE:HB | 1.97 | 0.45 |
| 9:CJ:80:THR:HB | 9:CJ:83:THR:OG1 | 2.16 | 0.45 |
| 9:CJ:6:ILE:O | 9:CJ:8:ILE:HD12 | 2.16 | 0.45 |
| 12:CM:64:VAL:HA | 12:CM:68:LEU:CD1 | 2.43 | 0.45 |
| 13:CN:20:PHE:CD2 | 13:CN:55:SER:HA | 2.52 | 0.45 |
| 13:CN:30:ILE:CG2 | 13:CN:41:TRP:HB2 | 2.45 | 0.45 |
| 18:CS:40:PHE:HB2 | 18:CS:43:MET:CE | 2.47 | 0.45 |
| 50:D3:61:LEU:N | 50:D3:62:PRO:HD3 | 2.32 | 0.45 |
| 23:DB:121:G:H2' | 23:DB:122:G:H8 | 1.81 | 0.45 |
| 23:DB:1432:G:O2' | 23:DB:1433:A:H5' | 2.17 | 0.45 |
| 23:DB:2261:C:O2' | 23:DB:2262:U:H5' | 2.17 | 0.45 |
| 23:DB:2306:C:C5 | 23:DB:2307:G:H2' | 2.52 | 0.45 |
| 23:DB:2655:G:N2 | 23:DB:2664:G:H2' | 2.32 | 0.45 |
| 23:DB:274:C:O5' | 23:DB:274:C:H6 | 2.00 | 0.45 |
| 23:DB:277:G:H4' | 23:DB:278:A:C6 | 2.51 | 0.45 |
| 23:DB:942:G:H2' | 23:DB:943:A:O4' | 2.16 | 0.45 |
| 25:DC:129:LEU:HD21 | 25:DC:133:ASN:HB2 | 1.99 | 0.45 |
| 27:DE:149:ILE:HG23 | 27:DE:188:MET:HA | 1.99 | 0.45 |
| 27:DE:48:THR:O | 27:DE:52:VAL:HG23 | 2.17 | 0.45 |
| 29:DG:156:TYR:O | 29:DG:157:LYS:HD2 | 2.17 | 0.45 |
| 30:DH:14:SER:C | 30:DH:16:GLY:H | 2.18 | 0.45 |
| 31:DJ:57:LEU:HG | 31:DJ:128:ASN:N | 2.31 | 0.45 |
| 35:DN:65:LEU:HD11 | 35:DN:69:ARG:NH2 | 2.31 | 0.45 |
| 38:DQ:23:TYR:CD2 | 38:DQ:23:TYR:N | 2.83 | 0.45 |
| 40:DS:41:LYS:O | 40:DS:43:ALA:N | 2.49 | 0.45 |
| 42:DU:26:ASN:ND2 | 42:DU:34:ILE:HD12 | 2.28 | 0.45 |
| 24:DV:42:LEU:N | 24:DV:42:LEU:HD23 | 2.32 | 0.45 |
| 1:AA:1260:G:OP1 | 1:AA:1284:C:H4' | 2.16 | 0.45 |
| 1:AA:154:U:H2' | 1:AA:155:A:H8 | 1.77 | 0.45 |
| 2:AC:110:LEU:HD21 | 2:AC:140:ALA:O | 2.16 | 0.45 |
| 5:AF:68:GLN:HA | 5:AF:71:ILE:HD11 | 1.98 | 0.45 |
| 7:AH:58:LEU:CD2 | 7:AH:60:LEU:HB2 | 2.47 | 0.45 |
| 8:AI:49:GLN:HA | 8:AI:52:GLU:HG2 | 1.99 | 0.45 |
| 16:AQ:39:ARG:HG3 | 16:AQ:39:ARG:NH1 | 2.29 | 0.45 |
| 21:AU:26:GLY:O | 21:AU:30:GLU:HB3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1177:G:H2' | 23:BB:1178:C:C6 | 2.52 | 0.45 |
| 23:BB:1444:G:H2' | 23:BB:1445:G:H8 | 1.80 | 0.45 |
| 23:BB:1523:U:H5'' | 23:BB:1524:G:C8 | 2.51 | 0.45 |
| 23:BB:1849:G:H2' | 23:BB:1850:G:C8 | 2.51 | 0.45 |
| 23:BB:2146:C:C1' | 23:BB:2147:A:H5' | 2.45 | 0.45 |
| 23:BB:877:A:C2 | 23:BB:900:A:N7 | 2.84 | 0.45 |
| 25:BC:41:GLY:O | 25:BC:48:ILE:HA | 2.16 | 0.45 |
| 26:BD:101:PHE:O | 26:BD:180:VAL:HG11 | 2.16 | 0.45 |
| 27:BE:152:GLU:O | 27:BE:153:LEU:HB3 | 2.16 | 0.45 |
| 27:BE:5:LEU:HB2 | 27:BE:11:ALA:H | 1.82 | 0.45 |
| 28:BF:126:ASN:HB3 | 28:BF:156:THR:CB | 2.47 | 0.45 |
| 29:BG:148:ARG:HA | 29:BG:161:VAL:CB | 2.43 | 0.45 |
| 29:BG:39:ALA:O | 29:BG:54:ARG:HB2 | 2.17 | 0.45 |
| 29:BG:91:VAL:HG23 | 29:BG:92:GLY:H | 1.81 | 0.45 |
| 30:BH:61:VAL:O | 30:BH:63:ALA:N | 2.49 | 0.45 |
| 31:BJ:140:LEU:HD23 | 31:BJ:141:ASP:N | 2.32 | 0.45 |
| 32:BK:19:VAL:C | 32:BK:41:ILE:HD11 | 2.36 | 0.45 |
| 36:BO:68:LYS:H | 36:BO:102:ARG:HD3 | 1.82 | 0.45 |
| 36:BO:51:ALA:CB | 36:BO:78:VAL:HG13 | 2.47 | 0.45 |
| 37:BP:4:ILE:O | 37:BP:6:GLN:N | 2.46 | 0.45 |
| 39:BR:2:TYR:HB2 | 39:BR:42:ALA:CB | 2.40 | 0.45 |
| 41:BT:83:ALA:O | 41:BT:84:TYR:HB2 | 2.17 | 0.45 |
| 42:BU:11:ILE:CG2 | 42:BU:70:ALA:HB3 | 2.45 | 0.45 |
| 43:BW:23:LYS:O | 43:BW:66:VAL:HB | 2.17 | 0.45 |
| 44:BX:56:LEU:C | 44:BX:58:ASN:N | 2.70 | 0.45 |
| 1:CA:1013:G:H2' | 1:CA:1015:G:OP2 | 2.16 | 0.45 |
| 1:CA:1159:U:O4' | 1:CA:1182:G:N2 | 2.50 | 0.45 |
| 1:CA:1014:A:N3 | 1:CA:1219:A:H1' | 2.31 | 0.45 |
| 1:CA:1527:U:H2' | 1:CA:1528:U:C6 | 2.52 | 0.45 |
| 1:CA:16:A:N1 | 1:CA:919:A:H2 | 2.15 | 0.45 |
| 1:CA:25:C:C5' | 1:CA:524:G:H1' | 2.47 | 0.45 |
| 1:CA:429:U:H5' | 3:CD:8:LEU:CG | 2.38 | 0.45 |
| 1:CA:936:C:H2' | 1:CA:937:A:O4' | 2.16 | 0.45 |
| 20:CB:117:GLU:HA | 20:CB:140:LEU:CD2 | 2.45 | 0.45 |
| 3:CD:125:ASN:OD1 | 3:CD:140:ASP:HA | 2.17 | 0.45 |
| 3:CD:162:GLU:HA | 3:CD:166:LYS:NZ | 2.32 | 0.45 |
| 1:CA:409:U:OP1 | 3:CD:23:GLY:HA3 | 2.16 | 0.45 |
| 5:CF:47:LEU:HD21 | 5:CF:57:ALA:CB | 2.47 | 0.45 |
| 5:CF:93:LYS:O | 5:CF:94:HIS:HB2 | 2.16 | 0.45 |
| 6:CG:72:VAL:HG12 | 6:CG:89:GLU:CA | 2.47 | 0.45 |
| 8:CI:9:GLY:HA2 | 8:CI:80:HIS:HD2 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:CM:15:VAL:HG22 | 12:CM:33:LEU:CD1 | 2.47 | 0.45 |
| 15:CP:2:VAL:O | 15:CP:65:ALA:HA | 2.16 | 0.45 |
| 23:DB:1056:G:H5'' | 23:DB:1057:A:H5' | 1.98 | 0.45 |
| 23:DB:117:G:C5' | 23:DB:126:A:H8 | 2.20 | 0.45 |
| 23:DB:1482:G:N2 | 23:DB:1508:A:H1' | 2.31 | 0.45 |
| 23:DB:1515:A:H2' | 23:DB:1516:G:O4' | 2.16 | 0.45 |
| 23:DB:1737:G:H5' | 23:DB:1738:G:OP2 | 2.17 | 0.45 |
| 23:DB:178:G:O2' | 23:DB:179:C:H5' | 2.17 | 0.45 |
| 23:DB:2109:U:C2 | 23:DB:2110:G:H5'' | 2.51 | 0.45 |
| 23:DB:2557:G:H2' | 23:DB:2558:C:H6 | 1.79 | 0.45 |
| 23:DB:2594:C:O2' | 23:DB:2595:G:H5' | 2.17 | 0.45 |
| 23:DB:307:G:H2' | 23:DB:309:A:OP2 | 2.16 | 0.45 |
| 23:DB:503:A:C2 | 23:DB:505:A:C4 | 3.05 | 0.45 |
| 23:DB:904:G:H2' | 23:DB:905:A:C8 | 2.51 | 0.45 |
| 23:DB:990:A:H1' | 23:DB:1156:A:C2 | 2.52 | 0.45 |
| 27:DE:115:GLN:O | 27:DE:117:ARG:HG3 | 2.16 | 0.45 |
| 30:DH:119:ASN:O | 30:DH:121:VAL:HG23 | 2.16 | 0.45 |
| 32:DK:109:SER:OG | 32:DK:111:LYS:HG2 | 2.17 | 0.45 |
| 33:DL:50:PHE:CE2 | 33:DL:53:GLY:HA2 | 2.52 | 0.45 |
| 35:DN:31:HIS:O | 35:DN:32:GLU:HB2 | 2.17 | 0.45 |
| 36:DO:18:LEU:HD23 | 36:DO:25:ARG:HD2 | 1.99 | 0.45 |
| 39:DR:38:VAL:O | 39:DR:53:PHE:HB3 | 2.16 | 0.45 |
| 43:DW:50:VAL:HG23 | 43:DW:51:GLY:H | 1.80 | 0.45 |
| 46:DZ:70:GLU:O | 46:DZ:72:ARG:N | 2.46 | 0.45 |
| 1:AA:1266:G:N2 | 1:AA:1268:G:H3' | 2.32 | 0.45 |
| 1:AA:1363:A:H2' | 1:AA:1363:A:N3 | 2.31 | 0.45 |
| 1:AA:241:G:O2' | 1:AA:242:G:H5' | 2.16 | 0.45 |
| 1:AA:333:U:H2' | 1:AA:334:C:C6 | 2.52 | 0.45 |
| 1:AA:364:A:H2' | 1:AA:365:U:O2 | 2.16 | 0.45 |
| 1:AA:496:A:H2' | 1:AA:497:G:C8 | 2.51 | 0.45 |
| 1:AA:53:A:C2 | 1:AA:54:C:H1' | 2.52 | 0.45 |
| 1:AA:552:U:H5' | 11:AL:82:ARG:HH11 | 1.81 | 0.45 |
| 1:AA:79:G:C2' | 1:AA:80:A:N7 | 2.79 | 0.45 |
| 20:AB:160:LEU:HD22 | 20:AB:182:VAL:HA | 1.97 | 0.45 |
| 20:AB:94:ARG:N | 20:AB:94:ARG:HE | 2.15 | 0.45 |
| 6:AG:13:PRO:O | 6:AG:18:GLY:HA2 | 2.17 | 0.45 |
| 8:AI:9:GLY:HA2 | 8:AI:80:HIS:CD2 | 2.51 | 0.45 |
| 10:AK:122:PRO:HD2 | 21:AU:35:GLU:HG2 | 1.99 | 0.45 |
| 23:BB:111:A:H2' | 23:BB:112:U:O4' | 2.16 | 0.45 |
| 23:BB:1207:C:H2' | 23:BB:1208:C:H6 | 1.82 | 0.45 |
| 23:BB:726:G:H5'' | 23:BB:1432:G:O2' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:1689:A:O2' | 23:BB:1690:A:H5' | 2.17 | 0.45 |
| 23:BB:1730:C:H1' | 23:BB:1731:G:N2 | 2.32 | 0.45 |
| 23:BB:2201:G:O2' | 23:BB:2202:U:H5' | 2.16 | 0.45 |
| 23:BB:160:A:H1' | 23:BB:2208:C:O2' | 2.16 | 0.45 |
| 23:BB:220:G:H1 | 23:BB:427:U:H2' | 1.82 | 0.45 |
| 23:BB:242:G:H5' | 50:B3:63:TYR:CD1 | 2.52 | 0.45 |
| 23:BB:2489:U:O2' | 23:BB:2490:G:H5' | 2.16 | 0.45 |
| 23:BB:26:G:H1' | 23:BB:514:A:N6 | 2.31 | 0.45 |
| 23:BB:2808:G:O2' | 23:BB:2809:A:H8 | 1.99 | 0.45 |
| 23:BB:705:A:N6 | 23:BB:726:G:H1' | 2.31 | 0.45 |
| 23:BB:770:G:OP2 | 49:B2:11:LYS:HE2 | 2.17 | 0.45 |
| 25:BC:6:LYS:O | 25:BC:8:THR:HG23 | 2.16 | 0.45 |
| 27:BE:148:ILE:HA | 27:BE:187:VAL:HB | 1.98 | 0.45 |
| 27:BE:155:GLU:O | 27:BE:159:LEU:HB2 | 2.17 | 0.45 |
| 28:BF:169:LEU:O | 28:BF:174:PHE:HB2 | 2.16 | 0.45 |
| 28:BF:94:ARG:HD3 | 28:BF:97:GLU:OE2 | 2.17 | 0.45 |
| 30:BH:89:LYS:HE2 | 30:BH:123:ARG:HB3 | 1.98 | 0.45 |
| 30:BH:114:GLU:HB2 | 30:BH:132:PHE:CE1 | 2.52 | 0.45 |
| 30:BH:14:SER:C | 30:BH:16:GLY:N | 2.69 | 0.45 |
| 52:BI:107:GLU:HA | 52:BI:110:GLN:OE1 | 2.16 | 0.45 |
| 52:BI:52:LEU:HD21 | 52:BI:81:LYS:NZ | 2.31 | 0.45 |
| 32:BK:35:VAL:HG12 | 32:BK:69:VAL:CG2 | 2.47 | 0.45 |
| 35:BN:31:HIS:O | 35:BN:32:GLU:HB2 | 2.15 | 0.45 |
| 32:BK:120:PRO:HA | 37:BP:65:ASN:HD21 | 1.81 | 0.45 |
| 38:BQ:4:LYS:CE | 38:BQ:7:VAL:HG22 | 2.46 | 0.45 |
| 39:BR:43:ASN:ND2 | 39:BR:44:GLY:N | 2.64 | 0.45 |
| 39:BR:68:ARG:HG2 | 39:BR:92:TRP:HA | 1.99 | 0.45 |
| 41:BT:57:VAL:HG22 | 41:BT:58:VAL:N | 2.21 | 0.45 |
| 42:BU:86:PHE:HB3 | 42:BU:90:LYS:O | 2.17 | 0.45 |
| 24:BV:49:ASN:O | 24:BV:52:ALA:HB3 | 2.17 | 0.45 |
| 43:BW:70:VAL:HG13 | 43:BW:70:VAL:O | 2.16 | 0.45 |
| 1:CA:246:A:C2 | 1:CA:282:A:C5 | 3.05 | 0.45 |
| 1:CA:250:A:H1' | 1:CA:252:U:C5 | 2.52 | 0.45 |
| 1:CA:445:G:H2' | 1:CA:446:G:O4' | 2.17 | 0.45 |
| 1:CA:708:C:H2' | 1:CA:709:U:C6 | 2.52 | 0.45 |
| 1:CA:818:G:H3' | 1:CA:819:A:H5'' | 1.99 | 0.45 |
| 1:CA:864:A:H2' | 1:CA:865:A:C8 | 2.52 | 0.45 |
| 1:CA:949:A:H2' | 1:CA:950:U:O4' | 2.15 | 0.45 |
| 20:CB:83:ALA:HA | 20:CB:88:GLN:HE21 | 1.80 | 0.45 |
| 2:CC:19:SER:HB2 | 2:CC:39:ARG:NH2 | 2.32 | 0.45 |
| 5:CF:47:LEU:HD13 | 5:CF:51:ILE:HG22 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CF:1:MET:HG2 | 5:CF:67:PRO:HD3 | 1.99 | 0.45 |
| 8:CI:117:LEU:HD22 | 8:CI:123:ARG:HG2 | 1.98 | 0.45 |
| 11:CL:60:PHE:O | 11:CL:62:VAL:HG13 | 2.17 | 0.45 |
| 12:CM:52:ILE:HA | 12:CM:55:LEU:HG | 1.97 | 0.45 |
| 15:CP:67:ILE:HG23 | 15:CP:67:ILE:O | 2.17 | 0.45 |
| 23:DB:1181:U:O2' | 23:DB:1182:G:H5' | 2.16 | 0.45 |
| 23:DB:1390:U:O2' | 23:DB:1391:U:H5' | 2.17 | 0.45 |
| 23:DB:1439:A:C5 | 23:DB:1552:A:N6 | 2.85 | 0.45 |
| 23:DB:1472:C:H2' | 23:DB:1473:G:C8 | 2.52 | 0.45 |
| 23:DB:1516:G:O2' | 23:DB:1517:G:H5' | 2.16 | 0.45 |
| 23:DB:1565:C:H5'' | 25:DC:17:LYS:CE | 2.47 | 0.45 |
| 23:DB:1606:C:H5'' | 23:DB:1607:C:OP1 | 2.16 | 0.45 |
| 23:DB:2078:C:H2' | 23:DB:2079:U:H6 | 1.81 | 0.45 |
| 23:DB:219:A:O2' | 23:DB:220:G:H5' | 2.17 | 0.45 |
| 23:DB:2219:U:H2' | 23:DB:2220:U:C6 | 2.52 | 0.45 |
| 23:DB:2428:G:H5'' | 23:DB:2429:G:OP1 | 2.17 | 0.45 |
| 23:DB:992:C:H2' | 23:DB:993:G:C8 | 2.52 | 0.45 |
| 25:DC:144:GLU:HG3 | 25:DC:151:GLY:N | 2.08 | 0.45 |
| 25:DC:185:ALA:C | 25:DC:187:CYS:H | 2.19 | 0.45 |
| 26:DD:148:GLN:CB | 26:DD:152:PRO:HG2 | 2.40 | 0.45 |
| 26:DD:15:PHE:HD1 | 26:DD:15:PHE:H | 1.63 | 0.45 |
| 23:DB:2050:C:H1' | 26:DD:161:MET:CE | 2.47 | 0.45 |
| 26:DD:61:THR:OG1 | 26:DD:63:PRO:HD2 | 2.17 | 0.45 |
| 27:DE:157:LEU:O | 27:DE:160:ALA:HB3 | 2.17 | 0.45 |
| 28:DF:11:VAL:HG21 | 28:DF:172:PHE:HE1 | 1.81 | 0.45 |
| 29:DG:94:ARG:HA | 29:DG:128:THR:HG22 | 1.98 | 0.45 |
| 30:DH:125:THR:HA | 30:DH:146:VAL:CG1 | 2.45 | 0.45 |
| 52:DI:57:VAL:HG23 | 52:DI:71:LYS:HZ1 | 1.80 | 0.45 |
| 31:DJ:63:ALA:HA | 31:DJ:69:ARG:HH22 | 1.81 | 0.45 |
| 32:DK:105:ARG:H | 32:DK:122:VAL:HG12 | 1.82 | 0.45 |
| 32:DK:95:ILE:HG13 | 32:DK:95:ILE:O | 2.17 | 0.45 |
| 35:DN:12:ARG:HG2 | 35:DN:16:HIS:ND1 | 2.31 | 0.45 |
| 23:DB:140:C:OP1 | 41:DT:2:ILE:HD12 | 2.16 | 0.45 |
| 42:DU:85:ARG:HH11 | 42:DU:86:PHE:N | 2.14 | 0.45 |
| 42:DU:85:ARG:NH1 | 42:DU:86:PHE:N | 2.65 | 0.45 |
| 43:DW:28:GLU:H | 43:DW:31:LEU:HG | 1.82 | 0.45 |
| 45:DY:9:THR:HB | 45:DY:10:ARG:H | 1.59 | 0.45 |
| 46:DZ:65:ASP:O | 46:DZ:69:ALA:HB2 | 2.17 | 0.45 |
| 1:AA:1056:U:H2' | 1:AA:1057:G:H8 | 1.81 | 0.45 |
| 2:AC:63:ILE:O | 2:AC:65:VAL:HG23 | 2.15 | 0.45 |
| 3:AD:2:ARG:HG3 | 3:AD:114:ARG:CZ | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AD:11:SER:HA | 3:AD:18:LEU:HD22 | 1.99 | 0.45 |
| 1:AA:967:C:H5' | 8:AI:129:ARG:HA | 1.99 | 0.45 |
| 11:AL:15:VAL:O | 11:AL:16:ALA:C | 2.54 | 0.45 |
| 13:AN:26:LEU:HD23 | 13:AN:27:LYS:H | 1.81 | 0.45 |
| 17:AR:52:ARG:O | 17:AR:56:ARG:HG3 | 2.17 | 0.45 |
| 23:BB:2215:C:H2' | 23:BB:2216:G:C8 | 2.52 | 0.45 |
| 23:BB:2344:U:H2' | 48:B1:35:LEU:O | 2.16 | 0.45 |
| 23:BB:2391:G:HO2' | 23:BB:2424:C:H41 | 1.64 | 0.45 |
| 23:BB:2428:G:H5'' | 23:BB:2429:G:OP1 | 2.17 | 0.45 |
| 23:BB:2885:G:H21 | 47:B0:31:LYS:HG2 | 1.82 | 0.45 |
| 25:BC:102:TYR:O | 25:BC:103:ILE:HG13 | 2.17 | 0.45 |
| 25:BC:141:HIS:O | 25:BC:143:VAL:HG23 | 2.17 | 0.45 |
| 28:BF:102:LEU:O | 28:BF:103:ILE:CB | 2.64 | 0.45 |
| 29:BG:122:ALA:HA | 29:BG:131:VAL:O | 2.16 | 0.45 |
| 30:BH:90:LEU:HB3 | 30:BH:123:ARG:HD2 | 1.98 | 0.45 |
| 52:BI:116:MET:SD | 52:BI:124:MET:HB2 | 2.56 | 0.45 |
| 31:BJ:64:VAL:HG11 | 31:BJ:69:ARG:H | 1.82 | 0.45 |
| 23:BB:587:C:N3 | 33:BL:33:ARG:NH2 | 2.64 | 0.45 |
| 35:BN:114:GLU:CD | 35:BN:118:ARG:HH11 | 2.19 | 0.45 |
| 35:BN:116:VAL:HG13 | 35:BN:116:VAL:O | 2.17 | 0.45 |
| 36:BO:68:LYS:H | 36:BO:102:ARG:CD | 2.30 | 0.45 |
| 39:BR:61:ALA:CB | 39:BR:98:ILE:H | 2.30 | 0.45 |
| 40:BS:42:LYS:HG3 | 40:BS:43:ALA:N | 2.32 | 0.45 |
| 41:BT:68:LYS:HD3 | 41:BT:68:LYS:N | 2.32 | 0.45 |
| 24:BV:26:PHE:CE2 | 24:BV:44:HIS:HA | 2.52 | 0.45 |
| 43:BW:44:PHE:CE2 | 43:BW:76:ARG:HD3 | 2.51 | 0.45 |
| 43:BW:49:ASN:CB | 43:BW:61:LYS:H | 2.28 | 0.45 |
| 1:CA:175:C:H2' | 1:CA:176:C:C6 | 2.52 | 0.45 |
| 1:CA:201:G:O2' | 1:CA:202:G:H5' | 2.17 | 0.45 |
| 1:CA:332:G:H2' | 1:CA:333:U:H6 | 1.82 | 0.45 |
| 20:CB:95:TRP:CH2 | 20:CB:100:LEU:HD13 | 2.52 | 0.45 |
| 20:CB:53:LEU:HD13 | 20:CB:216:VAL:HG12 | 1.98 | 0.45 |
| 20:CB:221:ARG:HG3 | 20:CB:222:GLU:H | 1.81 | 0.45 |
| 20:CB:23:ASN:O | 20:CB:25:LYS:N | 2.49 | 0.45 |
| 20:CB:86:CYS:SG | 20:CB:87:ASP:N | 2.87 | 0.45 |
| 1:CA:1057:G:H5'' | 2:CC:153:SER:CB | 2.47 | 0.45 |
| 3:CD:104:MET:SD | 3:CD:179:GLY:HA3 | 2.56 | 0.45 |
| 3:CD:106:PHE:CD1 | 3:CD:158:LEU:HD21 | 2.52 | 0.45 |
| 4:CE:89:THR:HG22 | 4:CE:90:GLY:N | 2.31 | 0.45 |
| 1:CA:1152:A:H4' | 9:CJ:15:HIS:CD2 | 2.52 | 0.45 |
| 10:CK:83:VAL:CG2 | 10:CK:106:ILE:HD11 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:CO:23:SER:HB3 | 14:CO:26:VAL:CG2 | 2.47 | 0.45 |
| 48:D1:46:VAL:HG13 | 48:D1:47:ILE:N | 2.32 | 0.45 |
| 23:DB:135:U:H2' | 23:DB:136:G:C8 | 2.52 | 0.45 |
| 23:DB:1417:C:O5' | 23:DB:1588:G:H1' | 2.16 | 0.45 |
| 23:DB:2489:U:H2' | 23:DB:2490:G:O4' | 2.17 | 0.45 |
| 23:DB:2733:A:H2' | 23:DB:2734:A:O4' | 2.16 | 0.45 |
| 23:DB:2773:C:O2' | 23:DB:2774:C:H5' | 2.16 | 0.45 |
| 23:DB:771:G:OP1 | 49:D2:14:ARG:HD2 | 2.17 | 0.45 |
| 23:DB:826:U:H2' | 23:DB:828:U:O4' | 2.16 | 0.45 |
| 25:DC:54:GLY:O | 25:DC:214:GLY:HA2 | 2.16 | 0.45 |
| 26:DD:108:ASP:N | 26:DD:204:LYS:O | 2.49 | 0.45 |
| 26:DD:180:VAL:HG22 | 26:DD:187:LEU:HD12 | 1.99 | 0.45 |
| 28:DF:140:ILE:O | 28:DF:141:ASP:C | 2.56 | 0.45 |
| 28:DF:64:PRO:HA | 28:DF:88:VAL:HG22 | 1.99 | 0.45 |
| 29:DG:109:SER:O | 29:DG:110:HIS:HB3 | 2.17 | 0.45 |
| 30:DH:41:LYS:O | 30:DH:45:GLU:HG3 | 2.17 | 0.45 |
| 30:DH:61:VAL:C | 30:DH:63:ALA:H | 2.20 | 0.45 |
| 52:DI:17:ALA:C | 52:DI:19:PRO:HD3 | 2.37 | 0.45 |
| 31:DJ:64:VAL:HG11 | 31:DJ:69:ARG:H | 1.82 | 0.45 |
| 32:DK:6:THR:O | 32:DK:7:MET:HG2 | 2.17 | 0.45 |
| 33:DL:115:GLU:N | 33:DL:115:GLU:OE1 | 2.49 | 0.45 |
| 35:DN:30:ARG:NH2 | 35:DN:72:ASP:OD1 | 2.50 | 0.45 |
| 36:DO:52:SER:H | 36:DO:55:GLU:HG3 | 1.82 | 0.45 |
| 38:DQ:111:LYS:HB2 | 39:DR:48:LYS:HD2 | 1.98 | 0.45 |
| 39:DR:70:GLU:O | 39:DR:90:ARG:HD2 | 2.16 | 0.45 |
| 41:DT:13:ALA:O | 41:DT:33:LYS:N | 2.50 | 0.45 |
| 41:DT:38:ALA:HB3 | 41:DT:81:LYS:HZ1 | 1.79 | 0.45 |
| 41:DT:55:VAL:HG22 | 41:DT:87:LEU:CD2 | 2.47 | 0.45 |
| 23:DB:329:G:N1 | 42:DU:16:LYS:HG2 | 2.31 | 0.45 |
| 42:DU:11:ILE:HG12 | 42:DU:20:LYS:O | 2.17 | 0.45 |
| 24:DV:26:PHE:CE2 | 24:DV:44:HIS:HA | 2.52 | 0.45 |
| 1:AA:1148:U:O4' | 8:AI:17:ARG:HD3 | 2.17 | 0.45 |
| 1:AA:1352:C:H2' | 1:AA:1353:G:H8 | 1.82 | 0.45 |
| 1:AA:1459:G:H2' | 1:AA:1460:C:H6 | 1.80 | 0.45 |
| 1:AA:222:C:H2' | 1:AA:223:A:C8 | 2.52 | 0.45 |
| 1:AA:358:U:H2' | 1:AA:359:G:C8 | 2.52 | 0.45 |
| 1:AA:454:G:O2' | 1:AA:455:G:H5' | 2.17 | 0.45 |
| 1:AA:859:G:O2' | 1:AA:860:A:H5' | 2.16 | 0.45 |
| 1:AA:865:A:H5' | 1:AA:1078:U:C4 | 2.52 | 0.45 |
| 1:AA:968:A:H3' | 1:AA:969:A:C5' | 2.47 | 0.45 |
| 20:AB:48:MET:O | 20:AB:52:ALA:HB3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AE:89:THR:HG22 | 4:AE:90:GLY:N | 2.31 | 0.45 |
| 6:AG:21:LEU:H | 6:AG:21:LEU:CD2 | 2.24 | 0.45 |
| 8:AI:9:GLY:HA2 | 8:AI:80:HIS:HD2 | 1.81 | 0.45 |
| 10:AK:111:ASP:HB2 | 21:AU:19:LYS:HE3 | 1.99 | 0.45 |
| 16:AQ:52:CYS:SG | 16:AQ:77:VAL:HG22 | 2.57 | 0.45 |
| 21:AU:26:GLY:C | 21:AU:28:LEU:N | 2.71 | 0.45 |
| 23:BB:1064:C:H2' | 23:BB:1065:U:O4' | 2.17 | 0.45 |
| 23:BB:1207:C:H2' | 23:BB:1208:C:C6 | 2.52 | 0.45 |
| 23:BB:1599:U:H2' | 23:BB:1600:C:C6 | 2.52 | 0.45 |
| 23:BB:1695:G:N7 | 25:BC:13:ARG:NH2 | 2.65 | 0.45 |
| 23:BB:1796:U:O2' | 23:BB:1797:G:H5' | 2.17 | 0.45 |
| 23:BB:2211:A:H4' | 23:BB:2211:A:OP2 | 2.16 | 0.45 |
| 23:BB:2315:G:H2' | 23:BB:2316:G:H8 | 1.82 | 0.45 |
| 23:BB:2478:A:H2' | 23:BB:2479:U:O4' | 2.17 | 0.45 |
| 23:BB:292:U:H2' | 23:BB:293:U:O4' | 2.17 | 0.45 |
| 23:BB:584:C:OP1 | 38:BQ:5:ARG:HB3 | 2.16 | 0.45 |
| 23:BB:632:A:H2' | 23:BB:633:A:C8 | 2.52 | 0.45 |
| 23:BB:728:G:O2' | 23:BB:730:A:H8 | 2.00 | 0.45 |
| 23:BB:989:G:H5'' | 45:BY:13:ILE:HD11 | 1.99 | 0.45 |
| 25:BC:175:LEU:HD11 | 25:BC:181:ARG:HG3 | 1.98 | 0.45 |
| 23:BB:2591:C:OP1 | 25:BC:237:ARG:HG3 | 2.17 | 0.45 |
| 26:BD:114:LYS:HZ1 | 26:BD:116:LYS:HG3 | 1.81 | 0.45 |
| 26:BD:10:GLY:HA3 | 26:BD:26:VAL:H | 1.82 | 0.45 |
| 26:BD:46:ARG:HH22 | 26:BD:86:GLU:N | 2.15 | 0.45 |
| 27:BE:4:VAL:HG12 | 27:BE:5:LEU:H | 1.81 | 0.45 |
| 28:BF:141:ASP:O | 28:BF:144:LYS:N | 2.50 | 0.45 |
| 28:BF:2:LYS:O | 28:BF:6:TYR:HB2 | 2.17 | 0.45 |
| 28:BF:3:LEU:HD11 | 28:BF:172:PHE:CD1 | 2.52 | 0.45 |
| 29:BG:23:ILE:HG22 | 29:BG:25:ILE:HD11 | 1.99 | 0.45 |
| 30:BH:92:GLY:HA3 | 1:CA:360:G:OP1 | 2.17 | 0.45 |
| 33:BL:77:ILE:HD12 | 33:BL:125:LEU:HD21 | 1.99 | 0.45 |
| 23:BB:911:A:N6 | 34:BM:9:PHE:HB3 | 2.32 | 0.45 |
| 35:BN:90:ARG:HB3 | 35:BN:94:TYR:CE1 | 2.52 | 0.45 |
| 38:BQ:38:VAL:O | 38:BQ:39:ILE:C | 2.56 | 0.45 |
| 38:BQ:60:TRP:O | 38:BQ:63:ARG:HG3 | 2.16 | 0.45 |
| 40:BS:24:ILE:CG2 | 40:BS:71:VAL:HG11 | 2.45 | 0.45 |
| 40:BS:88:ARG:HH21 | 40:BS:88:ARG:HG3 | 1.82 | 0.45 |
| 46:BZ:49:LEU:HB2 | 46:BZ:51:VAL:HG23 | 1.99 | 0.45 |
| 1:CA:1020:G:N3 | 1:CA:1020:G:H2' | 2.32 | 0.45 |
| 1:CA:1243:C:O2' | 1:CA:1244:G:H5' | 2.16 | 0.45 |
| 1:CA:1330:U:H2' | 1:CA:1331:G:O4' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:356:A:H2' | 1:CA:357:G:O4' | 2.17 | 0.45 |
| 30:BH:8:LYS:HE3 | 1:CA:495:A:P | 2.57 | 0.45 |
| 1:CA:586:C:O2' | 1:CA:587:G:H5' | 2.17 | 0.45 |
| 1:CA:614:C:C2' | 1:CA:615:G:H5' | 2.47 | 0.45 |
| 1:CA:721:G:H4' | 1:CA:722:G:O4' | 2.17 | 0.45 |
| 1:CA:743:A:H2' | 1:CA:744:C:H6 | 1.80 | 0.45 |
| 20:CB:88:GLN:H | 20:CB:88:GLN:HG3 | 1.49 | 0.45 |
| 4:CE:19:ARG:HH12 | 4:CE:28:ARG:HH12 | 1.65 | 0.45 |
| 6:CG:11:ILE:HG22 | 6:CG:12:LEU:N | 2.32 | 0.45 |
| 7:CH:87:ARG:HD3 | 7:CH:90:GLU:OE1 | 2.17 | 0.45 |
| 1:CA:1342:C:O2' | 8:CI:125:GLN:HB3 | 2.17 | 0.45 |
| 15:CP:46:LYS:C | 15:CP:48:GLU:N | 2.70 | 0.45 |
| 16:CQ:80:LYS:O | 16:CQ:80:LYS:HD2 | 2.16 | 0.45 |
| 17:CR:63:TYR:C | 17:CR:64:LEU:HD12 | 2.37 | 0.45 |
| 21:CU:48:LYS:HG3 | 21:CU:49:ALA:N | 2.31 | 0.45 |
| 48:D1:36:LYS:HG2 | 48:D1:47:ILE:HA | 1.99 | 0.45 |
| 51:D4:4:ARG:N | 51:D4:37:GLN:HE22 | 2.15 | 0.45 |
| 23:DB:125:A:H4' | 23:DB:126:A:OP2 | 2.17 | 0.45 |
| 23:DB:1563:U:O2' | 23:DB:1564:C:H5' | 2.16 | 0.45 |
| 23:DB:1669:A:H2' | 23:DB:1669:A:N3 | 2.31 | 0.45 |
| 23:DB:218:A:C2' | 23:DB:219:A:H5' | 2.47 | 0.45 |
| 23:DB:2472:G:C2' | 23:DB:2475:C:H42 | 2.29 | 0.45 |
| 23:DB:512:G:OP2 | 23:DB:1234:U:O2' | 2.31 | 0.45 |
| 25:DC:107:LYS:N | 25:DC:193:GLU:O | 2.50 | 0.45 |
| 25:DC:83:ASP:HB3 | 25:DC:86:ARG:HG2 | 1.99 | 0.45 |
| 28:DF:108:PRO:O | 28:DF:110:ILE:HG23 | 2.17 | 0.45 |
| 28:DF:135:ILE:CD1 | 28:DF:137:PHE:HB3 | 2.44 | 0.45 |
| 28:DF:28:PRO:O | 28:DF:168:LEU:HG | 2.17 | 0.45 |
| 30:DH:60:GLU:C | 30:DH:62:LEU:H | 2.19 | 0.45 |
| 36:DO:7:ARG:HA | 36:DO:10:ARG:NH2 | 2.31 | 0.45 |
| 36:DO:88:LYS:HD2 | 36:DO:89:ASP:CB | 2.46 | 0.45 |
| 38:DQ:107:ALA:C | 39:DR:48:LYS:HD3 | 2.37 | 0.45 |
| 43:DW:45:HIS:ND1 | 43:DW:45:HIS:N | 2.65 | 0.45 |
| 1:AA:435:A:N3 | 1:AA:435:A:H2' | 2.31 | 0.45 |
| 1:AA:474:G:O2' | 1:AA:475:C:H5' | 2.17 | 0.45 |
| 1:AA:593:U:O2' | 1:AA:594:U:H5' | 2.17 | 0.45 |
| 1:AA:664:G:H5'' | 17:AR:52:ARG:HE | 1.82 | 0.45 |
| 1:AA:744:C:H2' | 1:AA:745:G:C8 | 2.52 | 0.45 |
| 1:AA:864:A:H2' | 1:AA:865:A:C8 | 2.52 | 0.45 |
| 1:AA:865:A:O2' | 1:AA:866:C:H5' | 2.17 | 0.45 |
| 1:AA:1073:U:O2' | 20:AB:102:ASN:OD1 | 2.28 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:AB:120:SER:HA | 20:AB:125:PHE:HB3 | 1.99 | 0.45 |
| 3:AD:188:SER:C | 3:AD:190:LEU:H | 2.19 | 0.45 |
| 4:AE:131:ASN:O | 4:AE:135:VAL:HG23 | 2.16 | 0.45 |
| 1:AA:642:A:C5 | 7:AH:106:SER:HA | 2.52 | 0.45 |
| 7:AH:74:ILE:CG1 | 7:AH:128:VAL:HG22 | 2.45 | 0.45 |
| 1:AA:1152:A:H4' | 9:AJ:15:HIS:CD2 | 2.52 | 0.45 |
| 9:AJ:55:PRO:O | 9:AJ:56:HIS:HB3 | 2.17 | 0.45 |
| 9:AJ:6:ILE:O | 9:AJ:75:ASP:HA | 2.17 | 0.45 |
| 10:AK:80:ASN:HB3 | 10:AK:105:ARG:HB3 | 1.99 | 0.45 |
| 13:AN:26:LEU:HD23 | 13:AN:27:LYS:N | 2.32 | 0.45 |
| 48:B1:47:ILE:H | 48:B1:47:ILE:HD12 | 1.82 | 0.45 |
| 22:BA:112:G:O2' | 22:BA:113:C:H5' | 2.17 | 0.45 |
| 22:BA:42:C:C4 | 28:BF:65:LEU:HD22 | 2.51 | 0.45 |
| 23:BB:1047:G:O2' | 23:BB:1110:G:N2 | 2.43 | 0.45 |
| 23:BB:1076:C:H2' | 23:BB:1077:A:C8 | 2.52 | 0.45 |
| 23:BB:1163:G:H4' | 39:BR:92:TRP:HE1 | 1.81 | 0.45 |
| 23:BB:1472:C:H2' | 23:BB:1473:G:H8 | 1.82 | 0.45 |
| 23:BB:1872:A:H2' | 23:BB:1873:G:O4' | 2.17 | 0.45 |
| 23:BB:2247:A:H2' | 23:BB:2248:C:H6 | 1.82 | 0.45 |
| 23:BB:2448:A:H4' | 23:BB:2449:U:OP2 | 2.17 | 0.45 |
| 23:BB:322:A:C2 | 23:BB:340:A:C6 | 3.05 | 0.45 |
| 23:BB:681:G:H2' | 23:BB:682:G:H8 | 1.82 | 0.45 |
| 23:BB:746:U:O3' | 40:BS:90:LYS:NZ | 2.50 | 0.45 |
| 23:BB:753:A:O2' | 23:BB:754:U:H5' | 2.17 | 0.45 |
| 26:BD:179:ARG:NH1 | 26:BD:179:ARG:HB3 | 2.31 | 0.45 |
| 26:BD:8:LYS:O | 26:BD:197:THR:HA | 2.17 | 0.45 |
| 27:BE:102:ARG:O | 27:BE:106:LYS:HG3 | 2.17 | 0.45 |
| 27:BE:132:LYS:O | 27:BE:135:ALA:HB3 | 2.17 | 0.45 |
| 28:BF:98:PHE:C | 28:BF:100:GLU:H | 2.20 | 0.45 |
| 30:BH:59:ALA:O | 30:BH:60:GLU:HB3 | 2.17 | 0.45 |
| 52:BI:44:LYS:O | 52:BI:48:ILE:HG13 | 2.16 | 0.45 |
| 36:BO:7:ARG:HH11 | 36:BO:7:ARG:CG | 2.30 | 0.45 |
| 23:BB:1010:A:OP1 | 38:BQ:61:ILE:HG22 | 2.17 | 0.45 |
| 40:BS:73:LYS:HD2 | 40:BS:73:LYS:HA | 1.67 | 0.45 |
| 43:BW:65:LYS:N | 43:BW:84:GLU:HB3 | 2.31 | 0.45 |
| 46:BZ:21:ALA:C | 46:BZ:22:LEU:HG | 2.37 | 0.45 |
| 1:CA:1283:U:H2' | 1:CA:1284:C:H6 | 1.82 | 0.45 |
| 1:CA:1411:C:O2' | 1:CA:1412:C:H5' | 2.17 | 0.45 |
| 1:CA:233:C:O2' | 1:CA:234:C:H5' | 2.17 | 0.45 |
| 1:CA:313:A:H2' | 1:CA:314:C:H6 | 1.81 | 0.45 |
| 1:CA:503:C:H2' | 1:CA:504:C:C6 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:885:G:O2' | 1:CA:886:G:H5' | 2.16 | 0.45 |
| 1:CA:921:U:H2' | 1:CA:922:G:H8 | 1.82 | 0.45 |
| 20:CB:11:ALA:C | 20:CB:13:VAL:H | 2.20 | 0.45 |
| 20:CB:83:ALA:O | 20:CB:88:GLN:HB2 | 2.16 | 0.45 |
| 3:CD:197:HIS:CE1 | 3:CD:198:LEU:HG | 2.52 | 0.45 |
| 3:CD:90:LEU:HD11 | 3:CD:194:ILE:HD11 | 1.99 | 0.45 |
| 4:CE:64:GLU:O | 4:CE:68:ARG:HG2 | 2.17 | 0.45 |
| 4:CE:71:ILE:HD12 | 4:CE:73:VAL:CG2 | 2.47 | 0.45 |
| 5:CF:97:THR:HG22 | 5:CF:98:GLU:N | 2.32 | 0.45 |
| 8:CI:20:ILE:CD1 | 8:CI:85:ALA:HB3 | 2.47 | 0.45 |
| 10:CK:72:ALA:O | 10:CK:75:GLU:HG2 | 2.17 | 0.45 |
| 11:CL:34:THR:O | 11:CL:35:ARG:HD2 | 2.17 | 0.45 |
| 15:CP:52:LEU:CD2 | 15:CP:75:ILE:HA | 2.46 | 0.45 |
| 49:D2:6:GLN:NE2 | 49:D2:6:GLN:HA | 2.32 | 0.45 |
| 23:DB:1488:C:O2' | 23:DB:1489:C:H5' | 2.16 | 0.45 |
| 23:DB:1877:A:H2' | 23:DB:1878:G:C8 | 2.52 | 0.45 |
| 23:DB:1904:G:H1' | 23:DB:1927:A:N1 | 2.32 | 0.45 |
| 23:DB:212:G:H2' | 23:DB:213:A:C8 | 2.52 | 0.45 |
| 23:DB:2296:U:H4' | 23:DB:2297:A:OP1 | 2.16 | 0.45 |
| 23:DB:2473:U:C2' | 23:DB:2473:U:O2 | 2.65 | 0.45 |
| 23:DB:2537:U:H2' | 23:DB:2538:C:H6 | 1.81 | 0.45 |
| 23:DB:2591:C:O2' | 23:DB:2592:G:H5' | 2.17 | 0.45 |
| 23:DB:264:C:H2' | 23:DB:265:A:H5'' | 1.98 | 0.45 |
| 23:DB:2808:G:O2' | 23:DB:2809:A:H8 | 1.98 | 0.45 |
| 23:DB:561:G:O5' | 23:DB:561:G:H8 | 2.00 | 0.45 |
| 23:DB:671:C:O2' | 23:DB:672:C:H5' | 2.17 | 0.45 |
| 23:DB:750:A:H2' | 23:DB:751:A:H5'' | 1.99 | 0.45 |
| 23:DB:962:G:H2' | 23:DB:963:U:C6 | 2.51 | 0.45 |
| 23:DB:2227:A:H5'' | 25:DC:260:LYS:HD2 | 1.97 | 0.45 |
| 26:DD:130:GLN:HB2 | 26:DD:139:SER:O | 2.16 | 0.45 |
| 26:DD:8:LYS:CA | 26:DD:201:LEU:HD11 | 2.47 | 0.45 |
| 27:DE:128:ALA:O | 27:DE:133:LEU:HD12 | 2.16 | 0.45 |
| 28:DF:139:GLU:OE2 | 28:DF:142:TYR:HA | 2.17 | 0.45 |
| 52:DI:23:VAL:HG12 | 52:DI:27:LEU:HD21 | 1.97 | 0.45 |
| 52:DI:5:GLN:HB2 | 52:DI:30:GLN:OE1 | 2.17 | 0.45 |
| 32:DK:15:GLY:HA3 | 32:DK:52:VAL:CG2 | 2.45 | 0.45 |
| 32:DK:35:VAL:HG12 | 32:DK:69:VAL:CG2 | 2.46 | 0.45 |
| 23:DB:1666:G:H4' | 32:DK:6:THR:HG23 | 1.99 | 0.45 |
| 36:DO:111:ARG:HG2 | 36:DO:117:PHE:CE2 | 2.52 | 0.45 |
| 41:DT:66:LYS:N | 41:DT:76:ARG:HH21 | 2.15 | 0.45 |
| 42:DU:49:PRO:O | 42:DU:50:ALA:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DU:11:ILE:CG2 | 42:DU:70:ALA:HB3 | 2.45 | 0.45 |
| 24:DV:60:VAL:HG22 | 24:DV:73:LYS:HE2 | 1.99 | 0.45 |
| 23:DB:2386:A:H2 | 43:DW:38:ARG:HB3 | 1.80 | 0.45 |
| 43:DW:77:LYS:HA | 43:DW:77:LYS:HD3 | 1.82 | 0.45 |
| 1:AA:1313:U:OP2 | 18:AS:5:LYS:HA | 2.17 | 0.44 |
| 1:AA:1469:C:H2' | 1:AA:1470:U:O4' | 2.16 | 0.44 |
| 1:AA:1498:U:H6 | 1:AA:1498:U:O5' | 1.99 | 0.44 |
| 1:AA:1499:A:H1' | 1:AA:1520:C:OP1 | 2.17 | 0.44 |
| 1:AA:1514:G:H2' | 1:AA:1515:G:H8 | 1.82 | 0.44 |
| 1:AA:1527:U:O2' | 1:AA:1528:U:H5' | 2.16 | 0.44 |
| 1:AA:477:C:H2' | 1:AA:478:A:C8 | 2.51 | 0.44 |
| 1:AA:503:C:H2' | 1:AA:504:C:H6 | 1.81 | 0.44 |
| 1:AA:64:G:OP1 | 1:AA:64:G:H3' | 2.17 | 0.44 |
| 1:AA:668:G:O2' | 1:AA:669:G:H5' | 2.16 | 0.44 |
| 1:AA:861:G:H2' | 1:AA:862:C:C6 | 2.52 | 0.44 |
| 20:AB:99:MET:CA | 20:AB:106:VAL:HG21 | 2.43 | 0.44 |
| 2:AC:129:PHE:CD2 | 2:AC:156:LEU:HD22 | 2.52 | 0.44 |
| 2:AC:171:ARG:CB | 2:AC:171:ARG:HH11 | 2.25 | 0.44 |
| 3:AD:29:THR:CG2 | 3:AD:30:LYS:HD3 | 2.47 | 0.44 |
| 4:AE:95:MET:HA | 4:AE:124:ALA:HB2 | 1.98 | 0.44 |
| 6:AG:125:ASP:HB3 | 6:AG:131:GLY:N | 2.33 | 0.44 |
| 8:AI:20:ILE:HD13 | 8:AI:85:ALA:HB3 | 1.99 | 0.44 |
| 15:AP:2:VAL:O | 15:AP:65:ALA:HA | 2.17 | 0.44 |
| 21:AU:26:GLY:C | 21:AU:28:LEU:H | 2.19 | 0.44 |
| 21:AU:25:ALA:O | 21:AU:27:VAL:N | 2.50 | 0.44 |
| 47:B0:55:ALA:C | 47:B0:56:LYS:HG3 | 2.37 | 0.44 |
| 23:BB:1249:U:O4' | 38:BQ:3:VAL:HG21 | 2.17 | 0.44 |
| 23:BB:1708:C:O2' | 23:BB:1709:U:H5' | 2.17 | 0.44 |
| 23:BB:1733:G:H5' | 23:BB:1733:G:H8 | 1.82 | 0.44 |
| 23:BB:2102:G:H2' | 23:BB:2103:C:H5' | 1.99 | 0.44 |
| 23:BB:218:A:O2' | 23:BB:219:A:H5' | 2.17 | 0.44 |
| 23:BB:2439:A:C8 | 23:BB:2586:U:H4' | 2.53 | 0.44 |
| 23:BB:2683:C:O2' | 23:BB:2684:U:H5' | 2.17 | 0.44 |
| 23:BB:2852:G:H2' | 23:BB:2853:C:O4' | 2.17 | 0.44 |
| 23:BB:441:U:O2' | 23:BB:442:G:H5' | 2.17 | 0.44 |
| 23:BB:453:A:H1' | 23:BB:457:A:O2' | 2.18 | 0.44 |
| 23:BB:561:G:O5' | 23:BB:561:G:H8 | 2.00 | 0.44 |
| 23:BB:904:G:H2' | 23:BB:905:A:C8 | 2.50 | 0.44 |
| 25:BC:221:GLY:O | 25:BC:223:ALA:N | 2.50 | 0.44 |
| 26:BD:109:VAL:CG1 | 26:BD:193:VAL:HB | 2.47 | 0.44 |
| 28:BF:126:ASN:CB | 28:BF:156:THR:HA | 2.44 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:29:ARG:HD3 | 28:BF:158:THR:OG1 | 2.16 | 0.44 |
| 30:BH:143:ILE:O | 30:BH:144:VAL:HG23 | 2.17 | 0.44 |
| 31:BJ:35:ARG:HG3 | 31:BJ:40:HIS:HE2 | 1.82 | 0.44 |
| 33:BL:125:LEU:HD23 | 33:BL:126:ARG:N | 2.32 | 0.44 |
| 33:BL:142:ILE:HD12 | 33:BL:142:ILE:N | 2.31 | 0.44 |
| 35:BN:7:GLY:HA2 | 35:BN:46:ARG:HH12 | 1.79 | 0.44 |
| 36:BO:100:HIS:HA | 36:BO:104:GLN:NE2 | 2.32 | 0.44 |
| 38:BQ:57:ARG:HH12 | 38:BQ:61:ILE:CD1 | 2.30 | 0.44 |
| 38:BQ:65:ASN:CG | 38:BQ:75:TYR:HB2 | 2.37 | 0.44 |
| 41:BT:55:VAL:HG13 | 41:BT:85:VAL:HG12 | 2.00 | 0.44 |
| 1:CA:1002:G:H2' | 1:CA:1003:G:O4' | 2.17 | 0.44 |
| 1:CA:1071:C:O2' | 1:CA:1072:G:H5' | 2.16 | 0.44 |
| 1:CA:1436:U:H2' | 1:CA:1437:A:C8 | 2.52 | 0.44 |
| 1:CA:1454:G:H2' | 1:CA:1455:G:H8 | 1.81 | 0.44 |
| 1:CA:202:G:H2' | 1:CA:203:G:C8 | 2.52 | 0.44 |
| 1:CA:669:G:H2' | 1:CA:670:G:C8 | 2.52 | 0.44 |
| 1:CA:797:C:O2' | 1:CA:798:U:H5' | 2.17 | 0.44 |
| 1:CA:87:C:H2' | 1:CA:88:U:C6 | 2.51 | 0.44 |
| 1:CA:968:A:H3' | 1:CA:969:A:C5' | 2.47 | 0.44 |
| 20:CB:129:THR:C | 20:CB:131:LYS:N | 2.69 | 0.44 |
| 20:CB:138:ARG:O | 20:CB:141:GLU:HB2 | 2.17 | 0.44 |
| 5:CF:40:GLU:CB | 5:CF:61:LEU:HB2 | 2.46 | 0.44 |
| 6:CG:101:ARG:HG2 | 6:CG:105:GLU:OE2 | 2.17 | 0.44 |
| 6:CG:14:ASP:HB2 | 6:CG:19:SER:O | 2.17 | 0.44 |
| 10:CK:88:PRO:HG3 | 21:CU:28:LEU:HD21 | 1.99 | 0.44 |
| 13:CN:16:ALA:O | 13:CN:20:PHE:HB3 | 2.17 | 0.44 |
| 23:DB:1251:C:O2' | 23:DB:1252:G:H3' | 2.17 | 0.44 |
| 23:DB:1505:A:H2' | 23:DB:1506:U:C6 | 2.52 | 0.44 |
| 23:DB:1734:G:O2' | 23:DB:1735:A:H5' | 2.17 | 0.44 |
| 23:DB:1932:A:H2' | 23:DB:1933:G:O4' | 2.17 | 0.44 |
| 23:DB:2107:G:H3' | 23:DB:2108:A:H8 | 1.82 | 0.44 |
| 23:DB:2215:C:H2' | 23:DB:2216:G:H8 | 1.81 | 0.44 |
| 23:DB:2578:G:O2' | 23:DB:2579:C:H5' | 2.16 | 0.44 |
| 23:DB:2439:A:C8 | 23:DB:2586:U:H4' | 2.52 | 0.44 |
| 23:DB:2742:G:O2' | 23:DB:2743:U:H5' | 2.17 | 0.44 |
| 23:DB:522:A:H2' | 23:DB:523:C:H6 | 1.80 | 0.44 |
| 23:DB:643:A:N7 | 23:DB:644:A:N7 | 2.65 | 0.44 |
| 23:DB:817:C:O2' | 23:DB:839:U:H5'' | 2.16 | 0.44 |
| 23:DB:921:C:H2' | 23:DB:922:C:C6 | 2.52 | 0.44 |
| 26:DD:101:PHE:CZ | 26:DD:204:LYS:HA | 2.51 | 0.44 |
| 27:DE:3:LEU:O | 27:DE:12:LEU:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:673:C:H5'' | 27:DE:76:PRO:HD2 | 1.99 | 0.44 |
| 52:DI:102:ARG:HG3 | 52:DI:141:ASP:CB | 2.47 | 0.44 |
| 31:DJ:18:VAL:CG1 | 31:DJ:54:ILE:HD11 | 2.46 | 0.44 |
| 35:DN:80:PHE:O | 35:DN:85:PRO:HD3 | 2.18 | 0.44 |
| 37:DP:31:VAL:CG1 | 37:DP:38:ARG:HB2 | 2.48 | 0.44 |
| 37:DP:61:ARG:HD3 | 37:DP:70:GLU:CG | 2.45 | 0.44 |
| 37:DP:75:THR:O | 37:DP:80:VAL:HG11 | 2.16 | 0.44 |
| 42:DU:86:PHE:CG | 42:DU:87:GLU:N | 2.85 | 0.44 |
| 24:DV:28:ALA:HA | 24:DV:88:HIS:ND1 | 2.32 | 0.44 |
| 24:DV:89:ILE:O | 24:DV:89:ILE:HD12 | 2.17 | 0.44 |
| 1:AA:1020:G:H2' | 1:AA:1020:G:N3 | 2.32 | 0.44 |
| 1:AA:1035:A:H2' | 1:AA:1036:A:C8 | 2.51 | 0.44 |
| 1:AA:1138:G:N3 | 1:AA:1138:G:H3' | 2.32 | 0.44 |
| 1:AA:1194:U:H2' | 1:AA:1195:C:C6 | 2.53 | 0.44 |
| 1:AA:1276:G:H2' | 1:AA:1277:C:C6 | 2.53 | 0.44 |
| 1:AA:1342:C:O2' | 8:AI:125:GLN:HB3 | 2.17 | 0.44 |
| 1:AA:1408:A:O2' | 1:AA:1409:C:H5' | 2.17 | 0.44 |
| 1:AA:25:C:C5' | 1:AA:524:G:H1' | 2.47 | 0.44 |
| 1:AA:284:C:O2' | 1:AA:285:C:H5' | 2.17 | 0.44 |
| 1:AA:58:C:O2' | 1:AA:59:A:H5' | 2.17 | 0.44 |
| 1:AA:967:C:H4' | 8:AI:129:ARG:HG2 | 1.99 | 0.44 |
| 20:AB:14:HIS:HD2 | 20:AB:202:ASN:H | 1.64 | 0.44 |
| 2:AC:35:ASP:O | 2:AC:39:ARG:HG3 | 2.16 | 0.44 |
| 5:AF:3:HIS:HA | 5:AF:64:VAL:O | 2.17 | 0.44 |
| 1:AA:653:U:C6 | 7:AH:55:LYS:HE2 | 2.52 | 0.44 |
| 8:AI:20:ILE:CD1 | 8:AI:85:ALA:HB3 | 2.48 | 0.44 |
| 12:AM:77:LYS:O | 12:AM:80:MET:HG2 | 2.16 | 0.44 |
| 5:AF:45:ARG:NH2 | 17:AR:25:ILE:HD13 | 2.32 | 0.44 |
| 17:AR:57:ALA:O | 17:AR:60:ARG:HG3 | 2.16 | 0.44 |
| 19:AT:56:ILE:O | 19:AT:60:GLN:HG2 | 2.16 | 0.44 |
| 47:B0:18:HIS:N | 47:B0:18:HIS:HD1 | 2.14 | 0.44 |
| 48:B1:7:LYS:NZ | 50:B3:33:THR:HG22 | 2.32 | 0.44 |
| 50:B3:6:VAL:HB | 50:B3:60:CYS:HB3 | 1.98 | 0.44 |
| 22:BA:35:C:H2' | 22:BA:36:C:O4' | 2.17 | 0.44 |
| 22:BA:93:C:O2' | 22:BA:94:A:H5' | 2.16 | 0.44 |
| 23:BB:156:A:O2' | 23:BB:157:C:H5' | 2.18 | 0.44 |
| 23:BB:19:A:H2' | 23:BB:20:C:C6 | 2.52 | 0.44 |
| 23:BB:2300:C:H2' | 23:BB:2301:C:H6 | 1.81 | 0.44 |
| 23:BB:2743:U:H3' | 23:BB:2744:G:H5'' | 1.99 | 0.44 |
| 23:BB:2884:U:H4' | 47:B0:49:ARG:NH2 | 2.32 | 0.44 |
| 23:BB:533:G:H2' | 23:BB:534:U:C6 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:616:A:H5'' | 56:BB:3449:HOH:O | 2.16 | 0.44 |
| 23:BB:786:C:H5'' | 23:BB:1780:A:C8 | 2.52 | 0.44 |
| 25:BC:185:ALA:C | 25:BC:187:CYS:H | 2.20 | 0.44 |
| 23:BB:729:G:C5 | 25:BC:206:LYS:HB2 | 2.52 | 0.44 |
| 25:BC:250:GLN:CD | 25:BC:254:LYS:HG2 | 2.37 | 0.44 |
| 26:BD:110:THR:HG21 | 26:BD:169:ARG:HH11 | 1.83 | 0.44 |
| 26:BD:16:THR:HG22 | 26:BD:17:GLU:N | 2.33 | 0.44 |
| 26:BD:35:THR:OG1 | 26:BD:49:GLN:HG2 | 2.17 | 0.44 |
| 26:BD:51:THR:HG22 | 26:BD:76:GLY:HA3 | 1.99 | 0.44 |
| 27:BE:149:ILE:HG23 | 27:BE:188:MET:HA | 1.99 | 0.44 |
| 29:BG:94:ARG:HB2 | 29:BG:127:GLN:HG2 | 1.98 | 0.44 |
| 30:BH:27:ARG:HH11 | 46:BZ:64:ILE:CD1 | 2.30 | 0.44 |
| 23:BB:1060:U:C4 | 52:BI:131:THR:HG22 | 2.51 | 0.44 |
| 31:BJ:103:ILE:HG13 | 31:BJ:104:ALA:N | 2.32 | 0.44 |
| 32:BK:87:LEU:HD12 | 32:BK:92:GLU:C | 2.37 | 0.44 |
| 34:BM:32:GLY:HA2 | 34:BM:117:PHE:CZ | 2.52 | 0.44 |
| 23:BB:2816:G:O3' | 35:BN:99:LYS:HE3 | 2.16 | 0.44 |
| 36:BO:52:SER:H | 36:BO:55:GLU:HG3 | 1.82 | 0.44 |
| 36:BO:9:ARG:HA | 36:BO:12:THR:OG1 | 2.17 | 0.44 |
| 39:BR:60:LYS:H | 39:BR:100:GLY:N | 2.15 | 0.44 |
| 46:BZ:53:ALA:C | 46:BZ:55:GLY:H | 2.18 | 0.44 |
| 1:CA:1081:A:O2' | 1:CA:1082:A:H5' | 2.17 | 0.44 |
| 1:CA:1138:G:H3' | 1:CA:1138:G:N3 | 2.33 | 0.44 |
| 1:CA:1313:U:OP2 | 18:CS:5:LYS:HA | 2.17 | 0.44 |
| 1:CA:227:G:H2' | 1:CA:228:A:C8 | 2.53 | 0.44 |
| 1:CA:366:A:H1' | 1:CA:395:C:O2 | 2.16 | 0.44 |
| 1:CA:454:G:O2' | 1:CA:455:G:H5' | 2.17 | 0.44 |
| 1:CA:473:U:H6 | 1:CA:473:U:O5' | 2.00 | 0.44 |
| 1:CA:526:C:OP2 | 11:CL:87:LYS:HE3 | 2.18 | 0.44 |
| 1:CA:647:C:H2' | 1:CA:648:A:C8 | 2.51 | 0.44 |
| 20:CB:16:GLY:HA2 | 20:CB:40:ILE:H | 1.80 | 0.44 |
| 2:CC:63:ILE:HD12 | 2:CC:90:VAL:HG12 | 1.99 | 0.44 |
| 5:CF:3:HIS:HA | 5:CF:64:VAL:O | 2.17 | 0.44 |
| 1:CA:716:A:H1' | 10:CK:119:GLY:HA2 | 1.99 | 0.44 |
| 11:CL:49:ARG:N | 11:CL:49:ARG:HD2 | 2.32 | 0.44 |
| 47:D0:9:ARG:HB2 | 47:D0:12:ARG:NH2 | 2.33 | 0.44 |
| 48:D1:47:ILE:H | 48:D1:47:ILE:HD12 | 1.82 | 0.44 |
| 22:DA:94:A:O2' | 22:DA:95:U:H5' | 2.17 | 0.44 |
| 23:DB:1210:G:H5' | 23:DB:1212:G:O4' | 2.17 | 0.44 |
| 23:DB:131:A:H2' | 23:DB:132:G:H8 | 1.82 | 0.44 |
| 23:DB:1374:G:O2' | 23:DB:1375:U:H5' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1641:A:H2' | 23:DB:1642:G:O4' | 2.18 | 0.44 |
| 23:DB:1874:C:H2' | 23:DB:1875:G:O4' | 2.18 | 0.44 |
| 23:DB:2027:G:O2' | 23:DB:2028:U:H5' | 2.18 | 0.44 |
| 23:DB:2156:G:C2' | 23:DB:2157:G:H4' | 2.45 | 0.44 |
| 23:DB:2230:G:H2' | 23:DB:2231:U:C6 | 2.52 | 0.44 |
| 23:DB:2369:A:H2' | 23:DB:2370:G:H8 | 1.83 | 0.44 |
| 23:DB:2611:C:O2' | 23:DB:2612:C:H5' | 2.18 | 0.44 |
| 23:DB:265:A:O2' | 23:DB:266:G:C4' | 2.64 | 0.44 |
| 23:DB:2869:G:H2' | 23:DB:2870:C:C6 | 2.52 | 0.44 |
| 23:DB:599:A:H2' | 23:DB:600:G:H8 | 1.83 | 0.44 |
| 23:DB:746:U:O3' | 40:DS:90:LYS:NZ | 2.49 | 0.44 |
| 25:DC:6:LYS:O | 25:DC:8:THR:HG23 | 2.17 | 0.44 |
| 27:DE:38:GLY:C | 27:DE:40:ARG:H | 2.19 | 0.44 |
| 52:DI:100:ILE:HG23 | 52:DI:104:GLN:OE1 | 2.17 | 0.44 |
| 52:DI:27:LEU:HD23 | 52:DI:27:LEU:N | 2.22 | 0.44 |
| 31:DJ:101:ILE:O | 31:DJ:104:ALA:HB3 | 2.16 | 0.44 |
| 32:DK:113:MET:HE1 | 32:DK:116:ILE:HD11 | 1.98 | 0.44 |
| 27:DE:108:ILE:HG13 | 33:DL:2:ARG:HH22 | 1.80 | 0.44 |
| 38:DQ:33:VAL:HG23 | 38:DQ:34:ALA:H | 1.81 | 0.44 |
| 39:DR:14:VAL:HG21 | 39:DR:98:ILE:HG12 | 2.00 | 0.44 |
| 41:DT:74:ILE:HG13 | 41:DT:75:GLY:N | 2.32 | 0.44 |
| 42:DU:13:LEU:HD12 | 42:DU:68:ASN:O | 2.17 | 0.44 |
| 42:DU:20:LYS:HB3 | 42:DU:21:ARG:H | 1.62 | 0.44 |
| 43:DW:30:VAL:O | 43:DW:30:VAL:HG22 | 2.16 | 0.44 |
| 1:AA:1163:A:H2' | 1:AA:1164:G:C8 | 2.51 | 0.44 |
| 1:AA:1212:U:H4' | 1:AA:1213:A:C8 | 2.53 | 0.44 |
| 1:AA:1222:G:H2' | 1:AA:1223:C:H5' | 1.99 | 0.44 |
| 1:AA:1451:U:O3' | 1:AA:1452:C:H6 | 2.00 | 0.44 |
| 1:AA:203:G:H1' | 1:AA:465:A:N6 | 2.32 | 0.44 |
| 1:AA:237:G:H2' | 1:AA:238:A:C8 | 2.51 | 0.44 |
| 1:AA:395:C:H2' | 1:AA:396:C:C6 | 2.52 | 0.44 |
| 1:AA:513:C:H2' | 1:AA:514:C:H6 | 1.83 | 0.44 |
| 1:AA:626:G:H2' | 1:AA:627:G:C8 | 2.53 | 0.44 |
| 1:AA:677:U:H1' | 10:AK:120:CYS:SG | 2.58 | 0.44 |
| 1:AA:781:A:H2' | 1:AA:782:A:C5' | 2.40 | 0.44 |
| 1:AA:817:C:H1' | 1:AA:819:A:C5' | 2.40 | 0.44 |
| 3:AD:97:LEU:HD13 | 3:AD:136:VAL:CG1 | 2.47 | 0.44 |
| 9:AJ:80:THR:HG21 | 9:AJ:82:LYS:NZ | 2.32 | 0.44 |
| 9:AJ:8:ILE:HA | 9:AJ:100:ILE:HG22 | 1.99 | 0.44 |
| 18:AS:33:TRP:C | 18:AS:35:ARG:H | 2.20 | 0.44 |
| 47:B0:18:HIS:C | 47:B0:20:ALA:H | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:B3:61:LEU:N | 50:B3:62:PRO:HD3 | 2.32 | 0.44 |
| 23:BB:1372:U:O2' | 23:BB:1373:A:H5' | 2.17 | 0.44 |
| 23:BB:1544:A:H2' | 23:BB:1545:A:C8 | 2.52 | 0.44 |
| 23:BB:1727:C:H2' | 23:BB:1728:C:H6 | 1.83 | 0.44 |
| 23:BB:118:A:N3 | 23:BB:178:G:H1' | 2.31 | 0.44 |
| 23:BB:1792:G:OP1 | 25:BC:204:LEU:HD12 | 2.17 | 0.44 |
| 23:BB:1803:A:H4' | 25:BC:256:THR:OG1 | 2.17 | 0.44 |
| 23:BB:1932:A:H2' | 23:BB:1933:G:O4' | 2.18 | 0.44 |
| 23:BB:2217:G:H2' | 23:BB:2218:G:H8 | 1.83 | 0.44 |
| 23:BB:2246:G:H2' | 23:BB:2247:A:H8 | 1.81 | 0.44 |
| 23:BB:2306:C:C5 | 23:BB:2307:G:H2' | 2.52 | 0.44 |
| 23:BB:240:C:H5'' | 23:BB:241:A:H5'' | 1.98 | 0.44 |
| 23:BB:264:C:H2' | 23:BB:265:A:H5'' | 2.00 | 0.44 |
| 23:BB:342:A:H2' | 23:BB:343:C:O4' | 2.17 | 0.44 |
| 23:BB:817:C:O2' | 23:BB:839:U:H5'' | 2.17 | 0.44 |
| 25:BC:199:HIS:C | 25:BC:201:LEU:H | 2.21 | 0.44 |
| 26:BD:108:ASP:N | 26:BD:204:LYS:O | 2.51 | 0.44 |
| 26:BD:11:MET:H | 26:BD:25:THR:HA | 1.82 | 0.44 |
| 23:BB:674:G:O3' | 27:BE:60:TRP:HZ2 | 2.01 | 0.44 |
| 28:BF:62:GLN:HE21 | 28:BF:91:ARG:NE | 2.15 | 0.44 |
| 30:BH:58:LEU:HG | 30:BH:62:LEU:HD23 | 2.00 | 0.44 |
| 32:BK:85:VAL:HG21 | 32:BK:115:ILE:HD11 | 1.99 | 0.44 |
| 33:BL:47:ARG:HG3 | 33:BL:48:ARG:N | 2.32 | 0.44 |
| 35:BN:61:ALA:C | 35:BN:63:ARG:N | 2.71 | 0.44 |
| 38:BQ:38:VAL:O | 38:BQ:41:ALA:N | 2.51 | 0.44 |
| 38:BQ:81:GLY:HA3 | 38:BQ:116:LEU:CD1 | 2.48 | 0.44 |
| 38:BQ:96:ASP:C | 38:BQ:98:ALA:H | 2.19 | 0.44 |
| 39:BR:39:LEU:CA | 39:BR:53:PHE:HA | 2.44 | 0.44 |
| 41:BT:54:GLU:HB3 | 41:BT:88:LYS:HB2 | 1.99 | 0.44 |
| 24:BV:66:ASP:HB2 | 24:BV:68:LYS:CE | 2.42 | 0.44 |
| 43:BW:18:LYS:H | 43:BW:35:ILE:CG2 | 2.29 | 0.44 |
| 43:BW:50:VAL:HG23 | 43:BW:51:GLY:H | 1.82 | 0.44 |
| 1:CA:996:A:H2 | 1:CA:1045:C:HO2' | 1.63 | 0.44 |
| 1:CA:938:A:H1' | 1:CA:1376:U:O2' | 2.17 | 0.44 |
| 1:CA:1498:U:H6 | 1:CA:1498:U:O5' | 2.00 | 0.44 |
| 1:CA:1514:G:H2' | 1:CA:1515:G:H8 | 1.83 | 0.44 |
| 1:CA:837:U:H2' | 1:CA:838:G:H8 | 1.82 | 0.44 |
| 1:CA:859:G:O2' | 1:CA:860:A:H5' | 2.16 | 0.44 |
| 2:CC:154:GLY:HA2 | 2:CC:163:ARG:H | 1.82 | 0.44 |
| 3:CD:13:ARG:HG3 | 3:CD:55:ARG:NH1 | 2.33 | 0.44 |
| 3:CD:20:LEU:C | 3:CD:21:LYS:HD2 | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CE:33:THR:HG22 | 4:CE:51:LYS:CB | 2.46 | 0.44 |
| 6:CG:67:ASN:ND2 | 6:CG:127:ALA:HA | 2.32 | 0.44 |
| 6:CG:49:LEU:HD21 | 6:CG:60:ALA:CB | 2.46 | 0.44 |
| 13:CN:26:LEU:HD23 | 13:CN:27:LYS:H | 1.81 | 0.44 |
| 1:CA:564:C:C4 | 16:CQ:32:ILE:HD11 | 2.52 | 0.44 |
| 18:CS:38:THR:HG22 | 18:CS:68:HIS:O | 2.16 | 0.44 |
| 50:D3:6:VAL:HB | 50:D3:60:CYS:HB3 | 1.99 | 0.44 |
| 23:DB:1098:A:O5' | 52:DI:3:LYS:HG2 | 2.17 | 0.44 |
| 23:DB:1244:A:H5'' | 33:DL:8:PRO:CD | 2.29 | 0.44 |
| 23:DB:138:U:O2' | 23:DB:140:C:OP1 | 2.34 | 0.44 |
| 23:DB:1444:G:H2' | 23:DB:1445:G:H8 | 1.82 | 0.44 |
| 23:DB:1727:C:H2' | 23:DB:1728:C:H6 | 1.82 | 0.44 |
| 23:DB:1803:A:O3' | 25:DC:256:THR:HB | 2.17 | 0.44 |
| 23:DB:2199:A:H3' | 23:DB:2200:C:C6 | 2.52 | 0.44 |
| 23:DB:2252:G:O2' | 23:DB:2253:G:H5' | 2.17 | 0.44 |
| 23:DB:2262:U:O2' | 23:DB:2263:C:H5' | 2.18 | 0.44 |
| 23:DB:2282:G:H5'' | 23:DB:2283:C:O4' | 2.17 | 0.44 |
| 23:DB:2768:U:H2' | 23:DB:2769:U:O4' | 2.17 | 0.44 |
| 23:DB:2886:A:H2' | 23:DB:2887:A:O4' | 2.17 | 0.44 |
| 23:DB:2901:C:O2' | 23:DB:2902:C:H5' | 2.18 | 0.44 |
| 23:DB:80:G:O5' | 23:DB:346:A:H1' | 2.16 | 0.44 |
| 23:DB:53:A:H2' | 23:DB:54:G:O4' | 2.17 | 0.44 |
| 25:DC:221:GLY:O | 25:DC:223:ALA:N | 2.51 | 0.44 |
| 26:DD:114:LYS:HZ1 | 26:DD:116:LYS:HG3 | 1.81 | 0.44 |
| 26:DD:178:VAL:HB | 26:DD:188:LEU:CB | 2.48 | 0.44 |
| 26:DD:7:LYS:HD2 | 26:DD:198:GLY:HA2 | 2.00 | 0.44 |
| 27:DE:150:THR:O | 27:DE:192:ALA:HB2 | 2.17 | 0.44 |
| 28:DF:121:PHE:HB2 | 28:DF:126:ASN:O | 2.18 | 0.44 |
| 28:DF:126:ASN:CB | 28:DF:156:THR:HA | 2.46 | 0.44 |
| 28:DF:71:LYS:HG2 | 28:DF:71:LYS:O | 2.18 | 0.44 |
| 30:DH:39:ALA:O | 30:DH:41:LYS:N | 2.49 | 0.44 |
| 52:DI:70:THR:O | 52:DI:70:THR:HG23 | 2.17 | 0.44 |
| 31:DJ:11:VAL:HG21 | 31:DJ:13:ARG:NH1 | 2.33 | 0.44 |
| 32:DK:35:VAL:CG2 | 32:DK:36:GLY:H | 2.07 | 0.44 |
| 37:DP:105:LYS:HD3 | 37:DP:105:LYS:HA | 1.81 | 0.44 |
| 38:DQ:57:ARG:HH12 | 38:DQ:61:ILE:CD1 | 2.31 | 0.44 |
| 38:DQ:81:GLY:O | 38:DQ:85:ALA:N | 2.50 | 0.44 |
| 39:DR:49:ILE:HD13 | 39:DR:53:PHE:H | 1.82 | 0.44 |
| 23:DB:1225:G:P | 39:DR:71:LYS:HZ2 | 2.41 | 0.44 |
| 23:DB:1161:C:H4' | 39:DR:8:GLY:O | 2.17 | 0.44 |
| 43:DW:19:ARG:NE | 43:DW:19:ARG:H | 2.15 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1178:G:H2' | 1:AA:1180:A:OP2 | 2.17 | 0.44 |
| 1:AA:1314:C:H2' | 1:AA:1315:U:C6 | 2.52 | 0.44 |
| 1:AA:1390:U:H2' | 1:AA:1391:U:C6 | 2.51 | 0.44 |
| 1:AA:338:A:H2' | 1:AA:339:C:C6 | 2.53 | 0.44 |
| 1:AA:473:U:H6 | 1:AA:473:U:O5' | 2.00 | 0.44 |
| 1:AA:488:C:O2' | 1:AA:489:C:H5' | 2.18 | 0.44 |
| 1:AA:596:A:H2' | 1:AA:597:G:C8 | 2.52 | 0.44 |
| 1:AA:938:A:H1' | 1:AA:1376:U:O2' | 2.18 | 0.44 |
| 1:AA:993:G:N2 | 1:AA:996:A:N6 | 2.65 | 0.44 |
| 20:AB:16:GLY:HA2 | 20:AB:40:ILE:H | 1.81 | 0.44 |
| 2:AC:174:LEU:HD11 | 2:AC:200:TRP:NE1 | 2.32 | 0.44 |
| 5:AF:67:PRO:O | 5:AF:70:VAL:HG22 | 2.17 | 0.44 |
| 6:AG:55:LYS:HG2 | 6:AG:55:LYS:H | 1.62 | 0.44 |
| 9:AJ:12:ALA:H | 9:AJ:18:ILE:HD13 | 1.82 | 0.44 |
| 11:AL:60:PHE:O | 11:AL:62:VAL:HG13 | 2.17 | 0.44 |
| 11:AL:71:HIS:HD2 | 11:AL:73:LEU:HG | 1.82 | 0.44 |
| 13:AN:20:PHE:CD2 | 13:AN:55:SER:HA | 2.51 | 0.44 |
| 13:AN:30:ILE:CG2 | 13:AN:41:TRP:HB2 | 2.44 | 0.44 |
| 16:AQ:10:ARG:NH2 | 16:AQ:55:GLY:HA2 | 2.33 | 0.44 |
| 18:AS:39:ILE:HG12 | 18:AS:70:LEU:CD1 | 2.48 | 0.44 |
| 23:BB:1059:G:H2' | 23:BB:1060:U:C6 | 2.52 | 0.44 |
| 23:BB:1173:U:N3 | 23:BB:1174:U:H1' | 2.32 | 0.44 |
| 23:BB:1341:G:O4' | 41:BT:61:LEU:HD23 | 2.16 | 0.44 |
| 23:BB:143:C:H2' | 23:BB:144:A:C8 | 2.51 | 0.44 |
| 23:BB:1387:A:H4' | 23:BB:1469:A:H1' | 1.98 | 0.44 |
| 23:BB:1541:C:O2' | 23:BB:1542:U:H5' | 2.17 | 0.44 |
| 23:BB:1640:A:O2' | 23:BB:1641:A:H5' | 2.18 | 0.44 |
| 23:BB:1870:C:H3' | 23:BB:1871:A:C8 | 2.52 | 0.44 |
| 23:BB:2526:G:H5' | 23:BB:2742:G:O2' | 2.16 | 0.44 |
| 23:BB:26:G:H2' | 23:BB:27:G:C1' | 2.48 | 0.44 |
| 23:BB:2880:C:C1' | 35:BN:91:ALA:HB3 | 2.46 | 0.44 |
| 23:BB:2886:A:H2' | 23:BB:2887:A:O4' | 2.16 | 0.44 |
| 23:BB:591:U:H1' | 50:B3:1:PRO:H2 | 1.77 | 0.44 |
| 23:BB:841:G:O2' | 23:BB:842:U:H5' | 2.17 | 0.44 |
| 23:BB:84:A:H4' | 23:BB:85:G:O5' | 2.16 | 0.44 |
| 25:BC:68:ARG:HB3 | 25:BC:128:THR:OG1 | 2.17 | 0.44 |
| 26:BD:3:GLY:HA2 | 26:BD:101:PHE:CZ | 2.53 | 0.44 |
| 28:BF:69:ALA:HB3 | 28:BF:80:GLN:O | 2.18 | 0.44 |
| 29:BG:94:ARG:HH21 | 29:BG:105:SER:H | 1.63 | 0.44 |
| 31:BJ:4:PHE:HB3 | 31:BJ:44:TYR:CD1 | 2.53 | 0.44 |
| 33:BL:132:ARG:O | 33:BL:136:GLU:HG2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BN:80:PHE:O | 35:BN:85:PRO:HD3 | 2.17 | 0.44 |
| 37:BP:33:GLU:OE2 | 37:BP:38:ARG:NE | 2.49 | 0.44 |
| 37:BP:31:VAL:CG1 | 37:BP:38:ARG:HB2 | 2.47 | 0.44 |
| 37:BP:61:ARG:HD3 | 37:BP:70:GLU:CG | 2.47 | 0.44 |
| 38:BQ:108:LEU:HA | 39:BR:48:LYS:HD3 | 1.99 | 0.44 |
| 38:BQ:7:VAL:O | 38:BQ:8:ILE:C | 2.56 | 0.44 |
| 38:BQ:91:ARG:HB2 | 39:BR:11:GLN:CD | 2.38 | 0.44 |
| 39:BR:38:VAL:O | 39:BR:53:PHE:HB3 | 2.17 | 0.44 |
| 39:BR:71:LYS:HG2 | 39:BR:73:LYS:HZ3 | 1.79 | 0.44 |
| 23:BB:329:G:N1 | 42:BU:16:LYS:HE3 | 2.30 | 0.44 |
| 42:BU:84:PHE:O | 42:BU:85:ARG:CB | 2.63 | 0.44 |
| 44:BX:7:ARG:HD2 | 44:BX:7:ARG:HA | 1.83 | 0.44 |
| 1:CA:1329:A:O2' | 1:CA:1330:U:H5' | 2.17 | 0.44 |
| 1:CA:175:C:O2 | 1:CA:1447:A:H2 | 2.01 | 0.44 |
| 1:CA:631:C:H3' | 1:CA:632:U:H5' | 1.99 | 0.44 |
| 1:CA:634:C:H2' | 1:CA:635:A:C8 | 2.52 | 0.44 |
| 1:CA:939:G:H2' | 1:CA:940:C:C6 | 2.52 | 0.44 |
| 1:CA:982:U:H5'' | 13:CN:5:MET:HE1 | 1.99 | 0.44 |
| 2:CC:78:LYS:HE3 | 2:CC:79:LYS:NZ | 2.32 | 0.44 |
| 1:CA:1069:C:H5'' | 4:CE:25:LYS:HZ3 | 1.82 | 0.44 |
| 8:CI:30:ASN:ND2 | 8:CI:65:THR:HA | 2.32 | 0.44 |
| 10:CK:126:ARG:HB2 | 21:CU:33:ARG:HD2 | 2.00 | 0.44 |
| 12:CM:37:GLY:O | 12:CM:38:ILE:HD13 | 2.18 | 0.44 |
| 13:CN:60:ARG:NH2 | 13:CN:69:PRO:HB3 | 2.32 | 0.44 |
| 13:CN:86:ALA:HA | 13:CN:91:GLU:HG3 | 1.99 | 0.44 |
| 16:CQ:60:ILE:HG22 | 16:CQ:74:LEU:HA | 1.99 | 0.44 |
| 5:CF:45:ARG:HH22 | 17:CR:25:ILE:HD13 | 1.81 | 0.44 |
| 10:CK:122:PRO:HD2 | 21:CU:35:GLU:HG2 | 2.00 | 0.44 |
| 48:D1:18:HIS:NE2 | 48:D1:40:PRO:HD2 | 2.31 | 0.44 |
| 49:D2:39:ARG:HG3 | 49:D2:39:ARG:HH11 | 1.81 | 0.44 |
| 22:DA:116:G:H4' | 36:DO:54:VAL:CG2 | 2.40 | 0.44 |
| 23:DB:1092:C:H2' | 23:DB:1093:G:C5' | 2.46 | 0.44 |
| 23:DB:108:G:O2' | 23:DB:109:C:H5' | 2.17 | 0.44 |
| 23:DB:1258:U:H2' | 23:DB:1259:G:C8 | 2.52 | 0.44 |
| 23:DB:1344:U:O2' | 23:DB:1385:A:H2' | 2.18 | 0.44 |
| 23:DB:1525:A:H2' | 23:DB:1526:C:O4' | 2.18 | 0.44 |
| 23:DB:159:G:O2' | 23:DB:160:A:H5'' | 2.17 | 0.44 |
| 23:DB:1711:A:O2' | 23:DB:1712:U:H5' | 2.17 | 0.44 |
| 23:DB:2104:C:H6 | 23:DB:2104:C:H3' | 1.81 | 0.44 |
| 23:DB:246:C:O2' | 23:DB:247:G:H5' | 2.17 | 0.44 |
| 23:DB:2531:A:O2' | 23:DB:2532:G:H5' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2693:G:H2' | 23:DB:2694:G:C8 | 2.48 | 0.44 |
| 23:DB:67:U:H2' | 23:DB:68:G:C8 | 2.52 | 0.44 |
| 23:DB:714:U:H2' | 23:DB:716:A:OP2 | 2.18 | 0.44 |
| 23:DB:993:G:N3 | 39:DR:91:GLN:NE2 | 2.57 | 0.44 |
| 25:DC:216:ARG:HH11 | 25:DC:216:ARG:HG3 | 1.81 | 0.44 |
| 28:DF:162:ASP:C | 28:DF:166:ARG:HH11 | 2.20 | 0.44 |
| 28:DF:3:LEU:O | 28:DF:3:LEU:HD13 | 2.17 | 0.44 |
| 28:DF:43:ILE:HG13 | 28:DF:44:ALA:N | 2.33 | 0.44 |
| 28:DF:70:ARG:HA | 28:DF:80:GLN:NE2 | 2.32 | 0.44 |
| 30:DH:101:ASP:O | 30:DH:104:THR:HB | 2.17 | 0.44 |
| 30:DH:112:LYS:HA | 30:DH:132:PHE:HE1 | 1.81 | 0.44 |
| 52:DI:140:GLU:CD | 52:DI:140:GLU:H | 2.21 | 0.44 |
| 31:DJ:40:HIS:HE1 | 31:DJ:41:LYS:HE3 | 1.82 | 0.44 |
| 32:DK:35:VAL:HG12 | 32:DK:69:VAL:HG22 | 1.98 | 0.44 |
| 33:DL:141:LYS:C | 33:DL:142:ILE:HD12 | 2.38 | 0.44 |
| 34:DM:10:ARG:HG3 | 34:DM:10:ARG:HH21 | 1.83 | 0.44 |
| 41:DT:65:GLY:HA3 | 41:DT:76:ARG:NH2 | 2.33 | 0.44 |
| 1:AA:1080:A:O3' | 4:AE:20:VAL:HG11 | 2.17 | 0.44 |
| 1:AA:1014:A:N3 | 1:AA:1219:A:H1' | 2.33 | 0.44 |
| 1:AA:1219:A:H2' | 1:AA:1220:G:H8 | 1.82 | 0.44 |
| 1:AA:1388:C:H2' | 1:AA:1389:C:H6 | 1.83 | 0.44 |
| 1:AA:1510:C:H2' | 1:AA:1511:G:H8 | 1.82 | 0.44 |
| 1:AA:458:U:H2' | 1:AA:459:A:C8 | 2.53 | 0.44 |
| 1:AA:486:U:O2' | 1:AA:487:A:H5' | 2.18 | 0.44 |
| 1:AA:537:G:H2' | 1:AA:538:G:C8 | 2.52 | 0.44 |
| 1:AA:586:C:O2' | 1:AA:587:G:H5' | 2.17 | 0.44 |
| 1:AA:940:C:H2' | 1:AA:941:G:C8 | 2.52 | 0.44 |
| 20:AB:18:GLN:HB2 | 20:AB:188:THR:OG1 | 2.17 | 0.44 |
| 20:AB:218:ALA:O | 20:AB:222:GLU:N | 2.51 | 0.44 |
| 3:AD:123:MET:HA | 3:AD:128:VAL:HA | 1.99 | 0.44 |
| 3:AD:25:ARG:HD3 | 3:AD:26:ALA:HB3 | 1.99 | 0.44 |
| 8:AI:10:ARG:CB | 8:AI:15:ALA:HA | 2.48 | 0.44 |
| 8:AI:19:PHE:HB2 | 8:AI:63:TYR:HB3 | 1.99 | 0.44 |
| 10:AK:74:LYS:HG3 | 10:AK:104:PHE:CZ | 2.52 | 0.44 |
| 13:AN:23:ARG:C | 13:AN:25:GLU:H | 2.21 | 0.44 |
| 2:AC:5:HIS:ND1 | 13:AN:88:MET:HB3 | 2.33 | 0.44 |
| 13:AN:86:ALA:HA | 13:AN:91:GLU:HG3 | 1.99 | 0.44 |
| 1:AA:751:U:O2' | 14:AO:24:THR:HG23 | 2.18 | 0.44 |
| 10:AK:112:VAL:HA | 17:AR:72:ARG:HH21 | 1.82 | 0.44 |
| 21:AU:39:LYS:N | 21:AU:40:PRO:CD | 2.81 | 0.44 |
| 49:B2:19:ARG:O | 49:B2:22:MET:HB2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1309:G:H4' | 49:B2:7:PRO:HB2 | 1.99 | 0.44 |
| 23:BB:1091:G:O2' | 23:BB:1092:C:H5' | 2.17 | 0.44 |
| 23:BB:1163:G:H4' | 39:BR:92:TRP:NE1 | 2.31 | 0.44 |
| 23:BB:1183:U:O2' | 23:BB:1184:U:H5' | 2.17 | 0.44 |
| 23:BB:124:G:C5 | 49:B2:19:ARG:NH1 | 2.85 | 0.44 |
| 23:BB:1439:A:H1' | 23:BB:1553:A:N6 | 2.33 | 0.44 |
| 23:BB:2300:C:H2' | 23:BB:2301:C:C6 | 2.52 | 0.44 |
| 23:BB:264:C:O2' | 23:BB:265:A:H5'' | 2.18 | 0.44 |
| 23:BB:601:C:O2 | 23:BB:605:G:H4' | 2.17 | 0.44 |
| 23:BB:629:G:O2' | 23:BB:630:G:H5' | 2.18 | 0.44 |
| 23:BB:935:C:H2' | 23:BB:936:A:C8 | 2.52 | 0.44 |
| 27:BE:29:HIS:CD2 | 33:BL:8:PRO:HA | 2.52 | 0.44 |
| 30:BH:114:GLU:O | 30:BH:115:VAL:HG13 | 2.17 | 0.44 |
| 31:BJ:57:LEU:HG | 31:BJ:128:ASN:N | 2.31 | 0.44 |
| 35:BN:9:GLN:O | 35:BN:17:ARG:HD3 | 2.17 | 0.44 |
| 31:BJ:44:TYR:HB2 | 38:BQ:63:ARG:HD2 | 1.99 | 0.44 |
| 38:BQ:91:ARG:HE | 38:BQ:94:LEU:CD2 | 2.30 | 0.44 |
| 39:BR:39:LEU:HD22 | 39:BR:53:PHE:CD1 | 2.53 | 0.44 |
| 42:BU:94:PHE:HB2 | 42:BU:101:THR:HA | 2.00 | 0.44 |
| 42:BU:11:ILE:N | 42:BU:70:ALA:O | 2.45 | 0.44 |
| 1:CA:1299:A:C2' | 1:CA:1301:U:H1' | 2.47 | 0.44 |
| 1:CA:1454:G:H2' | 1:CA:1455:G:C8 | 2.53 | 0.44 |
| 1:CA:1502:A:HO2' | 1:CA:1503:A:P | 2.40 | 0.44 |
| 1:CA:49:U:O2 | 1:CA:362:G:H1' | 2.18 | 0.44 |
| 1:CA:770:C:O2' | 1:CA:771:G:H5' | 2.17 | 0.44 |
| 1:CA:923:A:OP1 | 4:CE:25:LYS:HB3 | 2.17 | 0.44 |
| 20:CB:142:LYS:HA | 20:CB:145:ASN:CG | 2.38 | 0.44 |
| 20:CB:31:PHE:HB3 | 20:CB:39:ILE:CG2 | 2.48 | 0.44 |
| 4:CE:148:SER:HB2 | 4:CE:150:GLU:OE1 | 2.18 | 0.44 |
| 7:CH:5:PRO:HB2 | 7:CH:32:LYS:NZ | 2.32 | 0.44 |
| 8:CI:48:ARG:O | 8:CI:52:GLU:HG2 | 2.16 | 0.44 |
| 9:CJ:32:THR:O | 9:CJ:32:THR:HG23 | 2.17 | 0.44 |
| 9:CJ:50:THR:HG22 | 9:CJ:62:ARG:HD2 | 2.00 | 0.44 |
| 11:CL:89:LEU:HD22 | 11:CL:89:LEU:N | 2.33 | 0.44 |
| 12:CM:57:ASP:O | 12:CM:61:LYS:HE2 | 2.16 | 0.44 |
| 13:CN:50:LEU:CG | 13:CN:51:PRO:HD3 | 2.48 | 0.44 |
| 16:CQ:47:ASP:CG | 16:CQ:50:ASN:HA | 2.38 | 0.44 |
| 1:CA:254:G:OP1 | 16:CQ:68:LYS:O | 2.36 | 0.44 |
| 18:CS:40:PHE:HB3 | 18:CS:41:PRO:HD2 | 1.98 | 0.44 |
| 47:D0:18:HIS:N | 47:D0:18:HIS:HD1 | 2.16 | 0.44 |
| 48:D1:3:GLY:C | 48:D1:5:ARG:N | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:2419:U:OP2 | 50:D3:32:LEU:HD13 | 2.17 | 0.44 |
| 23:DB:1153:C:H2' | 23:DB:1154:G:O4' | 2.17 | 0.44 |
| 23:DB:1183:U:O2' | 23:DB:1184:U:H5' | 2.18 | 0.44 |
| 23:DB:1403:A:H2' | 23:DB:1404:C:H6 | 1.83 | 0.44 |
| 23:DB:1465:G:H2' | 23:DB:1466:U:C6 | 2.52 | 0.44 |
| 23:DB:1496:A:H2' | 23:DB:1498:C:C5 | 2.53 | 0.44 |
| 23:DB:1593:A:H2' | 23:DB:1594:U:H6 | 1.78 | 0.44 |
| 23:DB:188:G:H5'' | 46:DZ:14:THR:CG2 | 2.47 | 0.44 |
| 23:DB:1904:G:O2' | 23:DB:1905:C:H5' | 2.18 | 0.44 |
| 23:DB:2246:G:H2' | 23:DB:2247:A:H8 | 1.83 | 0.44 |
| 23:DB:2448:A:H4' | 23:DB:2449:U:OP2 | 2.16 | 0.44 |
| 23:DB:2456:C:H2' | 23:DB:2457:U:O4' | 2.17 | 0.44 |
| 23:DB:302:C:H2' | 23:DB:303:G:H8 | 1.83 | 0.44 |
| 23:DB:309:A:N3 | 23:DB:329:G:O2' | 2.45 | 0.44 |
| 23:DB:407:G:O2' | 23:DB:408:G:H5' | 2.16 | 0.44 |
| 23:DB:644:A:H2 | 23:DB:646:U:O4 | 1.99 | 0.44 |
| 23:DB:84:A:H4' | 23:DB:85:G:O5' | 2.18 | 0.44 |
| 25:DC:140:VAL:HG12 | 25:DC:141:HIS:N | 2.22 | 0.44 |
| 26:DD:33:ARG:HG2 | 26:DD:33:ARG:NH2 | 2.32 | 0.44 |
| 28:DF:59:ILE:HG12 | 28:DF:137:PHE:CE2 | 2.53 | 0.44 |
| 28:DF:29:ARG:HD3 | 28:DF:158:THR:OG1 | 2.17 | 0.44 |
| 28:DF:46:LYS:NZ | 28:DF:83:PRO:HD2 | 2.33 | 0.44 |
| 29:DG:154:GLU:OE1 | 29:DG:157:LYS:HB2 | 2.18 | 0.44 |
| 30:DH:57:LYS:HG3 | 30:DH:58:LEU:N | 2.32 | 0.44 |
| 23:DB:1100:C:H41 | 52:DI:1:ALA:H2 | 1.66 | 0.44 |
| 52:DI:21:PRO:HB2 | 52:DI:22:PRO:CD | 2.43 | 0.44 |
| 35:DN:33:ILE:C | 35:DN:34:ILE:HG13 | 2.38 | 0.44 |
| 35:DN:31:HIS:C | 35:DN:33:ILE:H | 2.21 | 0.44 |
| 39:DR:6:GLN:HE22 | 39:DR:9:GLY:C | 2.21 | 0.44 |
| 39:DR:75:VAL:O | 39:DR:76:LYS:HD2 | 2.17 | 0.44 |
| 40:DS:4:ILE:CG2 | 40:DS:106:VAL:HG22 | 2.48 | 0.44 |
| 40:DS:60:HIS:ND1 | 40:DS:60:HIS:O | 2.50 | 0.44 |
| 40:DS:61:ASN:HB3 | 40:DS:62:ASP:H | 1.56 | 0.44 |
| 42:DU:84:PHE:HE2 | 42:DU:93:ARG:HG2 | 1.82 | 0.44 |
| 24:DV:71:LYS:HB2 | 24:DV:94:ALA:OXT | 2.16 | 0.44 |
| 43:DW:23:LYS:HZ3 | 43:DW:24:ARG:CG | 2.27 | 0.44 |
| 1:AA:1105:A:O2' | 1:AA:1106:G:H5' | 2.17 | 0.44 |
| 1:AA:1134:G:N2 | 1:AA:1135:U:H1' | 2.32 | 0.44 |
| 1:AA:1175:G:O2' | 1:AA:1176:A:H5' | 2.18 | 0.44 |
| 1:AA:1318:A:H4' | 18:AS:9:PHE:CE1 | 2.53 | 0.44 |
| 1:AA:1456:A:H2' | 1:AA:1457:G:O4' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:356:A:H2' | 1:AA:357:G:O4' | 2.18 | 0.44 |
| 1:AA:44:A:O2' | 1:AA:45:G:H5' | 2.18 | 0.44 |
| 1:AA:618:C:N3 | 1:AA:622:A:N6 | 2.63 | 0.44 |
| 20:AB:187:ASP:OD1 | 20:AB:203:ASP:HB3 | 2.17 | 0.44 |
| 2:AC:129:PHE:HD2 | 2:AC:156:LEU:HD22 | 1.83 | 0.44 |
| 4:AE:104:ILE:CG2 | 4:AE:111:ARG:HH12 | 2.23 | 0.44 |
| 5:AF:35:LYS:HB2 | 5:AF:65:GLU:HB3 | 2.00 | 0.44 |
| 9:AJ:18:ILE:HG13 | 9:AJ:72:ARG:HG2 | 1.98 | 0.44 |
| 10:AK:47:GLY:C | 10:AK:49:SER:H | 2.21 | 0.44 |
| 15:AP:67:ILE:HG23 | 15:AP:67:ILE:O | 2.18 | 0.44 |
| 1:AA:107:G:O6 | 19:AT:9:ARG:HD3 | 2.17 | 0.44 |
| 48:B1:3:GLY:O | 48:B1:5:ARG:N | 2.50 | 0.44 |
| 49:B2:39:ARG:NH1 | 49:B2:39:ARG:HG3 | 2.32 | 0.44 |
| 23:BB:1286:A:H1' | 23:BB:1288:G:OP2 | 2.18 | 0.44 |
| 23:BB:1637:A:H5' | 23:BB:1760:C:O2' | 2.17 | 0.44 |
| 23:BB:182:A:H1' | 23:BB:434:U:H5' | 2.00 | 0.44 |
| 23:BB:212:G:H2' | 23:BB:213:A:H8 | 1.81 | 0.44 |
| 23:BB:2301:C:H2' | 23:BB:2302:U:H6 | 1.82 | 0.44 |
| 23:BB:2389:G:H5'' | 23:BB:2390:U:O4' | 2.18 | 0.44 |
| 23:BB:2571:U:O2' | 26:BD:152:PRO:HG3 | 2.18 | 0.44 |
| 23:BB:2646:C:H2' | 23:BB:2647:U:O4' | 2.18 | 0.44 |
| 23:BB:309:A:N3 | 23:BB:329:G:O2' | 2.48 | 0.44 |
| 23:BB:311:A:H3' | 23:BB:312:G:C8 | 2.52 | 0.44 |
| 23:BB:483:A:H2' | 23:BB:484:C:H5' | 2.00 | 0.44 |
| 23:BB:538:A:H2' | 23:BB:539:G:O4' | 2.17 | 0.44 |
| 23:BB:599:A:H2' | 23:BB:600:G:H8 | 1.82 | 0.44 |
| 25:BC:180:MET:O | 25:BC:267:VAL:HG23 | 2.17 | 0.44 |
| 32:BK:106:GLU:N | 32:BK:106:GLU:OE1 | 2.47 | 0.44 |
| 36:BO:36:TYR:CD2 | 36:BO:36:TYR:N | 2.86 | 0.44 |
| 38:BQ:94:LEU:C | 38:BQ:96:ASP:N | 2.71 | 0.44 |
| 39:BR:59:ILE:HA | 39:BR:100:GLY:HA3 | 1.99 | 0.44 |
| 39:BR:6:GLN:HE22 | 39:BR:9:GLY:N | 2.16 | 0.44 |
| 41:BT:11:LEU:CD2 | 41:BT:46:ALA:HB1 | 2.44 | 0.44 |
| 41:BT:54:GLU:CB | 41:BT:88:LYS:HB2 | 2.48 | 0.44 |
| 41:BT:7:LEU:C | 41:BT:9:LYS:H | 2.20 | 0.44 |
| 42:BU:49:PRO:O | 42:BU:50:ALA:HB2 | 2.16 | 0.44 |
| 42:BU:73:ASN:HD21 | 42:BU:76:THR:H | 1.66 | 0.44 |
| 43:BW:70:VAL:CG2 | 43:BW:75:ASN:HD21 | 2.31 | 0.44 |
| 46:BZ:68:LEU:HD22 | 46:BZ:78:TYR:CE1 | 2.53 | 0.44 |
| 1:CA:1105:A:O2' | 1:CA:1106:G:H5' | 2.18 | 0.44 |
| 1:CA:1261:A:H1' | 1:CA:1275:A:N1 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1296:C:H5' | 12:CM:13:HIS:CE1 | 2.53 | 0.44 |
| 1:CA:570:G:H2' | 1:CA:571:U:C6 | 2.53 | 0.44 |
| 1:CA:57:G:H2' | 1:CA:58:C:C6 | 2.52 | 0.44 |
| 1:CA:594:U:O2' | 1:CA:595:A:H5' | 2.17 | 0.44 |
| 1:CA:861:G:H2' | 1:CA:862:C:C6 | 2.52 | 0.44 |
| 1:CA:948:C:O2' | 1:CA:949:A:H5' | 2.17 | 0.44 |
| 2:CC:35:ASP:O | 2:CC:39:ARG:HG3 | 2.17 | 0.44 |
| 5:CF:12:PRO:C | 5:CF:14:GLN:H | 2.21 | 0.44 |
| 5:CF:66:ALA:HB1 | 5:CF:70:VAL:HG21 | 2.00 | 0.44 |
| 6:CG:11:ILE:HD12 | 6:CG:11:ILE:N | 2.33 | 0.44 |
| 8:CI:118:ARG:NH1 | 8:CI:122:ARG:HE | 2.16 | 0.44 |
| 12:CM:84:CYS:O | 12:CM:88:LEU:HG | 2.16 | 0.44 |
| 12:CM:89:ARG:CB | 12:CM:96:VAL:HG22 | 2.47 | 0.44 |
| 19:CT:35:TYR:CG | 19:CT:36:ALA:N | 2.85 | 0.44 |
| 48:D1:38:PHE:O | 48:D1:40:PRO:HD3 | 2.18 | 0.44 |
| 49:D2:26:ASN:HA | 49:D2:29:GLN:HB3 | 1.99 | 0.44 |
| 23:DB:1062:G:H2' | 23:DB:1063:G:C8 | 2.53 | 0.44 |
| 23:DB:1201:U:O2' | 23:DB:1202:G:H5' | 2.18 | 0.44 |
| 23:DB:1535:A:C5' | 23:DB:1536:C:H5 | 2.30 | 0.44 |
| 23:DB:179:C:H2' | 23:DB:180:G:O4' | 2.17 | 0.44 |
| 23:DB:2049:G:O2' | 23:DB:2050:C:H5' | 2.18 | 0.44 |
| 23:DB:2233:U:H2' | 23:DB:2234:G:H8 | 1.83 | 0.44 |
| 23:DB:2247:A:H2' | 23:DB:2248:C:H6 | 1.83 | 0.44 |
| 23:DB:2304:G:N3 | 23:DB:2304:G:H2' | 2.31 | 0.44 |
| 23:DB:231:A:H3' | 23:DB:232:G:C8 | 2.53 | 0.44 |
| 23:DB:2409:G:H2' | 23:DB:2410:G:O4' | 2.16 | 0.44 |
| 23:DB:550:C:H2' | 23:DB:551:G:H8 | 1.82 | 0.44 |
| 23:DB:601:C:O2 | 23:DB:605:G:H4' | 2.17 | 0.44 |
| 23:DB:2730:C:H4' | 26:DD:174:SER:HB3 | 1.99 | 0.44 |
| 26:DD:202:ILE:HG22 | 26:DD:202:ILE:O | 2.16 | 0.44 |
| 23:DB:2786:U:H5' | 26:DD:70:LYS:HG3 | 1.99 | 0.44 |
| 26:DD:51:THR:HG22 | 26:DD:76:GLY:HA3 | 1.97 | 0.44 |
| 27:DE:200:LEU:HD22 | 27:DE:200:LEU:N | 2.33 | 0.44 |
| 28:DF:98:PHE:C | 28:DF:100:GLU:H | 2.20 | 0.44 |
| 29:DG:84:LYS:HB2 | 29:DG:132:LEU:H | 1.83 | 0.44 |
| 23:DB:1063:G:O2' | 52:DI:88:GLY:HA3 | 2.17 | 0.44 |
| 31:DJ:64:VAL:O | 31:DJ:65:THR:HG22 | 2.17 | 0.44 |
| 33:DL:125:LEU:HD23 | 33:DL:126:ARG:H | 1.82 | 0.44 |
| 33:DL:75:ALA:HB2 | 33:DL:101:ILE:HG23 | 2.00 | 0.44 |
| 40:DS:81:SER:CA | 40:DS:99:ARG:HA | 2.46 | 0.44 |
| 23:DB:83:A:H5'' | 42:DU:1:ALA:N | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DW:23:LYS:O | 43:DW:66:VAL:HB | 2.18 | 0.44 |
| 45:DY:3:THR:HB | 45:DY:36:GLU:CG | 2.48 | 0.44 |
| 46:DZ:32:ASN:O | 46:DZ:33:LEU:O | 2.35 | 0.44 |
| 1:AA:244:U:O4 | 1:AA:906:A:H1' | 2.17 | 0.44 |
| 1:AA:342:C:O2' | 1:AA:343:U:H5' | 2.18 | 0.44 |
| 1:AA:502:A:H2' | 1:AA:503:C:O4' | 2.17 | 0.44 |
| 1:AA:647:C:H2' | 1:AA:648:A:C8 | 2.52 | 0.44 |
| 20:AB:64:GLY:HA2 | 20:AB:158:ASP:OD1 | 2.17 | 0.44 |
| 20:AB:16:GLY:HA2 | 20:AB:40:ILE:CG1 | 2.48 | 0.44 |
| 20:AB:16:GLY:HA2 | 20:AB:40:ILE:HG13 | 2.00 | 0.44 |
| 20:AB:40:ILE:HD13 | 20:AB:201:GLY:CA | 2.47 | 0.44 |
| 2:AC:52:SER:O | 2:AC:113:LYS:HG2 | 2.18 | 0.44 |
| 3:AD:2:ARG:HH22 | 3:AD:132:ALA:CB | 2.30 | 0.44 |
| 6:AG:67:ASN:ND2 | 6:AG:127:ALA:HA | 2.32 | 0.44 |
| 1:AA:599:C:H4' | 7:AH:121:GLY:CA | 2.48 | 0.44 |
| 7:AH:29:SER:OG | 7:AH:32:LYS:HG3 | 2.17 | 0.44 |
| 10:AK:70:ALA:C | 10:AK:72:ALA:N | 2.71 | 0.44 |
| 11:AL:49:ARG:HD2 | 11:AL:49:ARG:N | 2.32 | 0.44 |
| 18:AS:10:ILE:HB | 18:AS:14:LEU:HD21 | 2.00 | 0.44 |
| 19:AT:49:ALA:CA | 19:AT:52:GLU:HB3 | 2.47 | 0.44 |
| 47:B0:26:SER:HB3 | 47:B0:39:ARG:NH2 | 2.33 | 0.44 |
| 23:BB:83:A:N1 | 23:BB:101:A:H5' | 2.32 | 0.44 |
| 23:BB:1076:C:H2' | 23:BB:1077:A:H8 | 1.82 | 0.44 |
| 23:BB:1147:A:O2' | 23:BB:1148:U:H5' | 2.18 | 0.44 |
| 23:BB:1439:A:C5 | 23:BB:1552:A:N6 | 2.85 | 0.44 |
| 23:BB:1591:A:O2' | 23:BB:1592:C:H5' | 2.17 | 0.44 |
| 23:BB:1656:C:H2' | 23:BB:1657:U:H6 | 1.82 | 0.44 |
| 23:BB:1826:G:H2' | 23:BB:1827:U:C6 | 2.51 | 0.44 |
| 23:BB:2459:A:H2' | 23:BB:2459:A:N3 | 2.33 | 0.44 |
| 23:BB:2466:C:O2' | 23:BB:2467:C:H5' | 2.18 | 0.44 |
| 23:BB:2618:G:H2' | 23:BB:2619:C:H6 | 1.83 | 0.44 |
| 23:BB:2848:G:N2 | 23:BB:2867:G:C2 | 2.86 | 0.44 |
| 23:BB:28:A:O2' | 23:BB:583:G:H5' | 2.17 | 0.44 |
| 23:BB:364:C:H6 | 23:BB:364:C:O5' | 2.01 | 0.44 |
| 23:BB:613:A:H4' | 23:BB:614:A:OP2 | 2.18 | 0.44 |
| 23:BB:64:A:H2' | 23:BB:65:U:H6 | 1.81 | 0.44 |
| 23:BB:765:C:H2' | 23:BB:766:U:H6 | 1.83 | 0.44 |
| 25:BC:52:HIS:O | 25:BC:53:ILE:HB | 2.17 | 0.44 |
| 26:BD:14:ILE:O | 26:BD:14:ILE:HG23 | 2.18 | 0.44 |
| 26:BD:8:LYS:HA | 26:BD:201:LEU:HD11 | 1.99 | 0.44 |
| 28:BF:140:ILE:O | 28:BF:141:ASP:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BF:24:VAL:O | 28:BF:27:VAL:HG22 | 2.18 | 0.44 |
| 28:BF:43:ILE:CG2 | 28:BF:44:ALA:H | 2.16 | 0.44 |
| 52:BI:102:ARG:HA | 52:BI:105:LEU:HD12 | 1.99 | 0.44 |
| 33:BL:89:VAL:O | 33:BL:89:VAL:HG13 | 2.17 | 0.44 |
| 33:BL:93:ASN:HB2 | 33:BL:94:THR:H | 1.66 | 0.44 |
| 37:BP:26:GLU:HB2 | 37:BP:86:LYS:HD3 | 2.00 | 0.44 |
| 38:BQ:104:ALA:HA | 39:BR:46:GLU:OE2 | 2.18 | 0.44 |
| 41:BT:12:ARG:HA | 44:BX:29:ARG:NH2 | 2.26 | 0.44 |
| 23:BB:137:U:H2' | 41:BT:1:MET:N | 2.33 | 0.44 |
| 41:BT:61:LEU:HG | 41:BT:82:LYS:HB2 | 1.99 | 0.44 |
| 42:BU:51:LEU:HD22 | 42:BU:52:ASN:OD1 | 2.17 | 0.44 |
| 24:BV:2:PHE:HD1 | 24:BV:50:MET:HE2 | 1.83 | 0.44 |
| 43:BW:18:LYS:HA | 43:BW:18:LYS:HD2 | 1.72 | 0.44 |
| 43:BW:37:VAL:HB | 43:BW:38:ARG:HD3 | 1.98 | 0.44 |
| 45:BY:50:VAL:O | 45:BY:54:VAL:HG22 | 2.17 | 0.44 |
| 1:CA:338:A:H2' | 1:CA:339:C:C6 | 2.53 | 0.44 |
| 1:CA:669:G:H2' | 1:CA:670:G:H8 | 1.83 | 0.44 |
| 1:CA:686:U:O4 | 1:CA:703:G:H1' | 2.18 | 0.44 |
| 3:CD:25:ARG:O | 3:CD:27:ILE:N | 2.51 | 0.44 |
| 3:CD:48:SER:O | 3:CD:49:ASP:C | 2.56 | 0.44 |
| 5:CF:81:ASN:O | 5:CF:84:VAL:HG12 | 2.18 | 0.44 |
| 1:CA:600:A:OP2 | 7:CH:87:ARG:HG2 | 2.18 | 0.44 |
| 9:CJ:49:PHE:HB2 | 9:CJ:65:TYR:HB2 | 1.99 | 0.44 |
| 9:CJ:80:THR:O | 9:CJ:84:VAL:HG23 | 2.18 | 0.44 |
| 11:CL:105:GLY:HA3 | 11:CL:117:GLY:O | 2.17 | 0.44 |
| 18:CS:33:TRP:C | 18:CS:35:ARG:H | 2.21 | 0.44 |
| 18:CS:52:ASN:ND2 | 18:CS:53:GLY:H | 2.15 | 0.44 |
| 21:CU:39:LYS:N | 21:CU:40:PRO:CD | 2.81 | 0.44 |
| 22:DA:65:U:C2' | 22:DA:66:A:H5' | 2.48 | 0.44 |
| 23:DB:1286:A:H1' | 23:DB:1288:G:OP2 | 2.18 | 0.44 |
| 23:DB:1537:G:H5'' | 23:DB:1537:G:N3 | 2.33 | 0.44 |
| 23:DB:1749:A:H2' | 23:DB:1750:G:H8 | 1.83 | 0.44 |
| 23:DB:1851:U:H2' | 23:DB:1852:U:H6 | 1.83 | 0.44 |
| 23:DB:2156:G:H2' | 23:DB:2157:G:C4' | 2.45 | 0.44 |
| 23:DB:2248:C:H2' | 23:DB:2249:U:O4' | 2.18 | 0.44 |
| 23:DB:24:G:H1' | 40:DS:77:ASP:HB3 | 2.00 | 0.44 |
| 23:DB:2580:U:C5' | 26:DD:136:ASN:H | 2.31 | 0.44 |
| 23:DB:2693:G:O2' | 23:DB:2694:G:H5' | 2.18 | 0.44 |
| 23:DB:357:C:H2' | 23:DB:358:U:C6 | 2.53 | 0.44 |
| 23:DB:39:G:O2' | 23:DB:40:U:H5' | 2.18 | 0.44 |
| 23:DB:729:G:H5'' | 23:DB:730:A:H5'' | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:2073:C:C5' | 25:DC:227:VAL:HG12 | 2.45 | 0.44 |
| 26:DD:171:THR:OG1 | 26:DD:172:VAL:N | 2.50 | 0.44 |
| 28:DF:111:ARG:CD | 28:DF:111:ARG:N | 2.80 | 0.44 |
| 28:DF:42:ALA:O | 28:DF:44:ALA:N | 2.50 | 0.44 |
| 29:DG:28:LYS:O | 29:DG:30:GLY:N | 2.50 | 0.44 |
| 29:DG:58:ALA:C | 29:DG:60:GLY:H | 2.21 | 0.44 |
| 31:DJ:20:ALA:CB | 31:DJ:28:LEU:HD22 | 2.48 | 0.44 |
| 32:DK:19:VAL:HG13 | 32:DK:43:ILE:HA | 1.99 | 0.44 |
| 23:DB:1754:A:OP1 | 37:DP:93:LYS:HD3 | 2.18 | 0.44 |
| 39:DR:26:ASP:O | 39:DR:27:ILE:HD13 | 2.18 | 0.44 |
| 39:DR:86:GLN:HB2 | 39:DR:86:GLN:HE21 | 1.53 | 0.44 |
| 42:DU:86:PHE:HE1 | 42:DU:88:ASP:OD1 | 2.01 | 0.44 |
| 1:AA:1245:C:H2' | 1:AA:1246:A:H8 | 1.81 | 0.44 |
| 1:AA:570:G:H2' | 1:AA:571:U:C6 | 2.52 | 0.44 |
| 1:AA:708:C:H2' | 1:AA:709:U:C6 | 2.53 | 0.44 |
| 20:AB:46:VAL:HA | 20:AB:49:PHE:HD2 | 1.82 | 0.44 |
| 2:AC:122:GLN:O | 2:AC:127:VAL:HG13 | 2.17 | 0.44 |
| 4:AE:21:SER:CB | 4:AE:28:ARG:HE | 2.22 | 0.44 |
| 5:AF:71:ILE:HG13 | 5:AF:72:ASP:N | 2.33 | 0.44 |
| 6:AG:129:ASN:HD22 | 6:AG:137:ARG:HH22 | 1.63 | 0.44 |
| 6:AG:46:LEU:O | 6:AG:57:GLU:HG3 | 2.18 | 0.44 |
| 1:AA:643:C:H5' | 7:AH:31:LEU:HD13 | 2.00 | 0.44 |
| 8:AI:52:GLU:C | 8:AI:53:LEU:HD22 | 2.38 | 0.44 |
| 8:AI:82:ILE:O | 8:AI:86:LEU:HB2 | 2.17 | 0.44 |
| 12:AM:57:ASP:O | 12:AM:61:LYS:HE2 | 2.17 | 0.44 |
| 16:AQ:47:ASP:CG | 16:AQ:50:ASN:HA | 2.38 | 0.44 |
| 17:AR:63:TYR:C | 17:AR:64:LEU:HD12 | 2.37 | 0.44 |
| 18:AS:77:ARG:HG2 | 18:AS:77:ARG:H | 1.56 | 0.44 |
| 49:B2:6:GLN:NE2 | 49:B2:6:GLN:HA | 2.33 | 0.44 |
| 23:BB:1210:G:H5' | 23:BB:1212:G:C4' | 2.47 | 0.44 |
| 23:BB:1336:A:H3' | 23:BB:1337:G:H8 | 1.81 | 0.44 |
| 23:BB:1463:C:H2' | 23:BB:1464:G:H8 | 1.82 | 0.44 |
| 23:BB:1821:A:H2' | 23:BB:1822:C:H6 | 1.81 | 0.44 |
| 23:BB:1933:G:H2' | 23:BB:1934:C:C6 | 2.53 | 0.44 |
| 23:BB:1998:A:H2' | 23:BB:1999:C:C6 | 2.53 | 0.44 |
| 23:BB:231:A:H3' | 23:BB:232:G:C8 | 2.53 | 0.44 |
| 23:BB:2369:A:H2' | 23:BB:2370:G:H8 | 1.83 | 0.44 |
| 23:BB:2462:C:H2' | 23:BB:2463:C:H6 | 1.82 | 0.44 |
| 23:BB:2487:G:H2' | 23:BB:2488:G:H8 | 1.83 | 0.44 |
| 23:BB:2699:C:H2' | 23:BB:2700:A:C8 | 2.53 | 0.44 |
| 23:BB:59:U:H5' | 23:BB:73:A:N1 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:866:A:O2' | 23:BB:867:C:H5' | 2.18 | 0.44 |
| 28:BF:135:ILE:CD1 | 28:BF:137:PHE:HB3 | 2.45 | 0.44 |
| 28:BF:64:PRO:HA | 28:BF:88:VAL:HG22 | 1.99 | 0.44 |
| 28:BF:74:ALA:C | 28:BF:76:PHE:H | 2.21 | 0.44 |
| 34:BM:10:ARG:HH11 | 34:BM:89:VAL:HG23 | 1.83 | 0.44 |
| 35:BN:90:ARG:HB3 | 35:BN:94:TYR:HE1 | 1.82 | 0.44 |
| 37:BP:88:ARG:HB2 | 37:BP:112:ARG:HH12 | 1.78 | 0.44 |
| 40:BS:66:ILE:CD1 | 40:BS:66:ILE:H | 2.26 | 0.44 |
| 44:BX:59:GLU:OE2 | 44:BX:59:GLU:N | 2.51 | 0.44 |
| 46:BZ:49:LEU:HD11 | 46:BZ:68:LEU:HD21 | 2.00 | 0.44 |
| 1:CA:865:A:O2' | 1:CA:866:C:H5' | 2.17 | 0.44 |
| 20:CB:99:MET:CA | 20:CB:106:VAL:HG21 | 2.44 | 0.44 |
| 20:CB:112:ARG:O | 20:CB:116:LEU:HB2 | 2.17 | 0.44 |
| 20:CB:150:ILE:O | 20:CB:150:ILE:HG12 | 2.17 | 0.44 |
| 20:CB:16:GLY:HA3 | 20:CB:40:ILE:H | 1.83 | 0.44 |
| 2:CC:46:LEU:HB3 | 2:CC:49:ALA:CB | 2.48 | 0.44 |
| 2:CC:6:PRO:HB3 | 2:CC:174:LEU:HD21 | 1.99 | 0.44 |
| 4:CE:11:GLN:HB2 | 4:CE:116:VAL:HB | 2.00 | 0.44 |
| 6:CG:22:LEU:O | 6:CG:25:PHE:HB3 | 2.18 | 0.44 |
| 6:CG:72:VAL:HG12 | 6:CG:89:GLU:CB | 2.45 | 0.44 |
| 6:CG:87:PRO:O | 6:CG:152:HIS:HB3 | 2.18 | 0.44 |
| 9:CJ:8:ILE:CD1 | 9:CJ:76:ILE:HG13 | 2.48 | 0.44 |
| 21:CU:44:ARG:HH11 | 21:CU:44:ARG:HG3 | 1.83 | 0.44 |
| 47:D0:41:HIS:CD2 | 47:D0:41:HIS:N | 2.85 | 0.44 |
| 47:D0:55:ALA:C | 47:D0:56:LYS:HG3 | 2.38 | 0.44 |
| 23:DB:101:A:O2' | 23:DB:102:U:P | 2.75 | 0.44 |
| 23:DB:107:G:O2' | 23:DB:108:G:H5' | 2.17 | 0.44 |
| 23:DB:52:A:C5 | 23:DB:118:A:C2 | 3.06 | 0.44 |
| 23:DB:1324:G:N1 | 23:DB:1331:G:C6 | 2.86 | 0.44 |
| 23:DB:1387:A:H4' | 23:DB:1469:A:H1' | 1.99 | 0.44 |
| 23:DB:1599:U:H2' | 23:DB:1600:C:H6 | 1.82 | 0.44 |
| 23:DB:177:G:H3' | 23:DB:178:G:H8 | 1.83 | 0.44 |
| 23:DB:2393:U:H2' | 23:DB:2394:C:C6 | 2.52 | 0.44 |
| 23:DB:2450:A:C2' | 23:DB:2451:A:H5' | 2.47 | 0.44 |
| 23:DB:2646:C:H2' | 23:DB:2647:U:O4' | 2.17 | 0.44 |
| 23:DB:28:A:N6 | 23:DB:512:G:O2' | 2.51 | 0.44 |
| 23:DB:181:A:H1' | 23:DB:435:C:H5' | 1.98 | 0.44 |
| 23:DB:4:U:O2' | 23:DB:5:A:H5' | 2.17 | 0.44 |
| 23:DB:540:C:H2' | 23:DB:541:A:H8 | 1.83 | 0.44 |
| 23:DB:538:A:N6 | 23:DB:555:G:O2' | 2.51 | 0.44 |
| 23:DB:576:U:H5 | 56:DB:3400:HOH:O | 2.01 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:64:A:H2' | 23:DB:65:U:H6 | 1.79 | 0.44 |
| 23:DB:859:G:HO2' | 23:DB:916:G:H1 | 1.65 | 0.44 |
| 25:DC:63:ILE:HD13 | 25:DC:63:ILE:HA | 1.77 | 0.44 |
| 23:DB:600:G:H1' | 27:DE:100:MET:CG | 2.48 | 0.44 |
| 27:DE:148:ILE:HA | 27:DE:187:VAL:HB | 1.99 | 0.44 |
| 23:DB:659:G:H21 | 27:DE:30:GLN:CD | 2.21 | 0.44 |
| 27:DE:37:ALA:C | 27:DE:39:ALA:H | 2.20 | 0.44 |
| 52:DI:2:LYS:HB3 | 52:DI:2:LYS:HZ2 | 1.83 | 0.44 |
| 52:DI:78:LEU:HD23 | 52:DI:81:LYS:HE2 | 2.00 | 0.44 |
| 32:DK:87:LEU:HB2 | 32:DK:93:GLN:C | 2.36 | 0.44 |
| 34:DM:108:VAL:HG22 | 34:DM:109:PRO:HD2 | 1.98 | 0.44 |
| 35:DN:118:ARG:HE | 35:DN:118:ARG:HB3 | 1.50 | 0.44 |
| 37:DP:54:LEU:HD12 | 37:DP:76:HIS:HB2 | 1.99 | 0.44 |
| 23:DB:30:G:OP1 | 38:DQ:4:LYS:HG2 | 2.17 | 0.44 |
| 38:DQ:96:ASP:C | 38:DQ:98:ALA:N | 2.70 | 0.44 |
| 42:DU:89:GLY:O | 42:DU:90:LYS:HG3 | 2.17 | 0.44 |
| 24:DV:80:HIS:CD2 | 24:DV:81:PRO:HD2 | 2.53 | 0.44 |
| 43:DW:18:LYS:H | 43:DW:35:ILE:CG2 | 2.29 | 0.44 |
| 1:AA:1057:G:H4' | 2:AC:196:GLY:N | 2.27 | 0.44 |
| 1:AA:1086:U:H3 | 1:AA:1099:G:N2 | 1.94 | 0.44 |
| 1:AA:159:G:N1 | 1:AA:163:C:N4 | 2.66 | 0.44 |
| 1:AA:167:A:O2' | 1:AA:168:G:H5' | 2.17 | 0.44 |
| 1:AA:186:C:H2' | 1:AA:187:G:O4' | 2.18 | 0.44 |
| 1:AA:284:C:H2' | 1:AA:285:C:C6 | 2.52 | 0.44 |
| 1:AA:308:C:H2' | 1:AA:309:A:C8 | 2.52 | 0.44 |
| 1:AA:584:G:H2' | 1:AA:585:G:H8 | 1.83 | 0.44 |
| 1:AA:683:G:O2' | 1:AA:684:U:H5' | 2.17 | 0.44 |
| 1:AA:746:A:N1 | 1:AA:747:A:N6 | 2.66 | 0.44 |
| 1:AA:915:A:H2' | 1:AA:916:U:H5' | 2.00 | 0.44 |
| 20:AB:102:ASN:ND2 | 20:AB:105:THR:HB | 2.32 | 0.44 |
| 20:AB:22:TRP:CZ3 | 20:AB:24:PRO:HA | 2.53 | 0.44 |
| 3:AD:187:ARG:CZ | 3:AD:191:SER:HB3 | 2.48 | 0.44 |
| 4:AE:95:MET:HA | 4:AE:124:ALA:CB | 2.47 | 0.44 |
| 6:AG:30:MET:HG3 | 6:AG:35:LYS:HA | 2.00 | 0.44 |
| 10:AK:57:SER:O | 10:AK:90:PRO:HG3 | 2.18 | 0.44 |
| 11:AL:98:ARG:HD2 | 11:AL:103:CYS:SG | 2.58 | 0.44 |
| 18:AS:10:ILE:CD1 | 18:AS:14:LEU:HD11 | 2.47 | 0.44 |
| 23:BB:1171:G:H2' | 23:BB:1172:C:O4' | 2.18 | 0.44 |
| 23:BB:1292:G:H2' | 23:BB:1293:C:H6 | 1.82 | 0.44 |
| 23:BB:1338:G:H4' | 41:BT:18:GLU:CG | 2.29 | 0.44 |
| 23:BB:152:A:H2' | 23:BB:153:U:C5 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1708:C:H2' | 23:BB:1709:U:H6 | 1.82 | 0.44 |
| 23:BB:177:G:H3' | 23:BB:178:G:H8 | 1.83 | 0.44 |
| 23:BB:2860:A:H2' | 23:BB:2861:U:O4' | 2.18 | 0.44 |
| 23:BB:30:G:OP1 | 38:BQ:4:LYS:HG2 | 2.18 | 0.44 |
| 23:BB:470:A:H2' | 23:BB:471:A:C8 | 2.53 | 0.44 |
| 23:BB:4:U:O2' | 23:BB:5:A:H5' | 2.18 | 0.44 |
| 23:BB:69:C:H2' | 23:BB:70:G:H8 | 1.83 | 0.44 |
| 25:BC:64:VAL:HG22 | 25:BC:90:ILE:HD11 | 2.00 | 0.44 |
| 28:BF:65:LEU:HD23 | 28:BF:87:LYS:CD | 2.43 | 0.44 |
| 28:BF:74:ALA:HB3 | 28:BF:77:LYS:O | 2.17 | 0.44 |
| 29:BG:154:GLU:O | 29:BG:156:TYR:N | 2.51 | 0.44 |
| 29:BG:89:VAL:HG21 | 29:BG:162:ARG:HH11 | 1.83 | 0.44 |
| 30:BH:141:LYS:HE2 | 30:BH:141:LYS:HB2 | 1.75 | 0.44 |
| 52:BI:129:GLU:CB | 52:BI:133:ARG:HH12 | 2.18 | 0.44 |
| 34:BM:101:VAL:HG13 | 34:BM:101:VAL:O | 2.18 | 0.44 |
| 42:BU:11:ILE:HB | 42:BU:72:PHE:HD1 | 1.83 | 0.44 |
| 44:BX:21:LEU:HD23 | 44:BX:21:LEU:N | 2.33 | 0.44 |
| 1:CA:503:C:H2' | 1:CA:504:C:H6 | 1.82 | 0.44 |
| 1:CA:5:U:H1' | 1:CA:6:G:C2 | 2.53 | 0.44 |
| 1:CA:607:A:H2' | 1:CA:608:A:C8 | 2.53 | 0.44 |
| 1:CA:83:C:OP1 | 1:CA:83:C:H4' | 2.18 | 0.44 |
| 2:CC:126:ARG:HA | 2:CC:126:ARG:NE | 2.33 | 0.44 |
| 2:CC:178:ARG:O | 2:CC:178:ARG:HG2 | 2.18 | 0.44 |
| 5:CF:71:ILE:HG13 | 5:CF:72:ASP:N | 2.33 | 0.44 |
| 8:CI:42:THR:O | 8:CI:46:VAL:HG22 | 2.18 | 0.44 |
| 11:CL:54:VAL:CG2 | 11:CL:79:ILE:HD11 | 2.48 | 0.44 |
| 11:CL:65:TYR:HB3 | 11:CL:95:HIS:CD2 | 2.52 | 0.44 |
| 12:CM:18:LEU:HD13 | 12:CM:33:LEU:HD21 | 2.00 | 0.44 |
| 12:CM:2:ARG:HD3 | 12:CM:2:ARG:N | 2.31 | 0.44 |
| 18:CS:12:LEU:O | 18:CS:16:LYS:HE2 | 2.17 | 0.44 |
| 1:CA:958:A:N1 | 18:CS:53:GLY:C | 2.71 | 0.44 |
| 18:CS:77:ARG:HB3 | 18:CS:77:ARG:HE | 1.64 | 0.44 |
| 19:CT:69:ASN:O | 19:CT:70:LYS:C | 2.57 | 0.44 |
| 21:CU:40:PRO:HG2 | 21:CU:41:THR:H | 1.83 | 0.44 |
| 49:D2:4:THR:O | 49:D2:5:PHE:HB2 | 2.16 | 0.44 |
| 50:D3:7:ARG:HG3 | 50:D3:7:ARG:HH11 | 1.82 | 0.44 |
| 22:DA:111:U:H2' | 22:DA:112:G:C8 | 2.53 | 0.44 |
| 22:DA:32:U:H2' | 22:DA:33:G:O4' | 2.18 | 0.44 |
| 22:DA:43:C:H1' | 28:DF:91:ARG:NH2 | 2.31 | 0.44 |
| 23:DB:1563:U:H2' | 23:DB:1564:C:C6 | 2.53 | 0.44 |
| 23:DB:1764:C:H2' | 23:DB:1765:U:H6 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1774:C:C2' | 23:DB:1774:C:O2 | 2.66 | 0.44 |
| 23:DB:1843:C:H5'' | 25:DC:250:GLN:NE2 | 2.30 | 0.44 |
| 23:DB:2277:G:C5' | 34:DM:86:LYS:HB2 | 2.48 | 0.44 |
| 23:DB:784:G:OP1 | 23:DB:2588:G:H5'' | 2.18 | 0.44 |
| 23:DB:2654:A:N6 | 23:DB:2666:C:OP2 | 2.50 | 0.44 |
| 23:DB:90:U:OP2 | 23:DB:91:A:H3' | 2.18 | 0.44 |
| 25:DC:103:ILE:HG22 | 25:DC:105:ALA:N | 2.32 | 0.44 |
| 26:DD:11:MET:H | 26:DD:25:THR:HA | 1.83 | 0.44 |
| 27:DE:101:TYR:O | 27:DE:104:ALA:HB3 | 2.17 | 0.44 |
| 28:DF:55:ASP:OD2 | 28:DF:149:ARG:HD2 | 2.18 | 0.44 |
| 30:DH:14:SER:HB2 | 30:DH:17:ASP:CB | 2.47 | 0.44 |
| 34:DM:69:PRO:HA | 34:DM:94:ALA:CA | 2.48 | 0.44 |
| 36:DO:51:ALA:CB | 36:DO:78:VAL:HG13 | 2.48 | 0.44 |
| 37:DP:46:VAL:HA | 37:DP:60:VAL:HG12 | 2.00 | 0.44 |
| 32:DK:75:SER:HA | 37:DP:72:VAL:O | 2.17 | 0.44 |
| 38:DQ:18:LYS:C | 38:DQ:20:ALA:N | 2.71 | 0.44 |
| 38:DQ:7:VAL:O | 38:DQ:8:ILE:C | 2.56 | 0.44 |
| 39:DR:6:GLN:HE22 | 39:DR:9:GLY:N | 2.16 | 0.44 |
| 41:DT:39:THR:HG22 | 41:DT:42:GLU:HG2 | 2.00 | 0.44 |
| 42:DU:32:LYS:HD3 | 42:DU:32:LYS:H | 1.83 | 0.44 |
| 43:DW:37:VAL:HB | 43:DW:38:ARG:HD3 | 2.00 | 0.44 |
| 44:DX:24:GLU:O | 44:DX:28:LEU:HD23 | 2.18 | 0.44 |
| 44:DX:56:LEU:C | 44:DX:58:ASN:N | 2.72 | 0.44 |
| 46:DZ:10:LYS:O | 46:DZ:31:PRO:HG2 | 2.18 | 0.44 |
| 46:DZ:53:ALA:O | 46:DZ:54:LYS:HB3 | 2.18 | 0.44 |
| 1:AA:1102:A:H2' | 1:AA:1103:C:C6 | 2.53 | 0.43 |
| 1:AA:1200:C:H4' | 1:AA:1201:A:H3' | 2.00 | 0.43 |
| 1:AA:1406:U:O2' | 1:AA:1407:C:H5' | 2.18 | 0.43 |
| 1:AA:178:C:O2' | 1:AA:179:A:H5' | 2.17 | 0.43 |
| 1:AA:201:G:O2' | 1:AA:469:C:H4' | 2.17 | 0.43 |
| 1:AA:516:U:O2' | 1:AA:517:G:H5' | 2.17 | 0.43 |
| 1:AA:791:G:C5 | 1:AA:792:A:N7 | 2.86 | 0.43 |
| 1:AA:837:U:H2' | 1:AA:838:G:H8 | 1.83 | 0.43 |
| 1:AA:845:A:H5'' | 1:AA:846:G:C8 | 2.53 | 0.43 |
| 1:AA:885:G:O2' | 1:AA:886:G:H5' | 2.17 | 0.43 |
| 1:AA:90:C:OP2 | 1:AA:90:C:H6 | 2.01 | 0.43 |
| 1:AA:987:G:H2' | 1:AA:988:G:H8 | 1.83 | 0.43 |
| 3:AD:123:MET:HG3 | 3:AD:143:SER:OG | 2.18 | 0.43 |
| 3:AD:7:LYS:HB3 | 3:AD:20:LEU:HB3 | 1.99 | 0.43 |
| 3:AD:29:THR:HB | 3:AD:30:LYS:HZ2 | 1.81 | 0.43 |
| 5:AF:18:VAL:N | 5:AF:19:PRO:HD2 | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:878:A:C5' | 7:AH:80:PRO:HG2 | 2.48 | 0.43 |
| 8:AI:20:ILE:CD1 | 8:AI:20:ILE:H | 2.30 | 0.43 |
| 11:AL:54:VAL:CG2 | 11:AL:79:ILE:HD11 | 2.48 | 0.43 |
| 13:AN:50:LEU:CG | 13:AN:51:PRO:HD3 | 2.47 | 0.43 |
| 13:AN:69:PRO:HG2 | 13:AN:70:HIS:H | 1.83 | 0.43 |
| 15:AP:21:VAL:HG12 | 15:AP:33:ILE:HD12 | 1.98 | 0.43 |
| 15:AP:40:ASN:ND2 | 15:AP:43:ALA:HB2 | 2.33 | 0.43 |
| 18:AS:52:ASN:ND2 | 18:AS:53:GLY:H | 2.16 | 0.43 |
| 10:AK:126:ARG:HB2 | 21:AU:33:ARG:HD2 | 1.99 | 0.43 |
| 21:AU:40:PRO:HG2 | 21:AU:41:THR:H | 1.83 | 0.43 |
| 22:BA:75:G:N1 | 22:BA:102:G:N2 | 2.47 | 0.43 |
| 22:BA:115:A:O2' | 22:BA:116:G:H5' | 2.17 | 0.43 |
| 22:BA:22:U:H2' | 22:BA:23:G:C8 | 2.53 | 0.43 |
| 22:BA:27:C:C2' | 22:BA:28:C:H5' | 2.48 | 0.43 |
| 23:BB:1241:A:O4' | 23:BB:1241:A:N3 | 2.51 | 0.43 |
| 23:BB:1299:G:H5'' | 23:BB:1300:G:OP1 | 2.17 | 0.43 |
| 23:BB:1902:C:H2' | 23:BB:1903:G:O4' | 2.18 | 0.43 |
| 23:BB:1904:G:H1' | 23:BB:1927:A:N1 | 2.32 | 0.43 |
| 23:BB:1912:A:H4' | 23:BB:1913:A:OP1 | 2.18 | 0.43 |
| 23:BB:2133:G:N3 | 23:BB:2133:G:C2' | 2.80 | 0.43 |
| 23:BB:2140:G:H8 | 23:BB:2140:G:OP2 | 2.01 | 0.43 |
| 23:BB:55:G:H2' | 23:BB:56:A:H8 | 1.83 | 0.43 |
| 23:BB:560:C:H2' | 23:BB:561:G:O4' | 2.19 | 0.43 |
| 23:BB:596:U:O2' | 23:BB:597:G:H5' | 2.18 | 0.43 |
| 23:BB:643:A:C5 | 23:BB:644:A:N7 | 2.86 | 0.43 |
| 23:BB:67:U:H2' | 23:BB:68:G:C8 | 2.53 | 0.43 |
| 25:BC:226:PRO:HA | 25:BC:232:GLY:HA3 | 2.00 | 0.43 |
| 27:BE:104:ALA:C | 27:BE:106:LYS:H | 2.21 | 0.43 |
| 27:BE:134:LEU:HD21 | 27:BE:161:ALA:HB2 | 2.00 | 0.43 |
| 23:BB:588:U:H1' | 27:BE:85:PHE:CG | 2.53 | 0.43 |
| 28:BF:148:VAL:O | 28:BF:149:ARG:HG2 | 2.18 | 0.43 |
| 28:BF:71:LYS:HG2 | 28:BF:71:LYS:O | 2.18 | 0.43 |
| 28:BF:87:LYS:C | 28:BF:88:VAL:HG23 | 2.38 | 0.43 |
| 28:BF:33:ILE:H | 28:BF:95:MET:HG3 | 1.83 | 0.43 |
| 29:BG:58:ALA:C | 29:BG:60:GLY:H | 2.21 | 0.43 |
| 52:BI:12:VAL:HG23 | 52:BI:41:PHE:CE2 | 2.54 | 0.43 |
| 52:BI:4:VAL:O | 52:BI:4:VAL:HG13 | 2.17 | 0.43 |
| 31:BJ:59:ALA:C | 31:BJ:61:LYS:N | 2.71 | 0.43 |
| 23:BB:1244:A:C5' | 33:BL:8:PRO:HD3 | 2.34 | 0.43 |
| 35:BN:33:ILE:C | 35:BN:34:ILE:HG13 | 2.37 | 0.43 |
| 39:BR:19:THR:HG22 | 39:BR:97:LYS:HD2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:BS:81:SER:CA | 40:BS:99:ARG:HA | 2.46 | 0.43 |
| 44:BX:35:GLY:O | 44:BX:36:GLN:C | 2.57 | 0.43 |
| 45:BY:35:VAL:HG21 | 45:BY:37:ARG:NH2 | 2.33 | 0.43 |
| 1:CA:1065:U:H1' | 1:CA:1066:C:OP2 | 2.18 | 0.43 |
| 1:CA:1114:C:O2' | 1:CA:1115:U:H5' | 2.18 | 0.43 |
| 1:CA:1473:G:O2' | 1:CA:1474:U:H5' | 2.18 | 0.43 |
| 1:CA:926:G:H3' | 1:CA:1505:G:H21 | 1.82 | 0.43 |
| 1:CA:317:U:H2' | 1:CA:318:G:C8 | 2.53 | 0.43 |
| 1:CA:328:C:H4' | 1:CA:329:A:C5' | 2.47 | 0.43 |
| 1:CA:599:C:H4' | 7:CH:121:GLY:CA | 2.47 | 0.43 |
| 1:CA:69:G:H21 | 1:CA:71:A:H62 | 1.65 | 0.43 |
| 1:CA:993:G:O2' | 1:CA:994:A:N7 | 2.51 | 0.43 |
| 1:CA:993:G:N2 | 1:CA:996:A:N6 | 2.66 | 0.43 |
| 3:CD:123:MET:HA | 3:CD:128:VAL:HA | 2.00 | 0.43 |
| 3:CD:160:LEU:CD1 | 3:CD:160:LEU:H | 2.16 | 0.43 |
| 5:CF:47:LEU:HD13 | 5:CF:51:ILE:CG2 | 2.47 | 0.43 |
| 10:CK:23:HIS:HB3 | 10:CK:30:ILE:HG12 | 2.00 | 0.43 |
| 11:CL:54:VAL:HG12 | 11:CL:55:ARG:H | 1.83 | 0.43 |
| 12:CM:5:GLY:O | 12:CM:6:ILE:HB | 2.18 | 0.43 |
| 21:CU:36:PHE:HB3 | 21:CU:40:PRO:CD | 2.41 | 0.43 |
| 21:CU:39:LYS:H | 21:CU:39:LYS:HD3 | 1.82 | 0.43 |
| 22:DA:106:G:H2' | 22:DA:107:G:C8 | 2.53 | 0.43 |
| 22:DA:30:C:H1' | 22:DA:58:A:N1 | 2.33 | 0.43 |
| 23:DB:1249:U:C4' | 38:DQ:3:VAL:HG21 | 2.47 | 0.43 |
| 23:DB:1315:C:O2' | 23:DB:1316:U:H5' | 2.18 | 0.43 |
| 23:DB:1495:A:H2' | 23:DB:1496:A:H8 | 1.82 | 0.43 |
| 23:DB:1767:G:O2' | 23:DB:1768:C:H5' | 2.18 | 0.43 |
| 23:DB:1817:G:OP1 | 25:DC:86:ARG:NH2 | 2.50 | 0.43 |
| 23:DB:2496:C:C2' | 23:DB:2497:A:H5' | 2.48 | 0.43 |
| 23:DB:2617:U:H2' | 23:DB:2618:G:H5' | 1.99 | 0.43 |
| 23:DB:2716:C:H2' | 23:DB:2717:C:H6 | 1.83 | 0.43 |
| 23:DB:327:G:O2' | 23:DB:328:U:H5' | 2.18 | 0.43 |
| 23:DB:470:A:H2' | 23:DB:471:A:C8 | 2.53 | 0.43 |
| 23:DB:483:A:H5' | 42:DU:44:HIS:O | 2.18 | 0.43 |
| 23:DB:704:G:O2' | 23:DB:727:A:N6 | 2.51 | 0.43 |
| 23:DB:939:G:O2' | 23:DB:940:G:H5' | 2.18 | 0.43 |
| 23:DB:963:U:H2' | 23:DB:964:C:C6 | 2.52 | 0.43 |
| 25:DC:226:PRO:HA | 25:DC:232:GLY:HA3 | 2.00 | 0.43 |
| 25:DC:77:VAL:HG23 | 25:DC:77:VAL:O | 2.18 | 0.43 |
| 25:DC:78:GLU:OE1 | 25:DC:94:LEU:HD22 | 2.18 | 0.43 |
| 26:DD:148:GLN:HG3 | 26:DD:152:PRO:HB3 | 1.98 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DD:34:VAL:HG23 | 26:DD:48:ILE:HG13 | 2.00 | 0.43 |
| 26:DD:8:LYS:O | 26:DD:197:THR:HA | 2.18 | 0.43 |
| 26:DD:91:THR:HG23 | 26:DD:92:VAL:N | 2.32 | 0.43 |
| 28:DF:62:GLN:HE21 | 28:DF:91:ARG:NE | 2.15 | 0.43 |
| 29:DG:4:ALA:HA | 29:DG:65:GLY:HA2 | 2.00 | 0.43 |
| 30:DH:4:ILE:HG23 | 30:DH:17:ASP:N | 2.33 | 0.43 |
| 32:DK:7:MET:CE | 32:DK:18:ARG:HB3 | 2.48 | 0.43 |
| 32:DK:31:ARG:HH11 | 32:DK:31:ARG:HG3 | 1.83 | 0.43 |
| 32:DK:24:VAL:CG1 | 32:DK:33:ALA:HB2 | 2.47 | 0.43 |
| 34:DM:53:MET:O | 34:DM:57:VAL:HG23 | 2.17 | 0.43 |
| 36:DO:116:GLN:O | 36:DO:117:PHE:HB3 | 2.18 | 0.43 |
| 38:DQ:38:VAL:O | 38:DQ:41:ALA:N | 2.52 | 0.43 |
| 39:DR:76:LYS:HB2 | 39:DR:85:LYS:HB3 | 2.00 | 0.43 |
| 23:DB:139:U:O2' | 41:DT:1:MET:HB3 | 2.18 | 0.43 |
| 43:DW:35:ILE:HA | 43:DW:57:THR:HA | 2.00 | 0.43 |
| 43:DW:49:ASN:CB | 43:DW:61:LYS:HB2 | 2.48 | 0.43 |
| 45:DY:6:ILE:HG23 | 45:DY:56:VAL:HG22 | 1.99 | 0.43 |
| 46:DZ:27:ARG:CG | 46:DZ:28:ARG:N | 2.81 | 0.43 |
| 46:DZ:40:VAL:O | 46:DZ:42:SER:N | 2.51 | 0.43 |
| 46:DZ:65:ASP:N | 46:DZ:65:ASP:OD2 | 2.51 | 0.43 |
| 1:AA:389:A:C6 | 1:AA:390:U:H1' | 2.53 | 0.43 |
| 1:AA:736:C:H2' | 1:AA:737:C:H6 | 1.83 | 0.43 |
| 1:AA:893:C:H2' | 1:AA:894:G:H8 | 1.82 | 0.43 |
| 20:AB:17:HIS:CG | 20:AB:18:GLN:H | 2.36 | 0.43 |
| 20:AB:17:HIS:CG | 20:AB:18:GLN:N | 2.86 | 0.43 |
| 2:AC:179:ALA:O | 2:AC:180:ASP:O | 2.36 | 0.43 |
| 3:AD:24:VAL:HA | 3:AD:27:ILE:CD1 | 2.45 | 0.43 |
| 1:AA:923:A:OP1 | 4:AE:25:LYS:HB3 | 2.18 | 0.43 |
| 4:AE:64:GLU:O | 4:AE:68:ARG:HG2 | 2.18 | 0.43 |
| 5:AF:47:LEU:HD13 | 5:AF:51:ILE:HG22 | 2.00 | 0.43 |
| 5:AF:40:GLU:CB | 5:AF:61:LEU:HB2 | 2.46 | 0.43 |
| 6:AG:137:ARG:HG2 | 6:AG:141:HIS:NE2 | 2.32 | 0.43 |
| 8:AI:95:SER:O | 8:AI:99:LYS:HB2 | 2.18 | 0.43 |
| 9:AJ:8:ILE:CD1 | 9:AJ:76:ILE:HG13 | 2.47 | 0.43 |
| 19:AT:42:ASP:OD1 | 19:AT:44:ALA:HB3 | 2.18 | 0.43 |
| 48:B1:3:GLY:C | 48:B1:5:ARG:N | 2.71 | 0.43 |
| 48:B1:6:GLU:HB2 | 48:B1:52:LYS:NZ | 2.32 | 0.43 |
| 22:BA:28:C:H2' | 22:BA:29:A:C8 | 2.53 | 0.43 |
| 23:BB:1182:G:H2' | 23:BB:1183:U:O4' | 2.18 | 0.43 |
| 23:BB:127:A:H5'' | 23:BB:128:C:C6 | 2.54 | 0.43 |
| 23:BB:1387:A:C5' | 23:BB:1469:A:H1' | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1745:A:H2' | 23:BB:1746:A:C8 | 2.53 | 0.43 |
| 23:BB:1973:G:O2' | 23:BB:1974:C:H5' | 2.18 | 0.43 |
| 23:BB:2485:G:O2' | 23:BB:2486:C:H5' | 2.18 | 0.43 |
| 23:BB:2667:C:H1' | 29:BG:108:PHE:CD2 | 2.53 | 0.43 |
| 23:BB:623:C:H2' | 23:BB:624:C:H6 | 1.83 | 0.43 |
| 25:BC:131:MET:HE3 | 25:BC:187:CYS:O | 2.17 | 0.43 |
| 25:BC:64:VAL:HG11 | 25:BC:66:PHE:CE2 | 2.52 | 0.43 |
| 26:BD:171:THR:OG1 | 26:BD:172:VAL:N | 2.50 | 0.43 |
| 26:BD:201:LEU:C | 26:BD:202:ILE:HD12 | 2.38 | 0.43 |
| 27:BE:192:ALA:O | 27:BE:196:VAL:HG23 | 2.18 | 0.43 |
| 27:BE:24:ASN:OD1 | 27:BE:27:LEU:HB2 | 2.19 | 0.43 |
| 32:BK:19:VAL:HG12 | 32:BK:41:ILE:CG1 | 2.44 | 0.43 |
| 33:BL:143:GLU:O | 33:BL:144:GLU:HB2 | 2.18 | 0.43 |
| 36:BO:74:VAL:O | 36:BO:77:ALA:HB3 | 2.18 | 0.43 |
| 41:BT:62:VAL:HG12 | 41:BT:63:VAL:H | 1.83 | 0.43 |
| 42:BU:21:ARG:HD3 | 42:BU:72:PHE:CG | 2.53 | 0.43 |
| 46:BZ:68:LEU:HD22 | 46:BZ:78:TYR:HE1 | 1.83 | 0.43 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C5 | 2.53 | 0.43 |
| 1:CA:1314:C:H2' | 1:CA:1315:U:C6 | 2.53 | 0.43 |
| 1:CA:35:G:H2' | 1:CA:36:C:H6 | 1.80 | 0.43 |
| 1:CA:789:U:O2' | 1:CA:791:G:N7 | 2.44 | 0.43 |
| 3:CD:169:TRP:O | 3:CD:182:LYS:HB2 | 2.17 | 0.43 |
| 4:CE:87:VAL:HG23 | 4:CE:91:SER:O | 2.18 | 0.43 |
| 5:CF:36:ILE:H | 5:CF:36:ILE:HD12 | 1.83 | 0.43 |
| 5:CF:67:PRO:O | 5:CF:70:VAL:HG22 | 2.17 | 0.43 |
| 7:CH:58:LEU:CD2 | 7:CH:60:LEU:HB2 | 2.47 | 0.43 |
| 8:CI:87:MET:HE2 | 8:CI:88:GLU:HA | 2.00 | 0.43 |
| 13:CN:48:GLN:H | 13:CN:48:GLN:HG3 | 1.68 | 0.43 |
| 14:CO:42:PHE:CD1 | 14:CO:55:LEU:HD22 | 2.53 | 0.43 |
| 16:CQ:45:VAL:HG11 | 16:CQ:60:ILE:HG21 | 2.00 | 0.43 |
| 21:CU:26:GLY:C | 21:CU:28:LEU:N | 2.71 | 0.43 |
| 51:D4:2:LYS:HD3 | 51:D4:4:ARG:HG3 | 2.00 | 0.43 |
| 23:DB:1182:G:H2' | 23:DB:1183:U:O4' | 2.18 | 0.43 |
| 23:DB:1309:G:H4' | 49:D2:7:PRO:HB2 | 2.00 | 0.43 |
| 23:DB:1322:A:C2' | 23:DB:1323:C:H5' | 2.48 | 0.43 |
| 23:DB:1472:C:H2' | 23:DB:1473:G:H8 | 1.82 | 0.43 |
| 23:DB:1528:A:H2' | 23:DB:1529:G:O4' | 2.18 | 0.43 |
| 23:DB:2630:G:O2' | 23:DB:2631:G:H5' | 2.18 | 0.43 |
| 23:DB:2760:C:H2' | 23:DB:2760:C:O2 | 2.18 | 0.43 |
| 23:DB:2860:A:H2' | 23:DB:2861:U:O4' | 2.18 | 0.43 |
| 23:DB:484:C:H2' | 23:DB:485:C:H6 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:493:G:H2' | 23:DB:494:G:O4' | 2.17 | 0.43 |
| 23:DB:538:A:H2' | 23:DB:539:G:O4' | 2.18 | 0.43 |
| 23:DB:619:G:H2' | 23:DB:620:G:H5'' | 2.00 | 0.43 |
| 23:DB:755:U:H2' | 23:DB:756:A:C8 | 2.53 | 0.43 |
| 23:DB:958:U:OP2 | 34:DM:14:LYS:NZ | 2.51 | 0.43 |
| 28:DF:19:PHE:CE1 | 28:DF:167:ALA:HB2 | 2.53 | 0.43 |
| 28:DF:79:ARG:O | 28:DF:81:GLY:N | 2.51 | 0.43 |
| 29:DG:104:LEU:HB3 | 29:DG:106:LEU:HD21 | 1.99 | 0.43 |
| 33:DL:135:ILE:HG12 | 33:DL:140:GLY:HA2 | 2.00 | 0.43 |
| 34:DM:135:VAL:O | 34:DM:135:VAL:HG12 | 2.18 | 0.43 |
| 35:DN:70:THR:OG1 | 35:DN:70:THR:O | 2.36 | 0.43 |
| 38:DQ:33:VAL:HG23 | 38:DQ:34:ALA:N | 2.34 | 0.43 |
| 38:DQ:68:ALA:C | 38:DQ:71:ASN:HB3 | 2.38 | 0.43 |
| 38:DQ:78:PHE:CZ | 38:DQ:82:LEU:HD11 | 2.53 | 0.43 |
| 41:DT:22:THR:O | 41:DT:25:GLU:HB3 | 2.18 | 0.43 |
| 24:DV:48:MET:SD | 24:DV:85:LYS:HA | 2.59 | 0.43 |
| 46:DZ:43:GLU:HG2 | 46:DZ:43:GLU:O | 2.18 | 0.43 |
| 46:DZ:49:LEU:HB2 | 46:DZ:51:VAL:HG23 | 2.00 | 0.43 |
| 1:AA:1069:C:O4' | 1:AA:1191:A:H2 | 2.00 | 0.43 |
| 1:AA:1241:G:O2' | 1:AA:1242:G:H5' | 2.18 | 0.43 |
| 1:AA:1292:G:H2' | 1:AA:1293:C:H6 | 1.78 | 0.43 |
| 1:AA:152:A:H3' | 1:AA:153:C:C6 | 2.54 | 0.43 |
| 1:AA:182:A:HO2' | 1:AA:183:C:H3' | 1.82 | 0.43 |
| 1:AA:138:G:C6 | 1:AA:226:G:C6 | 3.06 | 0.43 |
| 3:AD:169:TRP:O | 3:AD:182:LYS:HB2 | 2.18 | 0.43 |
| 3:AD:40:HIS:O | 3:AD:43:ARG:HG2 | 2.18 | 0.43 |
| 3:AD:47:LEU:HD13 | 3:AD:52:VAL:HG22 | 1.98 | 0.43 |
| 5:AF:45:ARG:HH22 | 17:AR:25:ILE:HD13 | 1.83 | 0.43 |
| 5:AF:80:PHE:CE2 | 25:BC:123:ILE:HG12 | 2.53 | 0.43 |
| 5:AF:98:GLU:CG | 5:AF:99:ALA:N | 2.80 | 0.43 |
| 6:AG:22:LEU:O | 6:AG:25:PHE:HB3 | 2.18 | 0.43 |
| 8:AI:119:LYS:C | 8:AI:121:ARG:H | 2.22 | 0.43 |
| 1:AA:1148:U:C4' | 8:AI:17:ARG:HD3 | 2.48 | 0.43 |
| 11:AL:51:VAL:HG12 | 11:AL:52:CYS:N | 2.30 | 0.43 |
| 11:AL:31:GLY:HA3 | 11:AL:54:VAL:HG11 | 2.00 | 0.43 |
| 1:AA:1320:C:H41 | 18:AS:36:ARG:HA | 1.83 | 0.43 |
| 48:B1:26:LYS:HB2 | 48:B1:52:LYS:NZ | 2.33 | 0.43 |
| 23:BB:643:A:N3 | 48:B1:43:ARG:NH2 | 2.65 | 0.43 |
| 23:BB:686:U:O4 | 49:B2:12:ARG:HB2 | 2.18 | 0.43 |
| 50:B3:11:LYS:C | 50:B3:12:ARG:HG3 | 2.39 | 0.43 |
| 23:BB:1432:G:O2' | 23:BB:1433:A:H5' | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:1946:U:O2' | 23:BB:1947:C:H5' | 2.18 | 0.43 |
| 23:BB:2037:A:C6 | 23:BB:2038:G:C6 | 3.07 | 0.43 |
| 23:BB:2096:C:H2' | 23:BB:2097:A:H8 | 1.84 | 0.43 |
| 23:BB:2492:U:O2' | 23:BB:2493:U:H5' | 2.18 | 0.43 |
| 23:BB:2500:U:H5' | 23:BB:2501:C:OP2 | 2.18 | 0.43 |
| 23:BB:2773:C:O2' | 23:BB:2774:C:H5' | 2.18 | 0.43 |
| 23:BB:27:G:HO2' | 23:BB:28:A:H8 | 1.60 | 0.43 |
| 23:BB:443:A:H1' | 23:BB:1201:U:O4' | 2.18 | 0.43 |
| 23:BB:566:U:H2' | 23:BB:567:U:O4' | 2.18 | 0.43 |
| 23:BB:672:C:H2' | 23:BB:673:C:C6 | 2.54 | 0.43 |
| 23:BB:743:A:C2' | 23:BB:744:U:H5' | 2.47 | 0.43 |
| 25:BC:123:ILE:HG13 | 25:BC:123:ILE:O | 2.17 | 0.43 |
| 23:BB:1820:U:H3 | 25:BC:197:ALA:HA | 1.83 | 0.43 |
| 26:BD:130:GLN:HB2 | 26:BD:139:SER:O | 2.17 | 0.43 |
| 26:BD:24:VAL:HG23 | 26:BD:189:VAL:N | 2.34 | 0.43 |
| 26:BD:33:ARG:NH2 | 26:BD:33:ARG:HG2 | 2.33 | 0.43 |
| 26:BD:55:LYS:HE3 | 26:BD:59:ARG:HB3 | 2.00 | 0.43 |
| 28:BF:19:PHE:CE1 | 28:BF:167:ALA:HB2 | 2.54 | 0.43 |
| 28:BF:74:ALA:CB | 28:BF:78:ILE:HD13 | 2.48 | 0.43 |
| 29:BG:154:GLU:OE1 | 29:BG:157:LYS:HB2 | 2.18 | 0.43 |
| 29:BG:60:GLY:O | 29:BG:62:ALA:N | 2.51 | 0.43 |
| 30:BH:133:GLN:CB | 30:BH:139:PHE:HA | 2.45 | 0.43 |
| 31:BJ:101:ILE:O | 31:BJ:104:ALA:HB3 | 2.18 | 0.43 |
| 34:BM:21:ALA:HB3 | 34:BM:99:GLY:O | 2.18 | 0.43 |
| 35:BN:48:VAL:O | 35:BN:51:LEU:N | 2.52 | 0.43 |
| 39:BR:49:ILE:HD13 | 39:BR:53:PHE:H | 1.81 | 0.43 |
| 40:BS:14:ALA:C | 40:BS:16:LYS:H | 2.22 | 0.43 |
| 40:BS:24:ILE:HG23 | 40:BS:32:ALA:CB | 2.48 | 0.43 |
| 42:BU:94:PHE:CA | 42:BU:101:THR:HA | 2.48 | 0.43 |
| 42:BU:23:LYS:HD2 | 42:BU:23:LYS:N | 2.34 | 0.43 |
| 42:BU:38:ILE:CG2 | 42:BU:39:ASN:H | 2.07 | 0.43 |
| 24:BV:21:ARG:NE | 24:BV:87:GLN:HB3 | 2.28 | 0.43 |
| 46:BZ:43:GLU:HG2 | 46:BZ:43:GLU:O | 2.18 | 0.43 |
| 1:CA:1057:G:H4' | 2:CC:196:GLY:N | 2.27 | 0.43 |
| 1:CA:1407:C:O2' | 1:CA:1408:A:H5' | 2.17 | 0.43 |
| 1:CA:1500:A:OP1 | 1:CA:1505:G:OP1 | 2.36 | 0.43 |
| 1:CA:153:C:H2' | 1:CA:154:U:H6 | 1.79 | 0.43 |
| 1:CA:307:C:H2' | 1:CA:308:C:H6 | 1.83 | 0.43 |
| 1:CA:394:G:H2' | 1:CA:395:C:C6 | 2.53 | 0.43 |
| 1:CA:795:C:H1' | 1:CA:1506:U:C5 | 2.53 | 0.43 |
| 20:CB:46:VAL:HA | 20:CB:49:PHE:HD2 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:CB:94:ARG:N | 20:CB:94:ARG:HE | 2.16 | 0.43 |
| 3:CD:121:ALA:C | 3:CD:122:ILE:HD13 | 2.39 | 0.43 |
| 1:CA:1080:A:H4' | 4:CE:20:VAL:HG13 | 1.98 | 0.43 |
| 8:CI:29:ILE:HG23 | 8:CI:64:ILE:C | 2.39 | 0.43 |
| 11:CL:43:LYS:CD | 11:CL:44:PRO:HD3 | 2.48 | 0.43 |
| 13:CN:51:PRO:HB2 | 13:CN:54:SER:CB | 2.33 | 0.43 |
| 16:CQ:30:HIS:CG | 16:CQ:33:TYR:HB2 | 2.53 | 0.43 |
| 16:CQ:60:ILE:HD13 | 16:CQ:60:ILE:N | 2.33 | 0.43 |
| 21:CU:15:LEU:C | 21:CU:17:ARG:H | 2.21 | 0.43 |
| 21:CU:26:GLY:O | 21:CU:30:GLU:HB3 | 2.17 | 0.43 |
| 51:D4:18:LYS:HE3 | 51:D4:21:GLY:HA2 | 2.00 | 0.43 |
| 22:DA:64:G:O2' | 22:DA:65:U:H5' | 2.19 | 0.43 |
| 23:DB:102:U:O4' | 23:DB:102:U:P | 2.76 | 0.43 |
| 23:DB:1112:G:H2' | 23:DB:1113:U:O4' | 2.18 | 0.43 |
| 23:DB:1387:A:C5' | 23:DB:1469:A:H1' | 2.48 | 0.43 |
| 23:DB:1528:A:H2' | 23:DB:1529:G:H5' | 2.00 | 0.43 |
| 23:DB:1674:G:N2 | 23:DB:1677:A:N1 | 2.67 | 0.43 |
| 23:DB:1973:G:H2' | 23:DB:1974:C:H6 | 1.83 | 0.43 |
| 23:DB:2025:C:H2' | 23:DB:2026:U:H6 | 1.78 | 0.43 |
| 23:DB:2211:A:H4' | 23:DB:2211:A:OP2 | 2.18 | 0.43 |
| 23:DB:2459:A:H2' | 23:DB:2459:A:N3 | 2.32 | 0.43 |
| 23:DB:2697:G:H2' | 23:DB:2698:U:O4' | 2.17 | 0.43 |
| 23:DB:611:C:H2' | 23:DB:612:G:O4' | 2.17 | 0.43 |
| 23:DB:719:C:O2' | 23:DB:720:U:H5' | 2.17 | 0.43 |
| 25:DC:157:ALA:C | 25:DC:159:THR:H | 2.22 | 0.43 |
| 25:DC:92:LEU:HG | 25:DC:93:VAL:H | 1.82 | 0.43 |
| 26:DD:197:THR:C | 26:DD:199:SER:H | 2.21 | 0.43 |
| 27:DE:91:ASP:C | 27:DE:93:SER:H | 2.21 | 0.43 |
| 29:DG:28:LYS:HG2 | 29:DG:79:THR:HA | 1.99 | 0.43 |
| 29:DG:83:THR:C | 29:DG:84:LYS:HD3 | 2.39 | 0.43 |
| 52:DI:11:GLN:NE2 | 52:DI:74:PRO:HG3 | 2.33 | 0.43 |
| 33:DL:120:VAL:O | 33:DL:135:ILE:HD11 | 2.17 | 0.43 |
| 33:DL:61:LEU:N | 33:DL:61:LEU:CD1 | 2.81 | 0.43 |
| 34:DM:28:PHE:HB3 | 34:DM:64:TRP:CE2 | 2.52 | 0.43 |
| 36:DO:67:ASN:H | 36:DO:70:ALA:CB | 2.29 | 0.43 |
| 36:DO:8:ILE:HG13 | 36:DO:8:ILE:H | 1.67 | 0.43 |
| 38:DQ:45:ALA:O | 38:DQ:49:ARG:N | 2.47 | 0.43 |
| 39:DR:39:LEU:CA | 39:DR:53:PHE:HA | 2.44 | 0.43 |
| 41:DT:32:LEU:H | 41:DT:83:ALA:CB | 2.30 | 0.43 |
| 42:DU:94:PHE:HB2 | 42:DU:101:THR:HA | 1.99 | 0.43 |
| 1:AA:1002:G:H2' | 1:AA:1003:G:O4' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1042:A:H2' | 1:AA:1043:G:O4' | 2.18 | 0.43 |
| 1:AA:1381:U:O2' | 1:AA:1382:C:H5' | 2.18 | 0.43 |
| 1:AA:1426:G:H2' | 1:AA:1427:C:O4' | 2.19 | 0.43 |
| 1:AA:394:G:H2' | 1:AA:395:C:C6 | 2.53 | 0.43 |
| 20:AB:31:PHE:HB3 | 20:AB:39:ILE:CG2 | 2.48 | 0.43 |
| 20:AB:48:MET:H | 20:AB:48:MET:HG2 | 1.58 | 0.43 |
| 4:AE:68:ARG:O | 4:AE:69:ASN:HB2 | 2.17 | 0.43 |
| 5:AF:10:VAL:HG12 | 5:AF:11:HIS:N | 2.33 | 0.43 |
| 6:AG:11:ILE:HG22 | 6:AG:12:LEU:N | 2.33 | 0.43 |
| 8:AI:18:VAL:HG12 | 8:AI:19:PHE:N | 2.33 | 0.43 |
| 8:AI:42:THR:O | 8:AI:46:VAL:HG22 | 2.18 | 0.43 |
| 1:AA:1150:A:O3' | 9:AJ:43:PRO:HA | 2.19 | 0.43 |
| 9:AJ:49:PHE:HB2 | 9:AJ:65:TYR:HB2 | 1.99 | 0.43 |
| 11:AL:16:ALA:HB1 | 11:AL:17:LYS:HZ1 | 1.82 | 0.43 |
| 11:AL:60:PHE:O | 11:AL:62:VAL:N | 2.51 | 0.43 |
| 12:AM:102:LYS:NZ | 12:AM:102:LYS:HB2 | 2.33 | 0.43 |
| 12:AM:30:LYS:HG3 | 12:AM:40:GLU:OE1 | 2.19 | 0.43 |
| 21:AU:44:ARG:HG3 | 21:AU:44:ARG:NH1 | 2.33 | 0.43 |
| 51:B4:3:VAL:O | 51:B4:4:ARG:HB2 | 2.19 | 0.43 |
| 23:BB:1053:C:H2' | 23:BB:1054:A:C8 | 2.53 | 0.43 |
| 23:BB:1411:U:H2' | 23:BB:1412:U:C6 | 2.54 | 0.43 |
| 23:BB:1706:C:H2' | 23:BB:1757:A:OP2 | 2.18 | 0.43 |
| 23:BB:2304:G:H2' | 23:BB:2304:G:N3 | 2.33 | 0.43 |
| 23:BB:252:G:O2' | 23:BB:253:C:H5' | 2.18 | 0.43 |
| 23:BB:2547:A:H2' | 23:BB:2548:U:H6 | 1.82 | 0.43 |
| 23:BB:2800:A:H2' | 23:BB:2801:G:C1' | 2.49 | 0.43 |
| 23:BB:416:U:H2' | 23:BB:417:C:H6 | 1.82 | 0.43 |
| 23:BB:514:A:N6 | 23:BB:515:A:N6 | 2.66 | 0.43 |
| 23:BB:673:C:C5' | 27:BE:76:PRO:HD2 | 2.47 | 0.43 |
| 23:BB:826:U:H2' | 23:BB:828:U:O4' | 2.18 | 0.43 |
| 23:BB:95:A:H4' | 44:BX:38:GLN:O | 2.18 | 0.43 |
| 23:BB:967:U:H2' | 23:BB:968:C:H6 | 1.82 | 0.43 |
| 25:BC:120:ASP:N | 25:BC:120:ASP:OD2 | 2.50 | 0.43 |
| 25:BC:255:LYS:C | 25:BC:256:THR:HG23 | 2.38 | 0.43 |
| 26:BD:109:VAL:HG11 | 26:BD:193:VAL:CB | 2.48 | 0.43 |
| 26:BD:202:ILE:HG22 | 26:BD:202:ILE:O | 2.17 | 0.43 |
| 27:BE:1:MET:HB3 | 27:BE:14:VAL:O | 2.19 | 0.43 |
| 30:BH:67:ALA:C | 30:BH:69:ALA:H | 2.21 | 0.43 |
| 52:BI:85:ILE:CD1 | 52:BI:137:LEU:HD21 | 2.47 | 0.43 |
| 52:BI:138:VAL:HG12 | 52:BI:139:VAL:N | 2.33 | 0.43 |
| 32:BK:79:PHE:CD2 | 37:BP:69:VAL:HG12 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BL:74:THR:HA | 33:BL:107:PHE:O | 2.19 | 0.43 |
| 35:BN:24:MET:CG | 35:BN:44:LEU:HD22 | 2.48 | 0.43 |
| 35:BN:29:VAL:HG21 | 35:BN:75:ILE:HB | 2.01 | 0.43 |
| 24:BV:60:VAL:HG22 | 24:BV:73:LYS:HE2 | 2.00 | 0.43 |
| 44:BX:22:LEU:O | 44:BX:24:GLU:N | 2.51 | 0.43 |
| 1:CA:409:U:O2' | 1:CA:410:G:H5' | 2.18 | 0.43 |
| 1:CA:451:A:H4' | 1:CA:452:A:O4' | 2.18 | 0.43 |
| 1:CA:496:A:H2' | 1:CA:497:G:C8 | 2.52 | 0.43 |
| 1:CA:502:A:H2' | 1:CA:503:C:O4' | 2.19 | 0.43 |
| 1:CA:78:A:H2' | 1:CA:79:G:C8 | 2.53 | 0.43 |
| 1:CA:845:A:H5'' | 1:CA:846:G:C8 | 2.53 | 0.43 |
| 1:CA:880:C:H2' | 1:CA:881:G:H8 | 1.84 | 0.43 |
| 1:CA:902:G:H2' | 1:CA:903:G:H8 | 1.84 | 0.43 |
| 20:CB:104:LYS:NZ | 20:CB:104:LYS:HB2 | 2.33 | 0.43 |
| 20:CB:116:LEU:HA | 20:CB:119:GLN:CG | 2.48 | 0.43 |
| 4:CE:11:GLN:O | 4:CE:38:VAL:HA | 2.18 | 0.43 |
| 5:CF:43:GLY:HA2 | 5:CF:58:HIS:CD2 | 2.53 | 0.43 |
| 7:CH:105:THR:HG21 | 7:CH:110:MET:SD | 2.59 | 0.43 |
| 8:CI:123:ARG:HB3 | 8:CI:123:ARG:NH1 | 2.32 | 0.43 |
| 9:CJ:5:ARG:N | 9:CJ:76:ILE:O | 2.52 | 0.43 |
| 12:CM:19:THR:HG22 | 12:CM:29:SER:HB3 | 2.01 | 0.43 |
| 13:CN:23:ARG:C | 13:CN:25:GLU:H | 2.20 | 0.43 |
| 50:D3:11:LYS:C | 50:D3:12:ARG:HG3 | 2.38 | 0.43 |
| 23:DB:1124:G:N3 | 51:D4:38:GLY:O | 2.51 | 0.43 |
| 23:DB:1042:G:H2' | 23:DB:1043:C:H6 | 1.82 | 0.43 |
| 23:DB:1103:A:H2' | 23:DB:1103:A:N3 | 2.34 | 0.43 |
| 23:DB:1184:U:O2' | 23:DB:1185:G:H5' | 2.19 | 0.43 |
| 23:DB:1370:C:H2' | 23:DB:1371:G:O4' | 2.19 | 0.43 |
| 23:DB:1545:A:H2' | 23:DB:1546:G:O4' | 2.19 | 0.43 |
| 23:DB:183:C:O2' | 23:DB:184:C:H5' | 2.19 | 0.43 |
| 23:DB:2249:U:H4' | 23:DB:2275:C:C5 | 2.54 | 0.43 |
| 23:DB:2297:A:H61 | 23:DB:2319:G:H1' | 1.83 | 0.43 |
| 23:DB:2315:G:H2' | 23:DB:2316:G:H8 | 1.83 | 0.43 |
| 23:DB:2466:C:OP1 | 51:D4:4:ARG:HB3 | 2.18 | 0.43 |
| 23:DB:2766:A:N3 | 23:DB:2766:A:H2' | 2.33 | 0.43 |
| 23:DB:2857:G:N2 | 23:DB:2859:G:H3' | 2.33 | 0.43 |
| 23:DB:342:A:H2' | 23:DB:343:C:O4' | 2.19 | 0.43 |
| 23:DB:699:A:H2' | 23:DB:700:G:O4' | 2.19 | 0.43 |
| 23:DB:708:G:N2 | 23:DB:724:U:H1' | 2.33 | 0.43 |
| 23:DB:91:A:H1' | 23:DB:92:U:C6 | 2.54 | 0.43 |
| 23:DB:937:C:H2' | 23:DB:938:G:H8 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:96:C:H2' | 23:DB:97:C:H6 | 1.83 | 0.43 |
| 25:DC:244:VAL:HB | 25:DC:249:VAL:H | 1.82 | 0.43 |
| 25:DC:75:ALA:HB1 | 25:DC:93:VAL:HG22 | 1.99 | 0.43 |
| 23:DB:2572:A:P | 26:DD:151:THR:HB | 2.59 | 0.43 |
| 26:DD:55:LYS:HE3 | 26:DD:59:ARG:HB3 | 1.99 | 0.43 |
| 28:DF:126:ASN:HB3 | 28:DF:156:THR:CB | 2.49 | 0.43 |
| 28:DF:24:VAL:O | 28:DF:27:VAL:HG22 | 2.18 | 0.43 |
| 30:DH:131:SER:OG | 30:DH:141:LYS:HE3 | 2.18 | 0.43 |
| 23:DB:1099:G:O5' | 52:DI:4:VAL:HG12 | 2.18 | 0.43 |
| 52:DI:54:ILE:HD11 | 52:DI:71:LYS:N | 2.33 | 0.43 |
| 31:DJ:55:ILE:HG13 | 31:DJ:55:ILE:O | 2.16 | 0.43 |
| 35:DN:96:ARG:NH2 | 35:DN:96:ARG:HG2 | 2.33 | 0.43 |
| 38:DQ:94:LEU:C | 38:DQ:96:ASP:N | 2.72 | 0.43 |
| 1:AA:1250:A:H2 | 1:AA:1370:G:H1' | 1.82 | 0.43 |
| 1:AA:1261:A:N7 | 1:AA:1274:A:H2 | 2.17 | 0.43 |
| 1:AA:1337:G:H5'' | 1:AA:1338:G:OP1 | 2.18 | 0.43 |
| 1:AA:1439:G:OP2 | 19:AT:32:LYS:HE2 | 2.18 | 0.43 |
| 1:AA:808:C:O2' | 1:AA:809:G:H5' | 2.18 | 0.43 |
| 20:AB:11:ALA:C | 20:AB:13:VAL:H | 2.22 | 0.43 |
| 20:AB:160:LEU:HG | 20:AB:161:PHE:N | 2.34 | 0.43 |
| 20:AB:184:ALA:HB3 | 20:AB:195:VAL:HG21 | 2.01 | 0.43 |
| 20:AB:96:LEU:HB2 | 20:AB:99:MET:HE2 | 1.98 | 0.43 |
| 2:AC:19:SER:HB2 | 2:AC:39:ARG:NH2 | 2.32 | 0.43 |
| 2:AC:8:GLY:HA3 | 13:AN:88:MET:SD | 2.58 | 0.43 |
| 3:AD:115:GLN:HG3 | 3:AD:119:HIS:CE1 | 2.53 | 0.43 |
| 3:AD:25:ARG:HE | 3:AD:25:ARG:HB2 | 1.57 | 0.43 |
| 9:AJ:12:ALA:CB | 9:AJ:96:VAL:HG12 | 2.43 | 0.43 |
| 10:AK:61:ALA:O | 10:AK:64:VAL:HG13 | 2.19 | 0.43 |
| 10:AK:88:PRO:HD3 | 21:AU:28:LEU:CD1 | 2.34 | 0.43 |
| 11:AL:21:PRO:HG2 | 11:AL:94:TYR:OH | 2.18 | 0.43 |
| 18:AS:40:PHE:HB3 | 18:AS:41:PRO:HD2 | 1.98 | 0.43 |
| 51:B4:9:LYS:N | 51:B4:9:LYS:HD3 | 2.31 | 0.43 |
| 23:BB:1369:G:H2' | 23:BB:1370:C:O4' | 2.19 | 0.43 |
| 23:BB:1525:A:H2' | 23:BB:1526:C:O4' | 2.18 | 0.43 |
| 23:BB:1573:G:H2' | 23:BB:1574:C:H5' | 2.01 | 0.43 |
| 23:BB:1496:A:H1' | 23:BB:1577:C:O2' | 2.17 | 0.43 |
| 23:BB:1704:C:H2' | 23:BB:1705:A:H8 | 1.84 | 0.43 |
| 23:BB:1749:A:H2' | 23:BB:1750:G:H8 | 1.84 | 0.43 |
| 23:BB:1874:C:H2' | 23:BB:1875:G:O4' | 2.17 | 0.43 |
| 23:BB:1933:G:H2' | 23:BB:1934:C:H6 | 1.82 | 0.43 |
| 23:BB:2147:A:H5'' | 23:BB:2148:G:O4' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:2496:C:H2' | 23:BB:2497:A:H5' | 2.01 | 0.43 |
| 23:BB:612:G:H2' | 23:BB:614:A:H5'' | 2.00 | 0.43 |
| 25:BC:149:LYS:HD3 | 25:BC:152:GLN:HE22 | 1.81 | 0.43 |
| 25:BC:259:ASN:OD1 | 25:BC:261:ARG:HB3 | 2.18 | 0.43 |
| 25:BC:71:ASP:O | 25:BC:73:ILE:HG12 | 2.18 | 0.43 |
| 25:BC:77:VAL:O | 25:BC:77:VAL:HG23 | 2.19 | 0.43 |
| 23:BB:2784:U:H4' | 26:BD:42:ASN:O | 2.18 | 0.43 |
| 23:BB:674:G:C4' | 27:BE:69:ARG:HB3 | 2.48 | 0.43 |
| 28:BF:3:LEU:HD13 | 28:BF:3:LEU:O | 2.18 | 0.43 |
| 29:BG:152:ARG:HE | 29:BG:152:ARG:HA | 1.83 | 0.43 |
| 29:BG:152:ARG:HA | 29:BG:152:ARG:NE | 2.33 | 0.43 |
| 30:BH:104:THR:HA | 30:BH:109:GLU:OE2 | 2.18 | 0.43 |
| 32:BK:54:LYS:H | 32:BK:54:LYS:CD | 2.29 | 0.43 |
| 23:BB:1203:U:C4' | 33:BL:3:LEU:HD12 | 2.49 | 0.43 |
| 34:BM:33:LEU:HD22 | 34:BM:128:THR:HB | 2.00 | 0.43 |
| 26:BD:13:ARG:HH12 | 37:BP:74:GLN:HE21 | 1.67 | 0.43 |
| 38:BQ:63:ARG:H | 38:BQ:63:ARG:HG3 | 1.60 | 0.43 |
| 38:BQ:93:ILE:O | 38:BQ:96:ASP:HB3 | 2.18 | 0.43 |
| 41:BT:14:PRO:HA | 41:BT:32:LEU:HB2 | 1.99 | 0.43 |
| 43:BW:54:ARG:HB3 | 43:BW:54:ARG:NH1 | 2.34 | 0.43 |
| 44:BX:51:ALA:O | 44:BX:55:THR:N | 2.46 | 0.43 |
| 1:CA:1026:G:O2' | 1:CA:1027:C:H5' | 2.19 | 0.43 |
| 1:CA:1060:U:H2' | 1:CA:1061:G:C8 | 2.52 | 0.43 |
| 1:CA:1290:G:H2' | 1:CA:1291:U:C6 | 2.54 | 0.43 |
| 1:CA:1393:U:O2' | 1:CA:1394:A:H2' | 2.19 | 0.43 |
| 1:CA:215:C:H2' | 1:CA:216:U:H6 | 1.82 | 0.43 |
| 1:CA:222:C:H2' | 1:CA:223:A:H8 | 1.82 | 0.43 |
| 1:CA:237:G:H2' | 1:CA:238:A:C8 | 2.53 | 0.43 |
| 1:CA:521:G:O2' | 1:CA:522:C:H5' | 2.18 | 0.43 |
| 1:CA:642:A:H2' | 1:CA:643:C:C6 | 2.53 | 0.43 |
| 1:CA:6:G:N3 | 1:CA:6:G:C3' | 2.81 | 0.43 |
| 1:CA:981:U:H2' | 1:CA:982:U:C5 | 2.53 | 0.43 |
| 3:CD:47:LEU:HD22 | 3:CD:51:GLY:O | 2.18 | 0.43 |
| 6:CG:129:ASN:CA | 6:CG:134:VAL:HG21 | 2.47 | 0.43 |
| 7:CH:9:MET:HG3 | 7:CH:26:MET:SD | 2.58 | 0.43 |
| 9:CJ:42:LEU:CD1 | 9:CJ:73:LEU:HB2 | 2.39 | 0.43 |
| 11:CL:31:GLY:HA3 | 11:CL:54:VAL:CG1 | 2.49 | 0.43 |
| 11:CL:33:CYS:N | 11:CL:54:VAL:HG13 | 2.33 | 0.43 |
| 13:CN:30:ILE:O | 13:CN:40:ARG:HA | 2.18 | 0.43 |
| 15:CP:21:VAL:O | 15:CP:33:ILE:HB | 2.18 | 0.43 |
| 16:CQ:28:VAL:O | 16:CQ:36:PHE:HA | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CK:111:ASP:HB3 | 21:CU:3:ILE:N | 2.34 | 0.43 |
| 50:D3:44:ARG:N | 50:D3:45:PRO:CD | 2.82 | 0.43 |
| 22:DA:52:A:H3' | 22:DA:53:A:H8 | 1.82 | 0.43 |
| 23:DB:1708:C:H2' | 23:DB:1709:U:H6 | 1.83 | 0.43 |
| 23:DB:1742:U:H2' | 23:DB:1743:G:H8 | 1.82 | 0.43 |
| 23:DB:1930:G:C2' | 23:DB:1931:U:OP2 | 2.67 | 0.43 |
| 23:DB:2217:G:H2' | 23:DB:2218:G:H8 | 1.82 | 0.43 |
| 23:DB:2320:U:H4' | 23:DB:2321:U:C2 | 2.54 | 0.43 |
| 23:DB:2341:G:H2' | 23:DB:2342:C:H6 | 1.81 | 0.43 |
| 23:DB:2636:C:H2' | 23:DB:2637:U:H6 | 1.83 | 0.43 |
| 23:DB:2676:C:O2' | 23:DB:2677:G:H5' | 2.19 | 0.43 |
| 23:DB:2677:G:H2' | 23:DB:2678:C:C6 | 2.53 | 0.43 |
| 23:DB:277:G:H1' | 23:DB:361:G:O6 | 2.19 | 0.43 |
| 23:DB:2852:G:H2' | 23:DB:2853:C:O4' | 2.18 | 0.43 |
| 23:DB:2835:A:H61 | 23:DB:2878:U:H2' | 1.83 | 0.43 |
| 23:DB:29:U:H2' | 23:DB:30:G:C8 | 2.54 | 0.43 |
| 23:DB:322:A:C2 | 23:DB:340:A:C6 | 3.07 | 0.43 |
| 23:DB:725:G:H2' | 23:DB:726:G:O4' | 2.19 | 0.43 |
| 26:DD:2:ILE:O | 26:DD:2:ILE:HD12 | 2.18 | 0.43 |
| 28:DF:76:PHE:O | 28:DF:77:LYS:HB2 | 2.18 | 0.43 |
| 23:DB:2748:A:H5' | 29:DG:3:VAL:HG21 | 2.00 | 0.43 |
| 52:DI:59:THR:O | 52:DI:59:THR:HG23 | 2.19 | 0.43 |
| 31:DJ:59:ALA:C | 31:DJ:61:LYS:N | 2.72 | 0.43 |
| 32:DK:106:GLU:OE1 | 32:DK:106:GLU:N | 2.49 | 0.43 |
| 34:DM:37:GLY:HA3 | 34:DM:126:ILE:HG23 | 2.00 | 0.43 |
| 34:DM:19:GLY:N | 34:DM:38:ARG:NH2 | 2.64 | 0.43 |
| 36:DO:35:ILE:HG13 | 36:DO:102:ARG:HE | 1.81 | 0.43 |
| 39:DR:2:TYR:N | 39:DR:42:ALA:HB2 | 2.34 | 0.43 |
| 40:DS:20:VAL:HG13 | 40:DS:21:ALA:N | 2.34 | 0.43 |
| 40:DS:25:ARG:HE | 40:DS:74:ILE:HG23 | 1.82 | 0.43 |
| 23:DB:483:A:O2' | 42:DU:56:GLY:N | 2.52 | 0.43 |
| 46:DZ:33:LEU:HD23 | 46:DZ:52:SER:HB3 | 2.01 | 0.43 |
| 46:DZ:7:VAL:HG13 | 46:DZ:8:THR:CG2 | 2.39 | 0.43 |
| 1:AA:1421:G:N2 | 1:AA:1479:C:O2 | 2.51 | 0.43 |
| 1:AA:332:G:O2' | 1:AA:333:U:H5' | 2.19 | 0.43 |
| 1:AA:541:G:H2' | 1:AA:542:G:H8 | 1.84 | 0.43 |
| 1:AA:642:A:H2' | 1:AA:643:C:C6 | 2.52 | 0.43 |
| 1:AA:721:G:H4' | 1:AA:722:G:O4' | 2.18 | 0.43 |
| 1:AA:767:A:H2' | 1:AA:768:A:H8 | 1.84 | 0.43 |
| 20:AB:172:ILE:CG2 | 20:AB:176:ASN:HD21 | 2.31 | 0.43 |
| 20:AB:95:TRP:CH2 | 20:AB:100:LEU:HD13 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:975:A:H61 | 9:AJ:50:THR:HG21 | 1.83 | 0.43 |
| 9:AJ:50:THR:HG22 | 9:AJ:62:ARG:HD2 | 2.00 | 0.43 |
| 11:AL:30:ARG:O | 11:AL:57:THR:HG23 | 2.18 | 0.43 |
| 11:AL:86:VAL:HG12 | 11:AL:89:LEU:H | 1.82 | 0.43 |
| 11:AL:89:LEU:HD22 | 11:AL:89:LEU:N | 2.33 | 0.43 |
| 12:AM:63:VAL:HG13 | 12:AM:67:ASP:CB | 2.48 | 0.43 |
| 23:BB:1270:C:H5'' | 23:BB:1271:G:O5' | 2.17 | 0.43 |
| 23:BB:1467:U:O2' | 23:BB:1468:U:H5' | 2.18 | 0.43 |
| 23:BB:1708:C:H2' | 23:BB:1709:U:C6 | 2.53 | 0.43 |
| 23:BB:1805:A:H5'' | 25:BC:247:TRP:CE2 | 2.54 | 0.43 |
| 23:BB:2026:U:H2' | 23:BB:2027:G:H8 | 1.83 | 0.43 |
| 23:BB:2694:G:H2' | 23:BB:2695:U:C6 | 2.54 | 0.43 |
| 23:BB:2716:C:H2' | 23:BB:2717:C:H6 | 1.82 | 0.43 |
| 23:BB:2742:G:O2' | 23:BB:2743:U:H5' | 2.19 | 0.43 |
| 23:BB:705:A:O2' | 25:BC:6:LYS:HD2 | 2.18 | 0.43 |
| 25:BC:156:SER:HB3 | 25:BC:159:THR:HG21 | 2.00 | 0.43 |
| 25:BC:224:MET:SD | 25:BC:229:HIS:HB2 | 2.58 | 0.43 |
| 27:BE:188:MET:HG2 | 27:BE:193:VAL:CG2 | 2.44 | 0.43 |
| 28:BF:107:VAL:HB | 28:BF:108:PRO:HD3 | 2.01 | 0.43 |
| 30:BH:131:SER:CB | 30:BH:141:LYS:HA | 2.46 | 0.43 |
| 52:BI:56:VAL:HG13 | 52:BI:58:ILE:HD11 | 2.01 | 0.43 |
| 31:BJ:64:VAL:HG22 | 31:BJ:68:LYS:CD | 2.49 | 0.43 |
| 32:BK:2:ILE:HD12 | 32:BK:2:ILE:N | 2.33 | 0.43 |
| 32:BK:7:MET:CE | 32:BK:18:ARG:HB3 | 2.49 | 0.43 |
| 34:BM:49:ALA:HA | 34:BM:123:LYS:HG3 | 2.00 | 0.43 |
| 22:BA:51:G:H5'' | 36:BO:64:TYR:CD2 | 2.53 | 0.43 |
| 37:BP:100:ARG:HB3 | 37:BP:101:GLU:OE2 | 2.19 | 0.43 |
| 37:BP:19:PHE:O | 37:BP:20:ARG:CB | 2.66 | 0.43 |
| 38:BQ:77:LYS:O | 38:BQ:80:ASN:HB3 | 2.19 | 0.43 |
| 39:BR:39:LEU:HD23 | 39:BR:39:LEU:H | 1.82 | 0.43 |
| 41:BT:40:LYS:O | 41:BT:43:ILE:HB | 2.18 | 0.43 |
| 41:BT:58:VAL:O | 41:BT:58:VAL:HG13 | 2.19 | 0.43 |
| 42:BU:73:ASN:ND2 | 42:BU:74:ALA:N | 2.67 | 0.43 |
| 43:BW:28:GLU:H | 43:BW:31:LEU:HG | 1.84 | 0.43 |
| 43:BW:55:ASP:C | 43:BW:57:THR:H | 2.21 | 0.43 |
| 45:BY:6:ILE:HG23 | 45:BY:56:VAL:HG22 | 2.01 | 0.43 |
| 46:BZ:70:GLU:O | 46:BZ:72:ARG:N | 2.42 | 0.43 |
| 46:BZ:77:LYS:HG3 | 46:BZ:78:TYR:H | 1.84 | 0.43 |
| 1:CA:1077:G:N1 | 1:CA:1081:A:C6 | 2.87 | 0.43 |
| 1:CA:1096:C:H2' | 1:CA:1097:C:C6 | 2.52 | 0.43 |
| 1:CA:1222:G:H2' | 1:CA:1223:C:H5' | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:126:G:H2' | 1:CA:127:G:O4' | 2.18 | 0.43 |
| 1:CA:186:C:H2' | 1:CA:187:G:O4' | 2.19 | 0.43 |
| 1:CA:375:U:O2' | 1:CA:376:G:H5' | 2.19 | 0.43 |
| 1:CA:386:C:O2' | 1:CA:387:U:H5' | 2.18 | 0.43 |
| 1:CA:562:U:H5'' | 1:CA:563:A:C4 | 2.54 | 0.43 |
| 1:CA:828:U:H2' | 1:CA:829:G:O5' | 2.19 | 0.43 |
| 1:CA:948:C:H2' | 1:CA:949:A:H8 | 1.83 | 0.43 |
| 20:CB:165:ALA:HB3 | 20:CB:186:VAL:HG11 | 2.01 | 0.43 |
| 20:CB:35:ASN:HD22 | 20:CB:35:ASN:HA | 1.53 | 0.43 |
| 20:CB:8:MET:SD | 20:CB:9:LEU:N | 2.92 | 0.43 |
| 3:CD:2:ARG:HG3 | 3:CD:114:ARG:CZ | 2.49 | 0.43 |
| 6:CG:30:MET:HG3 | 6:CG:35:LYS:HA | 2.00 | 0.43 |
| 7:CH:12:ARG:NH1 | 7:CH:12:ARG:HG3 | 2.34 | 0.43 |
| 10:CK:91:GLY:O | 10:CK:95:THR:HG22 | 2.19 | 0.43 |
| 11:CL:37:TYR:O | 11:CL:38:THR:HG23 | 2.18 | 0.43 |
| 17:CR:57:ALA:O | 17:CR:60:ARG:HG3 | 2.18 | 0.43 |
| 19:CT:4:LYS:HZ1 | 19:CT:6:ALA:CB | 2.30 | 0.43 |
| 48:D1:18:HIS:CG | 48:D1:19:PHE:N | 2.86 | 0.43 |
| 48:D1:46:VAL:HG22 | 48:D1:47:ILE:HD12 | 2.01 | 0.43 |
| 23:DB:1030:C:O2' | 23:DB:1031:G:H5' | 2.18 | 0.43 |
| 23:DB:1438:U:O2' | 23:DB:1439:A:H5' | 2.18 | 0.43 |
| 23:DB:1704:C:H2' | 23:DB:1705:A:H8 | 1.83 | 0.43 |
| 23:DB:1795:C:H2' | 23:DB:1796:U:C6 | 2.53 | 0.43 |
| 23:DB:1797:G:O3' | 25:DC:255:LYS:O | 2.37 | 0.43 |
| 23:DB:1831:G:H2' | 23:DB:1832:C:H6 | 1.82 | 0.43 |
| 23:DB:2485:G:O2' | 23:DB:2486:C:H5' | 2.19 | 0.43 |
| 23:DB:2655:G:H1' | 23:DB:2656:U:H5 | 1.84 | 0.43 |
| 23:DB:2722:G:O2' | 23:DB:2723:C:H5' | 2.19 | 0.43 |
| 23:DB:2743:U:C2' | 23:DB:2744:G:H5'' | 2.37 | 0.43 |
| 23:DB:39:G:H2' | 23:DB:40:U:H6 | 1.82 | 0.43 |
| 23:DB:463:G:N1 | 23:DB:467:G:C6 | 2.87 | 0.43 |
| 23:DB:672:C:H2' | 23:DB:673:C:C6 | 2.54 | 0.43 |
| 23:DB:811:U:OP2 | 33:DL:20:GLY:HA2 | 2.19 | 0.43 |
| 23:DB:989:G:H5'' | 45:DY:13:ILE:HD11 | 2.00 | 0.43 |
| 26:DD:161:MET:O | 26:DD:162:ALA:C | 2.57 | 0.43 |
| 26:DD:34:VAL:CG2 | 26:DD:48:ILE:HG13 | 2.49 | 0.43 |
| 26:DD:33:ARG:HE | 26:DD:74:GLU:HB3 | 1.83 | 0.43 |
| 26:DD:8:LYS:HA | 26:DD:201:LEU:HD11 | 2.01 | 0.43 |
| 30:DH:87:GLU:CD | 30:DH:87:GLU:H | 2.22 | 0.43 |
| 33:DL:54:GLN:O | 33:DL:56:PRO:HD3 | 2.18 | 0.43 |
| 34:DM:32:GLY:HA2 | 34:DM:117:PHE:CZ | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DN:116:VAL:HG13 | 35:DN:116:VAL:O | 2.19 | 0.43 |
| 36:DO:35:ILE:HG21 | 36:DO:71:ALA:HB1 | 2.00 | 0.43 |
| 36:DO:51:ALA:HB2 | 36:DO:81:ARG:HH11 | 1.84 | 0.43 |
| 38:DQ:9:ALA:O | 38:DQ:12:ARG:N | 2.51 | 0.43 |
| 38:DQ:30:VAL:HG12 | 38:DQ:33:VAL:HG22 | 1.99 | 0.43 |
| 38:DQ:65:ASN:CG | 38:DQ:75:TYR:HB2 | 2.39 | 0.43 |
| 40:DS:6:LYS:HB3 | 40:DS:104:THR:HA | 2.01 | 0.43 |
| 41:DT:12:ARG:HA | 44:DX:29:ARG:NH2 | 2.30 | 0.43 |
| 41:DT:58:VAL:O | 41:DT:58:VAL:HG13 | 2.18 | 0.43 |
| 24:DV:49:ASN:O | 24:DV:52:ALA:HB3 | 2.17 | 0.43 |
| 43:DW:70:VAL:O | 43:DW:70:VAL:HG13 | 2.19 | 0.43 |
| 1:AA:1140:C:O2' | 1:AA:1141:C:H5' | 2.18 | 0.43 |
| 1:AA:1329:A:O2' | 1:AA:1330:U:H5' | 2.18 | 0.43 |
| 1:AA:1409:C:H4' | 23:BB:1915:U:O4 | 2.19 | 0.43 |
| 1:AA:187:G:N2 | 1:AA:189:A:H3' | 2.34 | 0.43 |
| 1:AA:191:G:H2' | 1:AA:192:A:H8 | 1.84 | 0.43 |
| 1:AA:263:A:H2' | 1:AA:264:C:C6 | 2.53 | 0.43 |
| 1:AA:386:C:O2' | 1:AA:387:U:H5' | 2.18 | 0.43 |
| 1:AA:594:U:O2' | 1:AA:595:A:H5' | 2.17 | 0.43 |
| 1:AA:716:A:H1' | 10:AK:119:GLY:HA2 | 2.01 | 0.43 |
| 1:AA:71:A:O2' | 1:AA:72:A:H5'' | 2.18 | 0.43 |
| 1:AA:82:G:H1' | 1:AA:89:U:C2 | 2.54 | 0.43 |
| 2:AC:2:GLN:O | 2:AC:3:LYS:HB2 | 2.19 | 0.43 |
| 2:AC:50:SER:CB | 2:AC:70:ALA:HB3 | 2.48 | 0.43 |
| 3:AD:106:PHE:CD1 | 3:AD:158:LEU:HD21 | 2.54 | 0.43 |
| 5:AF:6:ILE:HG23 | 5:AF:62:MET:CB | 2.48 | 0.43 |
| 5:AF:81:ASN:O | 5:AF:84:VAL:HG12 | 2.18 | 0.43 |
| 8:AI:66:VAL:HG11 | 8:AI:78:ILE:HD11 | 2.01 | 0.43 |
| 8:AI:54:VAL:HG21 | 8:AI:86:LEU:HD21 | 2.00 | 0.43 |
| 8:AI:9:GLY:HA3 | 8:AI:81:GLY:N | 2.32 | 0.43 |
| 9:AJ:8:ILE:HB | 9:AJ:74:VAL:HB | 2.01 | 0.43 |
| 12:AM:72:ILE:O | 12:AM:76:ILE:HG13 | 2.18 | 0.43 |
| 48:B1:7:LYS:HD3 | 50:B3:33:THR:HG21 | 2.00 | 0.43 |
| 51:B4:2:LYS:HD3 | 51:B4:4:ARG:HG3 | 2.01 | 0.43 |
| 23:BB:1233:C:O2' | 23:BB:1234:U:H5' | 2.18 | 0.43 |
| 23:BB:1405:U:H2' | 23:BB:1406:U:H6 | 1.83 | 0.43 |
| 23:BB:1459:G:N3 | 23:BB:1459:G:O5' | 2.52 | 0.43 |
| 23:BB:1490:A:H2' | 25:BC:97:ASP:CG | 2.39 | 0.43 |
| 23:BB:1528:A:H2' | 23:BB:1529:G:H5' | 2.00 | 0.43 |
| 23:BB:1563:U:H2' | 23:BB:1564:C:C6 | 2.53 | 0.43 |
| 23:BB:1742:U:H2' | 23:BB:1743:G:H8 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1939:U:C6 | 23:BB:1939:U:H5' | 2.47 | 0.43 |
| 23:BB:1973:G:H2' | 23:BB:1974:C:H6 | 1.84 | 0.43 |
| 23:BB:2526:G:H2' | 23:BB:2527:C:H6 | 1.83 | 0.43 |
| 23:BB:2869:G:H2' | 23:BB:2870:C:C6 | 2.53 | 0.43 |
| 23:BB:504:A:HO2' | 23:BB:505:A:P | 2.41 | 0.43 |
| 23:BB:510:C:H2' | 23:BB:511:U:O4' | 2.19 | 0.43 |
| 23:BB:5:A:H2' | 23:BB:6:A:H8 | 1.82 | 0.43 |
| 23:BB:697:G:O2' | 23:BB:698:C:H5' | 2.18 | 0.43 |
| 23:BB:741:U:H2' | 23:BB:742:A:H8 | 1.84 | 0.43 |
| 23:BB:771:G:O2' | 23:BB:772:C:H5' | 2.19 | 0.43 |
| 23:BB:852:U:H2' | 23:BB:853:C:C6 | 2.53 | 0.43 |
| 23:BB:950:G:H2' | 23:BB:951:C:H6 | 1.84 | 0.43 |
| 25:BC:226:PRO:HG3 | 25:BC:233:GLY:N | 2.26 | 0.43 |
| 23:BB:1797:G:O3' | 25:BC:255:LYS:O | 2.37 | 0.43 |
| 23:BB:1798:U:H5'' | 25:BC:257:ARG:HB2 | 2.01 | 0.43 |
| 25:BC:36:ASN:ND2 | 25:BC:85:ASN:HD21 | 2.15 | 0.43 |
| 26:BD:187:LEU:O | 26:BD:188:LEU:HD23 | 2.19 | 0.43 |
| 23:BB:2786:U:H5' | 26:BD:70:LYS:HG3 | 2.00 | 0.43 |
| 28:BF:121:PHE:HE1 | 28:BF:162:ASP:CB | 2.32 | 0.43 |
| 29:BG:9:VAL:HA | 29:BG:48:THR:CG2 | 2.47 | 0.43 |
| 30:BH:78:VAL:HG11 | 30:BH:142:VAL:CG1 | 2.49 | 0.43 |
| 52:BI:49:GLU:HG3 | 52:BI:54:ILE:HD11 | 2.00 | 0.43 |
| 31:BJ:88:THR:HG22 | 31:BJ:91:GLU:OE1 | 2.19 | 0.43 |
| 33:BL:109:LYS:HE3 | 33:BL:111:ILE:HD11 | 2.01 | 0.43 |
| 33:BL:29:LYS:C | 33:BL:31:GLY:H | 2.22 | 0.43 |
| 35:BN:19:ALA:HA | 35:BN:22:ARG:CB | 2.47 | 0.43 |
| 38:BQ:96:ASP:C | 38:BQ:98:ALA:N | 2.71 | 0.43 |
| 1:CA:1111:A:O2' | 1:CA:1112:C:H5' | 2.19 | 0.43 |
| 1:CA:113:G:O2' | 1:CA:354:G:H5' | 2.19 | 0.43 |
| 1:CA:1366:C:H2' | 1:CA:1367:C:H6 | 1.83 | 0.43 |
| 1:CA:1390:U:H2' | 1:CA:1391:U:C6 | 2.53 | 0.43 |
| 1:CA:1469:C:H2' | 1:CA:1470:U:O4' | 2.18 | 0.43 |
| 1:CA:251:G:N3 | 1:CA:266:G:O6 | 2.51 | 0.43 |
| 1:CA:59:A:H3' | 1:CA:331:G:H22 | 1.83 | 0.43 |
| 1:CA:389:A:C6 | 1:CA:390:U:H1' | 2.53 | 0.43 |
| 1:CA:488:C:O2' | 1:CA:489:C:H5' | 2.19 | 0.43 |
| 1:CA:25:C:H5' | 1:CA:524:G:H1' | 2.00 | 0.43 |
| 1:CA:957:U:H2' | 1:CA:959:A:OP2 | 2.19 | 0.43 |
| 20:CB:44:LYS:O | 20:CB:47:PRO:HD2 | 2.18 | 0.43 |
| 2:CC:154:GLY:HA2 | 2:CC:163:ARG:N | 2.34 | 0.43 |
| 3:CD:31:CYS:O | 3:CD:32:LYS:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:CH:40:LYS:HD3 | 7:CH:48:PHE:CE1 | 2.53 | 0.43 |
| 7:CH:54:THR:HG23 | 7:CH:55:LYS:HG2 | 2.00 | 0.43 |
| 9:CJ:37:ARG:NH1 | 9:CJ:77:VAL:HG11 | 2.34 | 0.43 |
| 10:CK:106:ILE:O | 10:CK:107:THR:HG23 | 2.18 | 0.43 |
| 10:CK:36:ARG:HG3 | 10:CK:36:ARG:HH11 | 1.83 | 0.43 |
| 10:CK:59:PRO:HA | 10:CK:90:PRO:HB2 | 2.00 | 0.43 |
| 16:CQ:30:HIS:CB | 16:CQ:33:TYR:HB2 | 2.49 | 0.43 |
| 18:CS:41:PRO:C | 18:CS:43:MET:H | 2.22 | 0.43 |
| 19:CT:64:GLY:H | 19:CT:67:HIS:CD2 | 2.37 | 0.43 |
| 21:CU:20:ARG:C | 21:CU:22:CYS:H | 2.22 | 0.43 |
| 48:D1:3:GLY:O | 48:D1:5:ARG:N | 2.51 | 0.43 |
| 22:DA:91:C:H2' | 22:DA:92:C:C6 | 2.52 | 0.43 |
| 23:DB:1025:G:OP1 | 23:DB:1025:G:H8 | 2.01 | 0.43 |
| 23:DB:1027:A:N6 | 23:DB:1126:A:H1' | 2.33 | 0.43 |
| 23:DB:1059:G:H2' | 23:DB:1060:U:C5 | 2.53 | 0.43 |
| 23:DB:1708:C:H2' | 23:DB:1709:U:C6 | 2.54 | 0.43 |
| 23:DB:1930:G:H2' | 23:DB:1968:G:C6 | 2.54 | 0.43 |
| 23:DB:2052:A:N7 | 26:DD:146:ILE:HD11 | 2.34 | 0.43 |
| 23:DB:2391:G:HO2' | 23:DB:2392:A:P | 2.41 | 0.43 |
| 23:DB:2800:A:C2 | 23:DB:2801:G:H1' | 2.53 | 0.43 |
| 23:DB:2882:A:OP1 | 35:DN:96:ARG:HD2 | 2.18 | 0.43 |
| 23:DB:43:G:H2' | 23:DB:44:A:O4' | 2.19 | 0.43 |
| 23:DB:533:G:H2' | 23:DB:534:U:C6 | 2.53 | 0.43 |
| 23:DB:1803:A:H4' | 25:DC:256:THR:OG1 | 2.18 | 0.43 |
| 25:DC:36:ASN:ND2 | 25:DC:61:TYR:HB2 | 2.34 | 0.43 |
| 27:DE:134:LEU:CD2 | 27:DE:161:ALA:HB2 | 2.49 | 0.43 |
| 31:DJ:103:ILE:HG13 | 31:DJ:104:ALA:N | 2.33 | 0.43 |
| 32:DK:54:LYS:H | 32:DK:54:LYS:CD | 2.28 | 0.43 |
| 32:DK:88:ASN:ND2 | 32:DK:89:ASN:N | 2.66 | 0.43 |
| 35:DN:79:LEU:HA | 35:DN:83:LEU:HD12 | 2.00 | 0.43 |
| 38:DQ:63:ARG:HH12 | 38:DQ:96:ASP:HB2 | 1.84 | 0.43 |
| 39:DR:39:LEU:HD23 | 39:DR:39:LEU:H | 1.82 | 0.43 |
| 41:DT:39:THR:O | 41:DT:40:LYS:HB3 | 2.18 | 0.43 |
| 41:DT:69:ARG:HA | 41:DT:69:ARG:NH1 | 2.33 | 0.43 |
| 42:DU:73:ASN:ND2 | 42:DU:74:ALA:N | 2.67 | 0.43 |
| 43:DW:70:VAL:CG2 | 43:DW:75:ASN:HD21 | 2.32 | 0.43 |
| 45:DY:23:LEU:HD23 | 45:DY:50:VAL:HG11 | 2.00 | 0.43 |
| 46:DZ:64:ILE:HG22 | 46:DZ:68:LEU:CD1 | 2.48 | 0.43 |
| 1:AA:1120:C:H2' | 1:AA:1121:U:H6 | 1.82 | 0.43 |
| 1:AA:1305:G:H22 | 1:AA:1331:G:H2' | 1.83 | 0.43 |
| 1:AA:1527:U:H2' | 1:AA:1528:U:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:704:A:C2 | 1:AA:705:G:H1' | 2.54 | 0.43 |
| 5:AF:3:HIS:CD2 | 5:AF:65:GLU:HG3 | 2.53 | 0.43 |
| 6:AG:100:MET:O | 6:AG:104:VAL:HG23 | 2.18 | 0.43 |
| 8:AI:118:ARG:NH1 | 8:AI:122:ARG:HE | 2.17 | 0.43 |
| 12:AM:18:LEU:HD13 | 12:AM:33:LEU:HD21 | 2.01 | 0.43 |
| 15:AP:43:ALA:HB1 | 15:AP:46:LYS:HE3 | 2.01 | 0.43 |
| 16:AQ:34:GLY:O | 16:AQ:35:LYS:C | 2.57 | 0.43 |
| 19:AT:32:LYS:O | 19:AT:35:TYR:N | 2.51 | 0.43 |
| 47:B0:27:LEU:HD12 | 47:B0:27:LEU:H | 1.83 | 0.43 |
| 23:BB:1153:C:H2' | 23:BB:1154:G:O4' | 2.19 | 0.43 |
| 23:BB:1332:G:HO2' | 23:BB:1609:A:H2 | 1.65 | 0.43 |
| 23:BB:1454:C:C5 | 35:BN:64:ARG:HG2 | 2.54 | 0.43 |
| 23:BB:1636:U:O2' | 23:BB:1637:A:H5' | 2.18 | 0.43 |
| 23:BB:19:A:O2' | 23:BB:20:C:H5' | 2.19 | 0.43 |
| 23:BB:2219:U:O2' | 23:BB:2220:U:H5' | 2.17 | 0.43 |
| 23:BB:582:A:H2' | 23:BB:583:G:C8 | 2.54 | 0.43 |
| 23:BB:63:A:C8 | 23:BB:63:A:OP2 | 2.69 | 0.43 |
| 23:BB:754:U:H2' | 23:BB:755:U:H6 | 1.84 | 0.43 |
| 26:BD:117:GLY:HA2 | 26:BD:164:GLN:NE2 | 2.34 | 0.43 |
| 28:BF:111:ARG:O | 28:BF:112:ASP:HB2 | 2.18 | 0.43 |
| 28:BF:36:ASN:ND2 | 28:BF:152:ASP:HB2 | 2.10 | 0.43 |
| 29:BG:107:GLY:HA3 | 29:BG:151:ARG:NH2 | 2.34 | 0.43 |
| 29:BG:148:ARG:HD3 | 29:BG:152:ARG:NH1 | 2.33 | 0.43 |
| 30:BH:68:ARG:HB3 | 30:BH:132:PHE:HE2 | 1.84 | 0.43 |
| 30:BH:82:SER:HB2 | 30:BH:94:ILE:HG12 | 2.01 | 0.43 |
| 31:BJ:24:THR:O | 31:BJ:25:LEU:HB3 | 2.19 | 0.43 |
| 33:BL:50:PHE:CE2 | 33:BL:53:GLY:HA2 | 2.54 | 0.43 |
| 36:BO:34:HIS:HB3 | 36:BO:36:TYR:CE2 | 2.54 | 0.43 |
| 36:BO:78:VAL:HA | 36:BO:81:ARG:HB3 | 2.00 | 0.43 |
| 38:BQ:16:ILE:C | 38:BQ:18:LYS:H | 2.20 | 0.43 |
| 38:BQ:24:TYR:CD1 | 38:BQ:25:GLY:N | 2.86 | 0.43 |
| 24:BV:40:ILE:CD1 | 24:BV:40:ILE:H | 2.30 | 0.43 |
| 24:BV:71:LYS:HB2 | 24:BV:94:ALA:OXT | 2.19 | 0.43 |
| 24:BV:80:HIS:CD2 | 24:BV:81:PRO:HD2 | 2.54 | 0.43 |
| 44:BX:1:MET:CG | 44:BX:4:LYS:HD3 | 2.49 | 0.43 |
| 46:BZ:65:ASP:N | 46:BZ:65:ASP:OD2 | 2.52 | 0.43 |
| 1:CA:106:C:HO2' | 1:CA:107:G:H5' | 1.83 | 0.43 |
| 1:CA:116:A:O5' | 1:CA:116:A:H8 | 2.02 | 0.43 |
| 1:CA:1186:G:H4' | 8:CI:111:GLU:OE1 | 2.19 | 0.43 |
| 1:CA:1313:U:O2' | 1:CA:1314:C:H5' | 2.18 | 0.43 |
| 1:CA:1368:A:O2' | 1:CA:1369:C:H5' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1484:C:O2' | 1:CA:1485:U:H5' | 2.19 | 0.43 |
| 1:CA:138:G:C6 | 1:CA:226:G:C6 | 3.07 | 0.43 |
| 1:CA:282:A:H2' | 1:CA:282:A:N3 | 2.33 | 0.43 |
| 1:CA:300:A:H2' | 1:CA:301:G:O4' | 2.19 | 0.43 |
| 1:CA:38:G:O2' | 1:CA:39:G:H5' | 2.19 | 0.43 |
| 1:CA:542:G:O2' | 1:CA:543:U:H5' | 2.19 | 0.43 |
| 1:CA:967:C:H5' | 8:CI:129:ARG:HA | 2.01 | 0.43 |
| 1:CA:993:G:H21 | 1:CA:996:A:N6 | 2.17 | 0.43 |
| 20:CB:17:HIS:CG | 20:CB:18:GLN:H | 2.37 | 0.43 |
| 20:CB:46:VAL:CG1 | 20:CB:47:PRO:HD3 | 2.33 | 0.43 |
| 20:CB:48:MET:O | 20:CB:52:ALA:HB3 | 2.19 | 0.43 |
| 20:CB:95:TRP:HZ3 | 20:CB:174:GLU:CD | 2.22 | 0.43 |
| 2:CC:18:ASN:HB2 | 13:CN:90:GLY:HA3 | 1.99 | 0.43 |
| 3:CD:197:HIS:O | 3:CD:201:GLU:HG3 | 2.18 | 0.43 |
| 5:CF:54:LEU:C | 5:CF:56:LYS:H | 2.22 | 0.43 |
| 5:CF:97:THR:O | 5:CF:98:GLU:CD | 2.57 | 0.43 |
| 6:CG:46:LEU:HG | 6:CG:57:GLU:CB | 2.38 | 0.43 |
| 7:CH:106:SER:C | 7:CH:107:LYS:HE2 | 2.38 | 0.43 |
| 9:CJ:57:VAL:HG13 | 9:CJ:58:ASN:N | 2.33 | 0.43 |
| 10:CK:19:VAL:HG22 | 10:CK:34:THR:O | 2.18 | 0.43 |
| 10:CK:33:ILE:CG1 | 10:CK:73:VAL:HG21 | 2.46 | 0.43 |
| 11:CL:79:ILE:C | 11:CL:101:LEU:HD12 | 2.39 | 0.43 |
| 11:CL:86:VAL:HG12 | 11:CL:89:LEU:H | 1.83 | 0.43 |
| 14:CO:54:GLY:O | 14:CO:58:MET:HG2 | 2.19 | 0.43 |
| 49:D2:9:VAL:HG13 | 49:D2:10:LEU:N | 2.34 | 0.43 |
| 23:DB:1060:U:O4 | 52:DI:131:THR:HG22 | 2.18 | 0.43 |
| 23:DB:118:A:OP2 | 23:DB:119:A:H5'' | 2.18 | 0.43 |
| 23:DB:1897:G:O2' | 23:DB:1898:U:H5' | 2.19 | 0.43 |
| 23:DB:1994:C:O2' | 23:DB:1995:U:H5' | 2.19 | 0.43 |
| 23:DB:2571:U:O3' | 26:DD:151:THR:HB | 2.18 | 0.43 |
| 23:DB:2618:G:H2' | 23:DB:2619:C:H6 | 1.84 | 0.43 |
| 23:DB:2658:C:H2' | 23:DB:2659:G:H5' | 2.00 | 0.43 |
| 23:DB:2893:A:C5' | 23:DB:2894:G:H5' | 2.47 | 0.43 |
| 23:DB:426:C:O2' | 23:DB:427:U:H5' | 2.17 | 0.43 |
| 23:DB:523:C:O2' | 23:DB:524:G:H5' | 2.18 | 0.43 |
| 23:DB:560:C:H3' | 23:DB:561:G:C8 | 2.54 | 0.43 |
| 23:DB:876:C:H2' | 23:DB:877:A:C1' | 2.49 | 0.43 |
| 23:DB:866:A:H61 | 23:DB:913:U:C1' | 2.32 | 0.43 |
| 25:DC:45:ASN:H | 25:DC:45:ASN:ND2 | 2.15 | 0.43 |
| 25:DC:70:LYS:HB2 | 25:DC:101:ARG:NH2 | 2.33 | 0.43 |
| 26:DD:59:ARG:O | 26:DD:59:ARG:HD3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DF:107:VAL:HB | 28:DF:108:PRO:HD3 | 2.01 | 0.43 |
| 30:DH:110:VAL:O | 30:DH:110:VAL:HG22 | 2.17 | 0.43 |
| 30:DH:56:ALA:O | 30:DH:60:GLU:HB3 | 2.18 | 0.43 |
| 52:DI:90:GLY:C | 52:DI:91:LYS:HD2 | 2.38 | 0.43 |
| 33:DL:47:ARG:CB | 33:DL:47:ARG:HH21 | 2.31 | 0.43 |
| 33:DL:57:LEU:HD22 | 50:D3:53:ASP:HB3 | 2.01 | 0.43 |
| 32:DK:64:ARG:NH2 | 37:DP:67:GLU:HG3 | 2.34 | 0.43 |
| 38:DQ:68:ALA:HB1 | 38:DQ:73:ILE:CG2 | 2.46 | 0.43 |
| 38:DQ:81:GLY:HA3 | 38:DQ:116:LEU:HD11 | 2.00 | 0.43 |
| 41:DT:83:ALA:O | 41:DT:84:TYR:HB2 | 2.19 | 0.43 |
| 42:DU:86:PHE:HB3 | 42:DU:90:LYS:O | 2.19 | 0.43 |
| 1:AA:1065:U:H1' | 1:AA:1066:C:OP2 | 2.19 | 0.43 |
| 1:AA:1488:G:H2' | 1:AA:1489:G:O4' | 2.19 | 0.43 |
| 1:AA:1495:U:O2' | 1:AA:1496:C:H5' | 2.19 | 0.43 |
| 1:AA:152:A:H3' | 1:AA:153:C:H6 | 1.84 | 0.43 |
| 1:AA:307:C:H2' | 1:AA:308:C:H6 | 1.84 | 0.43 |
| 1:AA:425:G:H2' | 1:AA:426:U:C6 | 2.54 | 0.43 |
| 1:AA:523:A:H61 | 11:AL:88:ASP:HB2 | 1.83 | 0.43 |
| 1:AA:574:A:H1' | 1:AA:883:C:O4' | 2.18 | 0.43 |
| 1:AA:904:U:H2' | 1:AA:905:U:C6 | 2.53 | 0.43 |
| 1:AA:956:U:O2' | 1:AA:957:U:H5' | 2.19 | 0.43 |
| 20:AB:128:LEU:CD1 | 20:AB:132:GLU:HB3 | 2.48 | 0.43 |
| 20:AB:82:ALA:HB3 | 20:AB:213:LEU:HD22 | 2.00 | 0.43 |
| 6:AG:149:ALA:HB2 | 10:AK:55:ARG:CZ | 2.48 | 0.43 |
| 1:AA:779:C:H5'' | 10:AK:123:PRO:HB3 | 2.00 | 0.43 |
| 16:AQ:45:VAL:HG11 | 16:AQ:60:ILE:HG21 | 2.00 | 0.43 |
| 1:AA:1313:U:OP1 | 18:AS:6:LYS:HD3 | 2.19 | 0.43 |
| 49:B2:3:ARG:HA | 49:B2:3:ARG:CZ | 2.48 | 0.43 |
| 23:BB:1474:U:H2' | 23:BB:1475:G:H5'' | 2.00 | 0.43 |
| 23:BB:2219:U:H2' | 23:BB:2220:U:C6 | 2.54 | 0.43 |
| 23:BB:2231:U:O2' | 23:BB:2232:C:H5' | 2.19 | 0.43 |
| 23:BB:2258:C:O2' | 23:BB:2427:C:OP2 | 2.35 | 0.43 |
| 23:BB:2456:C:H2' | 23:BB:2457:U:O4' | 2.19 | 0.43 |
| 23:BB:2515:C:O2' | 23:BB:2516:A:H5' | 2.19 | 0.43 |
| 23:BB:2840:C:O2' | 23:BB:2841:C:H5' | 2.18 | 0.43 |
| 23:BB:2891:U:O2' | 23:BB:2892:G:H5' | 2.19 | 0.43 |
| 23:BB:2902:C:O2' | 23:BB:2903:U:H5' | 2.19 | 0.43 |
| 23:BB:91:A:H1' | 23:BB:92:U:C6 | 2.54 | 0.43 |
| 26:BD:202:ILE:HD12 | 26:BD:202:ILE:N | 2.34 | 0.43 |
| 26:BD:35:THR:N | 26:BD:49:GLN:O | 2.50 | 0.43 |
| 29:BG:166:GLU:CG | 29:BG:168:VAL:HG23 | 2.43 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:BG:4:ALA:HA | 29:BG:65:GLY:HA2 | 1.99 | 0.43 |
| 30:BH:65:ALA:O | 30:BH:67:ALA:N | 2.49 | 0.43 |
| 30:BH:94:ILE:HG23 | 30:BH:98:ASP:OD2 | 2.19 | 0.43 |
| 52:BI:19:PRO:HG2 | 52:BI:22:PRO:HB2 | 2.01 | 0.43 |
| 52:BI:63:ASP:O | 52:BI:65:SER:N | 2.52 | 0.43 |
| 23:BB:2548:U:H1' | 32:BK:23:LYS:NZ | 2.34 | 0.43 |
| 38:BQ:47:ARG:O | 38:BQ:51:GLN:HG3 | 2.18 | 0.43 |
| 44:BX:1:MET:HG2 | 44:BX:4:LYS:HD3 | 2.00 | 0.43 |
| 1:CA:373:A:O2' | 1:CA:374:A:H5' | 2.19 | 0.43 |
| 1:CA:402:G:O2' | 1:CA:403:C:H5' | 2.19 | 0.43 |
| 1:CA:537:G:H2' | 1:CA:538:G:H8 | 1.84 | 0.43 |
| 1:CA:591:U:OP2 | 7:CH:30:LYS:HE2 | 2.18 | 0.43 |
| 1:CA:618:C:H3' | 1:CA:620:C:OP2 | 2.19 | 0.43 |
| 1:CA:647:C:H2' | 1:CA:648:A:H8 | 1.84 | 0.43 |
| 1:CA:715:A:H2' | 1:CA:716:A:H8 | 1.80 | 0.43 |
| 20:CB:119:GLN:O | 20:CB:121:GLN:N | 2.41 | 0.43 |
| 20:CB:128:LEU:HB3 | 20:CB:132:GLU:HB2 | 2.01 | 0.43 |
| 21:AU:9:GLU:CG | 2:CC:108:PRO:HG3 | 2.47 | 0.43 |
| 3:CD:71:PHE:CE1 | 3:CD:89:LEU:HD11 | 2.54 | 0.43 |
| 1:CA:8:A:H1' | 4:CE:106:ALA:O | 2.18 | 0.43 |
| 5:CF:53:LYS:N | 5:CF:53:LYS:NZ | 2.66 | 0.43 |
| 1:CA:875:U:O2' | 7:CH:14:ARG:HD2 | 2.17 | 0.43 |
| 8:CI:11:ARG:NH2 | 8:CI:12:LYS:HD2 | 2.34 | 0.43 |
| 10:CK:80:ASN:HB3 | 10:CK:105:ARG:HB3 | 2.00 | 0.43 |
| 11:CL:21:PRO:HG2 | 11:CL:94:TYR:OH | 2.19 | 0.43 |
| 12:CM:100:ARG:HD3 | 12:CM:103:THR:OG1 | 2.19 | 0.43 |
| 14:CO:49:HIS:O | 14:CO:52:ARG:HB3 | 2.19 | 0.43 |
| 23:DB:1195:G:O2' | 23:DB:1196:C:H5' | 2.19 | 0.43 |
| 23:DB:443:A:H1' | 23:DB:1201:U:O4' | 2.19 | 0.43 |
| 23:DB:1229:C:H2' | 23:DB:1230:A:H8 | 1.81 | 0.43 |
| 23:DB:123:G:O3' | 23:DB:1376:C:H4' | 2.19 | 0.43 |
| 23:DB:164:C:H2' | 23:DB:165:A:H5' | 2.00 | 0.43 |
| 23:DB:2685:G:O2' | 23:DB:2686:G:H5' | 2.19 | 0.43 |
| 23:DB:277:G:O5' | 23:DB:278:A:N7 | 2.51 | 0.43 |
| 23:DB:2885:G:H2' | 23:DB:2886:A:H4' | 2.01 | 0.43 |
| 23:DB:31:C:C4 | 23:DB:32:C:C5 | 3.07 | 0.43 |
| 23:DB:495:G:H4' | 40:DS:4:ILE:O | 2.19 | 0.43 |
| 23:DB:876:C:H2' | 23:DB:877:A:H1' | 2.00 | 0.43 |
| 25:DC:34:GLU:HG3 | 25:DC:34:GLU:O | 2.19 | 0.43 |
| 27:DE:116:ASP:O | 27:DE:119:ILE:HD11 | 2.18 | 0.43 |
| 27:DE:4:VAL:HA | 27:DE:11:ALA:HA | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DE:4:VAL:HG12 | 27:DE:5:LEU:H | 1.84 | 0.43 |
| 28:DF:33:ILE:HG23 | 28:DF:155:ILE:HD12 | 2.00 | 0.43 |
| 29:DG:95:ALA:HB3 | 29:DG:124:CYS:SG | 2.59 | 0.43 |
| 31:DJ:12:LYS:O | 31:DJ:13:ARG:HB2 | 2.19 | 0.43 |
| 32:DK:64:ARG:HD2 | 32:DK:102:PRO:O | 2.19 | 0.43 |
| 33:DL:6:LEU:CD2 | 33:DL:6:LEU:H | 2.20 | 0.43 |
| 34:DM:38:ARG:HG3 | 34:DM:98:PRO:HD3 | 2.00 | 0.43 |
| 38:DQ:26:ALA:C | 38:DQ:28:SER:N | 2.72 | 0.43 |
| 38:DQ:94:LEU:O | 38:DQ:97:ILE:HG23 | 2.19 | 0.43 |
| 43:DW:16:GLU:H | 43:DW:16:GLU:CD | 2.20 | 0.43 |
| 1:AA:1113:C:O2' | 1:AA:1114:C:H5' | 2.19 | 0.43 |
| 1:AA:1296:C:H4' | 1:AA:1302:C:H42 | 1.83 | 0.43 |
| 1:AA:1464:U:OP2 | 37:BP:108:ARG:NH2 | 2.52 | 0.43 |
| 1:AA:250:A:H1' | 1:AA:252:U:C5 | 2.54 | 0.43 |
| 1:AA:256:U:H3' | 1:AA:257:G:H8 | 1.84 | 0.43 |
| 1:AA:59:A:H3' | 1:AA:331:G:H22 | 1.84 | 0.43 |
| 1:AA:994:A:C5 | 1:AA:1216:A:H4' | 2.54 | 0.43 |
| 2:AC:130:ARG:HA | 2:AC:130:ARG:HD2 | 1.90 | 0.43 |
| 3:AD:78:ALA:HA | 3:AD:81:LEU:HD12 | 2.01 | 0.43 |
| 3:AD:94:GLU:HG3 | 3:AD:99:ASN:ND2 | 2.33 | 0.43 |
| 3:AD:97:LEU:HA | 3:AD:100:VAL:CG2 | 2.49 | 0.43 |
| 4:AE:143:LEU:C | 4:AE:145:ASN:H | 2.22 | 0.43 |
| 6:AG:14:ASP:HB2 | 6:AG:19:SER:O | 2.19 | 0.43 |
| 1:AA:970:C:H42 | 8:AI:128:LYS:HG2 | 1.84 | 0.43 |
| 9:AJ:32:THR:HG23 | 9:AJ:32:THR:O | 2.18 | 0.43 |
| 9:AJ:57:VAL:HG13 | 9:AJ:58:ASN:N | 2.34 | 0.43 |
| 9:AJ:80:THR:O | 9:AJ:84:VAL:HG23 | 2.18 | 0.43 |
| 11:AL:28:GLN:HB3 | 11:AL:28:GLN:HE21 | 1.50 | 0.43 |
| 11:AL:43:LYS:CD | 11:AL:44:PRO:HD3 | 2.49 | 0.43 |
| 13:AN:30:ILE:O | 13:AN:40:ARG:HA | 2.18 | 0.43 |
| 14:AO:10:ILE:O | 14:AO:14:PHE:HD1 | 2.02 | 0.43 |
| 14:AO:42:PHE:CD1 | 14:AO:55:LEU:HD22 | 2.53 | 0.43 |
| 16:AQ:30:HIS:CB | 16:AQ:33:TYR:HB2 | 2.49 | 0.43 |
| 18:AS:41:PRO:C | 18:AS:43:MET:H | 2.22 | 0.43 |
| 47:B0:27:LEU:HB2 | 47:B0:28:SER:H | 1.63 | 0.43 |
| 48:B1:36:LYS:HG2 | 48:B1:47:ILE:HA | 2.01 | 0.43 |
| 23:BB:1131:G:O2' | 23:BB:1133:A:N7 | 2.52 | 0.43 |
| 23:BB:1557:C:H3' | 23:BB:1558:C:C5' | 2.46 | 0.43 |
| 23:BB:1641:A:H2' | 23:BB:1642:G:O4' | 2.19 | 0.43 |
| 23:BB:1939:U:O2 | 23:BB:1967:C:H4' | 2.19 | 0.43 |
| 23:BB:2282:G:O2' | 23:BB:2283:C:OP2 | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:2461:A:H2' | 23:BB:2462:C:H6 | 1.80 | 0.43 |
| 23:BB:2473:U:C2' | 23:BB:2473:U:O2 | 2.65 | 0.43 |
| 23:BB:2668:G:O2' | 23:BB:2669:G:H5' | 2.19 | 0.43 |
| 23:BB:2757:A:H2 | 29:BG:63:GLN:HE22 | 1.67 | 0.43 |
| 23:BB:2819:G:C6 | 23:BB:2828:G:C6 | 3.07 | 0.43 |
| 23:BB:506:G:H1' | 23:BB:507:A:C8 | 2.54 | 0.43 |
| 23:BB:687:C:H2' | 23:BB:688:U:O4' | 2.19 | 0.43 |
| 23:BB:915:C:H3' | 23:BB:916:G:H8 | 1.83 | 0.43 |
| 23:BB:2821:A:OP2 | 26:BD:115:GLY:HA3 | 2.19 | 0.43 |
| 23:BB:2052:A:N7 | 26:BD:146:ILE:HD11 | 2.34 | 0.43 |
| 27:BE:101:TYR:O | 27:BE:104:ALA:HB3 | 2.19 | 0.43 |
| 28:BF:120:SER:OG | 28:BF:129:MET:HB3 | 2.19 | 0.43 |
| 29:BG:14:VAL:O | 29:BG:16:VAL:HG23 | 2.19 | 0.43 |
| 38:BQ:18:LYS:C | 38:BQ:20:ALA:N | 2.72 | 0.43 |
| 38:BQ:26:ALA:C | 38:BQ:28:SER:N | 2.72 | 0.43 |
| 40:BS:60:HIS:ND1 | 40:BS:60:HIS:O | 2.50 | 0.43 |
| 41:BT:39:THR:HG22 | 41:BT:42:GLU:HG2 | 2.01 | 0.43 |
| 43:BW:16:GLU:H | 43:BW:16:GLU:CD | 2.21 | 0.43 |
| 44:BX:43:LEU:O | 44:BX:47:ARG:HG3 | 2.17 | 0.43 |
| 1:CA:1172:C:O2' | 1:CA:1173:U:H5' | 2.19 | 0.43 |
| 1:CA:218:U:H2' | 1:CA:219:U:H6 | 1.80 | 0.43 |
| 1:CA:377:G:H2' | 1:CA:378:G:H8 | 1.84 | 0.43 |
| 1:CA:493:A:H3' | 1:CA:494:G:H8 | 1.83 | 0.43 |
| 1:CA:643:C:H5' | 7:CH:31:LEU:HD13 | 2.00 | 0.43 |
| 1:CA:857:C:H2' | 1:CA:858:G:O4' | 2.19 | 0.43 |
| 1:CA:994:A:H2' | 1:CA:994:A:N3 | 2.34 | 0.43 |
| 20:CB:95:TRP:HH2 | 20:CB:100:LEU:HD22 | 1.83 | 0.43 |
| 20:CB:160:LEU:HG | 20:CB:161:PHE:N | 2.33 | 0.43 |
| 20:CB:165:ALA:H | 20:CB:186:VAL:HG12 | 1.83 | 0.43 |
| 20:CB:163:ILE:HD12 | 20:CB:185:ILE:HD12 | 2.00 | 0.43 |
| 20:CB:17:HIS:CG | 20:CB:18:GLN:N | 2.87 | 0.43 |
| 2:CC:54:ILE:O | 2:CC:54:ILE:HG23 | 2.19 | 0.43 |
| 4:CE:82:HIS:HE1 | 4:CE:147:ASN:H | 1.67 | 0.43 |
| 5:CF:79:ARG:HD3 | 5:CF:79:ARG:HA | 1.89 | 0.43 |
| 6:CG:78:ARG:HH11 | 6:CG:80:GLY:H | 1.67 | 0.43 |
| 8:CI:53:LEU:HD22 | 8:CI:53:LEU:N | 2.34 | 0.43 |
| 11:CL:30:ARG:O | 11:CL:57:THR:HG23 | 2.19 | 0.43 |
| 1:CA:1226:C:H3' | 12:CM:101:THR:OG1 | 2.18 | 0.43 |
| 49:D2:30:VAL:HG22 | 49:D2:33:ARG:NH2 | 2.24 | 0.43 |
| 22:DA:15:A:OP1 | 22:DA:108:A:H5' | 2.19 | 0.43 |
| 22:DA:22:U:H2' | 22:DA:23:G:C8 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:1241:A:N3 | 23:DB:1241:A:O4' | 2.51 | 0.43 |
| 23:DB:1411:U:H2' | 23:DB:1412:U:C6 | 2.54 | 0.43 |
| 23:DB:1474:U:H2' | 23:DB:1475:G:H5'' | 2.01 | 0.43 |
| 23:DB:1633:G:O2' | 23:DB:1634:A:H5'' | 2.19 | 0.43 |
| 23:DB:1946:U:O2' | 23:DB:1947:C:H5' | 2.18 | 0.43 |
| 23:DB:2149:U:H2' | 23:DB:2150:C:O4' | 2.18 | 0.43 |
| 23:DB:2780:G:H4' | 23:DB:2781:A:OP2 | 2.18 | 0.43 |
| 23:DB:716:A:C2' | 23:DB:717:C:H5'' | 2.48 | 0.43 |
| 23:DB:755:U:H2' | 23:DB:756:A:H8 | 1.83 | 0.43 |
| 23:DB:864:G:O2' | 23:DB:865:C:H5' | 2.18 | 0.43 |
| 23:DB:930:G:H1' | 45:DY:24:LEU:HD11 | 2.01 | 0.43 |
| 25:DC:180:MET:O | 25:DC:267:VAL:HG23 | 2.19 | 0.43 |
| 27:DE:104:ALA:C | 27:DE:106:LYS:H | 2.22 | 0.43 |
| 28:DF:31:GLU:HB2 | 28:DF:158:THR:CG2 | 2.48 | 0.43 |
| 28:DF:36:ASN:HD22 | 28:DF:152:ASP:CB | 2.12 | 0.43 |
| 28:DF:87:LYS:C | 28:DF:88:VAL:HG23 | 2.39 | 0.43 |
| 30:DH:83:LYS:HG3 | 30:DH:149:GLU:CG | 2.46 | 0.43 |
| 52:DI:126:ARG:NH1 | 52:DI:126:ARG:CB | 2.82 | 0.43 |
| 52:DI:72:THR:OG1 | 52:DI:73:PRO:HD2 | 2.18 | 0.43 |
| 31:DJ:29:ALA:O | 31:DJ:32:LEU:HB2 | 2.19 | 0.43 |
| 34:DM:126:ILE:HG22 | 34:DM:127:LYS:N | 2.34 | 0.43 |
| 34:DM:26:VAL:HG22 | 34:DM:133:LYS:HA | 2.00 | 0.43 |
| 35:DN:13:ASN:OD1 | 35:DN:16:HIS:HB2 | 2.19 | 0.43 |
| 38:DQ:93:ILE:HG23 | 38:DQ:94:LEU:H | 1.84 | 0.43 |
| 38:DQ:63:ARG:NH2 | 38:DQ:95:ALA:O | 2.52 | 0.43 |
| 39:DR:71:LYS:HG2 | 39:DR:73:LYS:HZ3 | 1.83 | 0.43 |
| 40:DS:41:LYS:HZ2 | 40:DS:41:LYS:HB3 | 1.82 | 0.43 |
| 41:DT:7:LEU:C | 41:DT:9:LYS:H | 2.21 | 0.43 |
| 24:DV:32:GLY:O | 24:DV:93:ARG:HB2 | 2.19 | 0.43 |
| 44:DX:59:GLU:N | 44:DX:59:GLU:OE2 | 2.52 | 0.43 |
| 1:AA:402:G:O2' | 1:AA:403:C:H5' | 2.19 | 0.42 |
| 1:AA:429:U:H5' | 3:AD:8:LEU:CG | 2.38 | 0.42 |
| 1:AA:927:G:H2' | 1:AA:928:G:H8 | 1.83 | 0.42 |
| 20:AB:93:HIS:O | 20:AB:94:ARG:HG2 | 2.19 | 0.42 |
| 1:AA:878:A:OP1 | 7:AH:80:PRO:HG2 | 2.18 | 0.42 |
| 16:AQ:18:LYS:H | 16:AQ:50:ASN:HD21 | 1.67 | 0.42 |
| 18:AS:30:LEU:HG | 18:AS:47:THR:O | 2.19 | 0.42 |
| 48:B1:18:HIS:CG | 48:B1:19:PHE:N | 2.87 | 0.42 |
| 23:BB:1208:C:C2' | 23:BB:1209:U:H5' | 2.49 | 0.42 |
| 23:BB:1238:G:O2' | 23:BB:1239:G:H5' | 2.19 | 0.42 |
| 23:BB:1535:A:C5' | 23:BB:1536:C:H5 | 2.30 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1565:C:H5'' | 25:BC:17:LYS:HZ1 | 1.83 | 0.42 |
| 23:BB:1637:A:H2' | 23:BB:1638:C:C6 | 2.54 | 0.42 |
| 23:BB:2146:C:O2' | 23:BB:2147:A:H5' | 2.17 | 0.42 |
| 23:BB:2590:A:O2' | 23:BB:2591:C:H5' | 2.18 | 0.42 |
| 23:BB:2655:G:N2 | 23:BB:2664:G:H2' | 2.34 | 0.42 |
| 23:BB:302:C:H2' | 23:BB:303:G:H8 | 1.84 | 0.42 |
| 23:BB:327:G:O2' | 23:BB:328:U:H5' | 2.19 | 0.42 |
| 23:BB:554:U:H2' | 23:BB:555:G:O4' | 2.19 | 0.42 |
| 23:BB:621:A:H2' | 23:BB:622:G:O4' | 2.19 | 0.42 |
| 23:BB:692:C:H2' | 23:BB:693:A:C8 | 2.54 | 0.42 |
| 23:BB:909:A:H2' | 23:BB:912:C:C5 | 2.53 | 0.42 |
| 23:BB:937:C:H2' | 23:BB:938:G:H8 | 1.84 | 0.42 |
| 23:BB:962:G:H2' | 23:BB:963:U:H6 | 1.84 | 0.42 |
| 26:BD:150:GLN:O | 26:BD:153:GLY:N | 2.52 | 0.42 |
| 26:BD:197:THR:C | 26:BD:199:SER:H | 2.21 | 0.42 |
| 27:BE:148:ILE:O | 27:BE:148:ILE:HG22 | 2.18 | 0.42 |
| 27:BE:12:LEU:HD11 | 27:BE:14:VAL:HG13 | 2.00 | 0.42 |
| 28:BF:76:PHE:O | 28:BF:77:LYS:HB2 | 2.19 | 0.42 |
| 29:BG:1:SER:HA | 29:BG:61:TRP:CZ3 | 2.54 | 0.42 |
| 34:BM:124:LEU:HA | 34:BM:125:PRO:HD3 | 1.87 | 0.42 |
| 24:BV:77:VAL:HG12 | 34:BM:136:MET:HG2 | 2.00 | 0.42 |
| 35:BN:116:VAL:O | 35:BN:117:ASP:CB | 2.59 | 0.42 |
| 22:BA:49:C:OP1 | 36:BO:101:GLY:HA3 | 2.19 | 0.42 |
| 36:BO:92:PHE:HB2 | 36:BO:117:PHE:CE1 | 2.53 | 0.42 |
| 36:BO:88:LYS:HD2 | 36:BO:89:ASP:CB | 2.48 | 0.42 |
| 37:BP:100:ARG:O | 37:BP:102:ARG:N | 2.52 | 0.42 |
| 39:BR:54:VAL:HG13 | 39:BR:56:GLY:O | 2.18 | 0.42 |
| 39:BR:63:VAL:O | 39:BR:63:VAL:HG23 | 2.19 | 0.42 |
| 41:BT:29:THR:HB | 41:BT:86:THR:HG22 | 2.01 | 0.42 |
| 42:BU:80:ASP:HB2 | 42:BU:95:PHE:CD2 | 2.54 | 0.42 |
| 42:BU:85:ARG:HH11 | 42:BU:86:PHE:H | 1.65 | 0.42 |
| 42:BU:84:PHE:HE2 | 42:BU:93:ARG:HG2 | 1.84 | 0.42 |
| 24:BV:2:PHE:HD2 | 24:BV:59:GLU:OE1 | 2.02 | 0.42 |
| 43:BW:35:ILE:HA | 43:BW:57:THR:HA | 2.01 | 0.42 |
| 46:BZ:11:ARG:HB3 | 46:BZ:12:PRO:HD2 | 2.00 | 0.42 |
| 1:CA:1014:A:C2 | 1:CA:1219:A:H1' | 2.54 | 0.42 |
| 1:CA:1056:U:H2' | 1:CA:1057:G:H8 | 1.84 | 0.42 |
| 1:CA:1187:G:OP1 | 8:CI:114:LYS:HE3 | 2.19 | 0.42 |
| 1:CA:977:A:O2' | 1:CA:1223:C:N4 | 2.52 | 0.42 |
| 1:CA:1320:C:H41 | 18:CS:36:ARG:HA | 1.84 | 0.42 |
| 1:CA:1352:C:H2' | 1:CA:1353:G:H8 | 1.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:201:G:H2' | 1:CA:202:G:C8 | 2.53 | 0.42 |
| 1:CA:51:A:H61 | 1:CA:314:C:H1' | 1.83 | 0.42 |
| 1:CA:623:C:H2' | 1:CA:624:C:C6 | 2.54 | 0.42 |
| 1:CA:695:A:H61 | 1:CA:797:C:C1' | 2.28 | 0.42 |
| 1:CA:822:U:H2' | 1:CA:823:C:H6 | 1.84 | 0.42 |
| 1:CA:915:A:H2' | 1:CA:916:U:H5' | 2.01 | 0.42 |
| 1:CA:986:U:H2' | 1:CA:987:G:C8 | 2.54 | 0.42 |
| 2:CC:174:LEU:HD23 | 2:CC:174:LEU:O | 2.18 | 0.42 |
| 4:CE:94:PHE:O | 4:CE:124:ALA:HB1 | 2.19 | 0.42 |
| 5:CF:9:MET:HB3 | 5:CF:59:TYR:CD2 | 2.54 | 0.42 |
| 6:CG:13:PRO:O | 6:CG:18:GLY:HA2 | 2.19 | 0.42 |
| 11:CL:35:ARG:NH2 | 11:CL:36:VAL:HG22 | 2.34 | 0.42 |
| 16:CQ:39:ARG:NH1 | 16:CQ:39:ARG:HG3 | 2.33 | 0.42 |
| 19:CT:54:GLN:O | 19:CT:57:VAL:HG23 | 2.19 | 0.42 |
| 49:D2:19:ARG:O | 49:D2:22:MET:HB2 | 2.19 | 0.42 |
| 23:DB:1109:C:H2' | 23:DB:1110:G:C4 | 2.53 | 0.42 |
| 23:DB:1205:A:N1 | 27:DE:165:HIS:HB2 | 2.34 | 0.42 |
| 23:DB:1270:C:H5'' | 23:DB:1271:G:O5' | 2.19 | 0.42 |
| 23:DB:1759:A:N3 | 23:DB:1759:A:H2' | 2.34 | 0.42 |
| 23:DB:1812:U:H4' | 25:DC:44:ASN:OD1 | 2.18 | 0.42 |
| 23:DB:1851:U:O2' | 23:DB:1852:U:H5' | 2.19 | 0.42 |
| 23:DB:2227:A:H2' | 23:DB:2228:G:O4' | 2.19 | 0.42 |
| 23:DB:2845:U:O2' | 23:DB:2846:G:H5' | 2.19 | 0.42 |
| 23:DB:554:U:H2' | 23:DB:555:G:O4' | 2.18 | 0.42 |
| 23:DB:616:A:H4' | 27:DE:101:TYR:CE2 | 2.54 | 0.42 |
| 23:DB:687:C:H2' | 23:DB:688:U:O4' | 2.19 | 0.42 |
| 23:DB:760:G:C2' | 23:DB:761:A:H5' | 2.49 | 0.42 |
| 23:DB:862:G:H2' | 23:DB:863:A:C8 | 2.54 | 0.42 |
| 25:DC:138:SER:O | 25:DC:140:VAL:HG23 | 2.19 | 0.42 |
| 25:DC:164:VAL:O | 25:DC:165:ALA:HB2 | 2.19 | 0.42 |
| 26:DD:13:ARG:HH21 | 37:DP:55:HIS:HA | 1.84 | 0.42 |
| 23:DB:2811:G:OP1 | 26:DD:62:LYS:HD2 | 2.19 | 0.42 |
| 27:DE:148:ILE:O | 27:DE:148:ILE:HG22 | 2.18 | 0.42 |
| 29:DG:60:GLY:O | 29:DG:62:ALA:N | 2.52 | 0.42 |
| 30:DH:138:VAL:O | 30:DH:138:VAL:HG12 | 2.18 | 0.42 |
| 30:DH:40:THR:O | 30:DH:41:LYS:HB2 | 2.17 | 0.42 |
| 52:DI:96:LYS:HD3 | 52:DI:138:VAL:HG21 | 2.00 | 0.42 |
| 52:DI:68:PHE:N | 52:DI:68:PHE:CD1 | 2.87 | 0.42 |
| 31:DJ:12:LYS:HG3 | 31:DJ:41:LYS:HZ3 | 1.83 | 0.42 |
| 35:DN:10:LEU:HD21 | 35:DN:43:GLU:HG3 | 2.01 | 0.42 |
| 37:DP:100:ARG:O | 37:DP:102:ARG:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DR:79:ARG:O | 39:DR:81:LYS:HG2 | 2.19 | 0.42 |
| 43:DW:55:ASP:C | 43:DW:57:THR:H | 2.22 | 0.42 |
| 1:AA:1078:U:H2' | 1:AA:1079:G:C8 | 2.54 | 0.42 |
| 1:AA:1229:A:H2' | 1:AA:1230:C:H6 | 1.82 | 0.42 |
| 1:AA:1324:A:H4' | 1:AA:1363:A:OP1 | 2.19 | 0.42 |
| 1:AA:174:A:O2' | 1:AA:175:C:H5' | 2.19 | 0.42 |
| 1:AA:175:C:O2 | 1:AA:1447:A:H2 | 2.03 | 0.42 |
| 1:AA:445:G:H2' | 1:AA:446:G:O4' | 2.18 | 0.42 |
| 20:AB:138:ARG:O | 20:AB:141:GLU:HB2 | 2.19 | 0.42 |
| 20:AB:150:ILE:O | 20:AB:150:ILE:HG12 | 2.18 | 0.42 |
| 2:AC:119:ILE:CG2 | 2:AC:197:VAL:HG11 | 2.46 | 0.42 |
| 3:AD:8:LEU:HD12 | 3:AD:31:CYS:SG | 2.59 | 0.42 |
| 3:AD:47:LEU:HD22 | 3:AD:51:GLY:O | 2.19 | 0.42 |
| 4:AE:11:GLN:O | 4:AE:38:VAL:HA | 2.19 | 0.42 |
| 5:AF:34:GLY:C | 5:AF:35:LYS:HD2 | 2.40 | 0.42 |
| 5:AF:92:THR:CG2 | 5:AF:94:HIS:H | 2.14 | 0.42 |
| 6:AG:11:ILE:N | 6:AG:11:ILE:HD12 | 2.33 | 0.42 |
| 6:AG:129:ASN:HA | 6:AG:134:VAL:CG1 | 2.39 | 0.42 |
| 7:AH:112:ASP:HB2 | 7:AH:116:ARG:NH2 | 2.35 | 0.42 |
| 10:AK:88:PRO:HG3 | 21:AU:28:LEU:HD21 | 2.00 | 0.42 |
| 11:AL:66:ILE:CG2 | 11:AL:71:HIS:HB3 | 2.44 | 0.42 |
| 12:AM:5:GLY:O | 12:AM:6:ILE:HB | 2.19 | 0.42 |
| 13:AN:45:LEU:O | 13:AN:45:LEU:HD23 | 2.19 | 0.42 |
| 14:AO:73:ASP:OD1 | 14:AO:75:ALA:HB3 | 2.19 | 0.42 |
| 15:AP:42:ILE:HG22 | 15:AP:43:ALA:N | 2.33 | 0.42 |
| 18:AS:52:ASN:CG | 18:AS:53:GLY:N | 2.71 | 0.42 |
| 22:BA:94:A:O2' | 22:BA:95:U:H5' | 2.18 | 0.42 |
| 23:BB:2311:A:H3' | 23:BB:2312:U:C6 | 2.54 | 0.42 |
| 23:BB:2722:G:O2' | 23:BB:2723:C:H5' | 2.18 | 0.42 |
| 23:BB:346:A:H2' | 23:BB:347:A:O4' | 2.19 | 0.42 |
| 23:BB:407:G:O2' | 23:BB:408:G:H5' | 2.20 | 0.42 |
| 23:BB:463:G:N2 | 23:BB:466:A:OP2 | 2.52 | 0.42 |
| 23:BB:649:G:H2' | 23:BB:650:C:C6 | 2.54 | 0.42 |
| 23:BB:693:A:H2' | 23:BB:694:U:H6 | 1.84 | 0.42 |
| 23:BB:725:G:H2' | 23:BB:726:G:O4' | 2.19 | 0.42 |
| 23:BB:962:G:H2' | 23:BB:963:U:C6 | 2.54 | 0.42 |
| 27:BE:194:LYS:O | 27:BE:197:GLU:HB3 | 2.19 | 0.42 |
| 30:BH:121:VAL:O | 30:BH:121:VAL:HG23 | 2.19 | 0.42 |
| 30:BH:68:ARG:CB | 30:BH:134:VAL:HB | 2.49 | 0.42 |
| 52:BI:52:LEU:O | 52:BI:54:ILE:HG13 | 2.19 | 0.42 |
| 52:BI:63:ASP:C | 52:BI:65:SER:H | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BI:5:GLN:HG2 | 52:BI:6:ALA:H | 1.81 | 0.42 |
| 33:BL:95:LEU:HB2 | 33:BL:101:ILE:CG1 | 2.48 | 0.42 |
| 35:BN:118:ARG:HE | 35:BN:118:ARG:HB3 | 1.52 | 0.42 |
| 35:BN:14:SER:O | 35:BN:18:GLN:HB2 | 2.20 | 0.42 |
| 35:BN:24:MET:CE | 35:BN:40:LYS:HB3 | 2.49 | 0.42 |
| 36:BO:52:SER:HA | 36:BO:74:VAL:CG1 | 2.48 | 0.42 |
| 43:BW:18:LYS:HE3 | 43:BW:19:ARG:NH2 | 2.34 | 0.42 |
| 1:CA:1035:A:H2' | 1:CA:1036:A:H8 | 1.84 | 0.42 |
| 1:CA:1150:A:O3' | 9:CJ:43:PRO:HA | 2.18 | 0.42 |
| 1:CA:1230:C:H2' | 1:CA:1231:G:H8 | 1.85 | 0.42 |
| 1:CA:1446:A:C2' | 1:CA:1447:A:H5'' | 2.48 | 0.42 |
| 1:CA:42:G:H2' | 1:CA:43:C:C6 | 2.53 | 0.42 |
| 1:CA:541:G:H2' | 1:CA:542:G:H8 | 1.84 | 0.42 |
| 1:CA:56:U:H2' | 1:CA:57:G:H8 | 1.84 | 0.42 |
| 1:CA:677:U:H1' | 10:CK:120:CYS:SG | 2.58 | 0.42 |
| 1:CA:878:A:OP1 | 7:CH:80:PRO:HG2 | 2.19 | 0.42 |
| 1:CA:979:C:H1' | 1:CA:1317:C:N4 | 2.26 | 0.42 |
| 3:CD:2:ARG:HH22 | 3:CD:132:ALA:CB | 2.32 | 0.42 |
| 6:CG:67:ASN:O | 6:CG:134:VAL:HA | 2.19 | 0.42 |
| 7:CH:112:ASP:HB2 | 7:CH:116:ARG:NH2 | 2.34 | 0.42 |
| 1:CA:826:C:H4' | 7:CH:12:ARG:NE | 2.34 | 0.42 |
| 9:CJ:6:ILE:HD12 | 9:CJ:76:ILE:HD11 | 1.99 | 0.42 |
| 10:CK:126:ARG:HE | 10:CK:126:ARG:HA | 1.84 | 0.42 |
| 16:CQ:34:GLY:O | 16:CQ:35:LYS:C | 2.57 | 0.42 |
| 18:CS:39:ILE:HG12 | 18:CS:70:LEU:CD1 | 2.49 | 0.42 |
| 19:CT:52:GLU:O | 19:CT:52:GLU:HG2 | 2.19 | 0.42 |
| 23:DB:1011:G:O2' | 23:DB:1013:C:H5'' | 2.19 | 0.42 |
| 23:DB:1106:G:H2' | 23:DB:1107:G:H8 | 1.83 | 0.42 |
| 23:DB:1214:A:H2' | 23:DB:1215:G:C8 | 2.54 | 0.42 |
| 23:DB:1366:A:H2' | 23:DB:1367:A:O4' | 2.20 | 0.42 |
| 23:DB:1389:G:O2' | 23:DB:1390:U:H5' | 2.19 | 0.42 |
| 23:DB:1479:G:O2' | 23:DB:1480:C:H5' | 2.19 | 0.42 |
| 23:DB:1636:U:O2' | 23:DB:1637:A:H5' | 2.18 | 0.42 |
| 23:DB:1683:U:O2' | 23:DB:1684:G:H5' | 2.19 | 0.42 |
| 23:DB:1764:C:H2' | 23:DB:1765:U:C6 | 2.54 | 0.42 |
| 23:DB:1891:G:H2' | 23:DB:1892:C:C6 | 2.54 | 0.42 |
| 23:DB:2201:G:O2' | 23:DB:2202:U:H5' | 2.20 | 0.42 |
| 23:DB:2734:A:C2' | 23:DB:2735:G:H5' | 2.44 | 0.42 |
| 23:DB:656:G:O2' | 23:DB:657:U:H5' | 2.19 | 0.42 |
| 26:DD:138:LEU:N | 26:DD:138:LEU:HD22 | 2.34 | 0.42 |
| 26:DD:110:THR:HG21 | 26:DD:169:ARG:HH11 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DE:152:GLU:O | 27:DE:153:LEU:HB3 | 2.18 | 0.42 |
| 28:DF:121:PHE:HE1 | 28:DF:162:ASP:CB | 2.33 | 0.42 |
| 30:DH:103:VAL:HA | 30:DH:106:ALA:HB3 | 2.00 | 0.42 |
| 52:DI:128:ILE:CA | 52:DI:131:THR:HG23 | 2.49 | 0.42 |
| 31:DJ:36:LEU:CD1 | 31:DJ:121:LYS:HE3 | 2.49 | 0.42 |
| 31:DJ:55:ILE:CG2 | 31:DJ:123:LYS:HB2 | 2.49 | 0.42 |
| 36:DO:79:ALA:O | 36:DO:83:LEU:HD13 | 2.19 | 0.42 |
| 36:DO:92:PHE:HB2 | 36:DO:117:PHE:CE1 | 2.55 | 0.42 |
| 40:DS:24:ILE:HG23 | 40:DS:32:ALA:CB | 2.49 | 0.42 |
| 40:DS:60:HIS:O | 40:DS:61:ASN:HB2 | 2.19 | 0.42 |
| 45:DY:6:ILE:HD13 | 45:DY:56:VAL:CG1 | 2.49 | 0.42 |
| 23:DB:2081:U:P | 46:DZ:19:SER:HB3 | 2.59 | 0.42 |
| 1:AA:1290:G:H2' | 1:AA:1291:U:C6 | 2.53 | 0.42 |
| 1:AA:43:C:H2' | 1:AA:44:A:O4' | 2.19 | 0.42 |
| 1:AA:731:G:H5' | 1:AA:766:A:H4' | 2.02 | 0.42 |
| 1:AA:74:A:H2' | 1:AA:75:G:H5'' | 2.01 | 0.42 |
| 1:AA:775:G:H2' | 1:AA:776:G:H8 | 1.84 | 0.42 |
| 1:AA:848:C:H2' | 1:AA:849:G:O4' | 2.18 | 0.42 |
| 1:AA:923:A:H2' | 1:AA:924:C:H6 | 1.82 | 0.42 |
| 20:AB:165:ALA:HB3 | 20:AB:186:VAL:HG11 | 2.00 | 0.42 |
| 2:AC:119:ILE:HD13 | 2:AC:136:ALA:HB2 | 2.00 | 0.42 |
| 3:AD:162:GLU:HB2 | 3:AD:166:LYS:HZ1 | 1.84 | 0.42 |
| 3:AD:64:TYR:CE2 | 3:AD:93:LEU:HB3 | 2.54 | 0.42 |
| 5:AF:36:ILE:H | 5:AF:36:ILE:HD12 | 1.84 | 0.42 |
| 5:AF:68:GLN:HA | 5:AF:71:ILE:HG12 | 2.00 | 0.42 |
| 8:AI:48:ARG:O | 8:AI:52:GLU:HG2 | 2.19 | 0.42 |
| 12:AM:85:TYR:HA | 12:AM:88:LEU:CD1 | 2.49 | 0.42 |
| 13:AN:79:SER:HG | 13:AN:82:LYS:HG2 | 1.83 | 0.42 |
| 14:AO:54:GLY:O | 14:AO:58:MET:HG2 | 2.19 | 0.42 |
| 16:AQ:10:ARG:HG3 | 16:AQ:10:ARG:O | 2.18 | 0.42 |
| 16:AQ:23:ALA:HA | 16:AQ:41:THR:O | 2.19 | 0.42 |
| 16:AQ:81:ALA:O | 16:AQ:82:VAL:HB | 2.19 | 0.42 |
| 19:AT:52:GLU:O | 19:AT:52:GLU:HG2 | 2.18 | 0.42 |
| 23:BB:107:G:O2' | 23:BB:108:G:H5' | 2.20 | 0.42 |
| 23:BB:1197:G:H2' | 23:BB:1198:U:C6 | 2.53 | 0.42 |
| 23:BB:1366:A:H2' | 23:BB:1367:A:O4' | 2.19 | 0.42 |
| 23:BB:1547:C:H2' | 23:BB:1548:A:C8 | 2.54 | 0.42 |
| 23:BB:1565:C:H5'' | 25:BC:17:LYS:CE | 2.49 | 0.42 |
| 23:BB:1727:C:H2' | 23:BB:1728:C:O4' | 2.20 | 0.42 |
| 23:BB:1767:G:O2' | 23:BB:1768:C:H5' | 2.18 | 0.42 |
| 23:BB:1803:A:O3' | 25:BC:256:THR:HB | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:182:A:O2' | 23:BB:183:C:H5' | 2.19 | 0.42 |
| 23:BB:2363:G:O2' | 23:BB:2364:C:H5' | 2.19 | 0.42 |
| 23:BB:2552:U:C2 | 23:BB:2554:U:H5' | 2.55 | 0.42 |
| 23:BB:673:C:OP1 | 27:BE:49:ARG:HD2 | 2.19 | 0.42 |
| 23:BB:465:G:N2 | 23:BB:684:G:H1' | 2.34 | 0.42 |
| 23:BB:992:C:H2' | 23:BB:993:G:C8 | 2.54 | 0.42 |
| 27:BE:148:ILE:HB | 27:BE:169:VAL:HG12 | 2.01 | 0.42 |
| 27:BE:29:HIS:O | 27:BE:32:VAL:HG22 | 2.19 | 0.42 |
| 28:BF:7:TYR:O | 28:BF:11:VAL:HB | 2.20 | 0.42 |
| 28:BF:42:ALA:O | 28:BF:43:ILE:C | 2.57 | 0.42 |
| 29:BG:167:VAL:HG23 | 29:BG:168:VAL:N | 2.26 | 0.42 |
| 30:BH:80:ILE:CD1 | 30:BH:99:ILE:HG23 | 2.49 | 0.42 |
| 34:BM:26:VAL:CG2 | 34:BM:133:LYS:HA | 2.50 | 0.42 |
| 34:BM:26:VAL:HB | 34:BM:104:GLU:OE2 | 2.19 | 0.42 |
| 35:BN:28:LEU:HD23 | 35:BN:28:LEU:HA | 1.85 | 0.42 |
| 37:BP:61:ARG:HE | 37:BP:100:ARG:HD2 | 1.83 | 0.42 |
| 37:BP:99:LEU:HD22 | 37:BP:99:LEU:HA | 1.92 | 0.42 |
| 39:BR:6:GLN:HE21 | 39:BR:6:GLN:C | 2.23 | 0.42 |
| 41:BT:39:THR:O | 41:BT:40:LYS:HB3 | 2.19 | 0.42 |
| 42:BU:98:ASN:OD1 | 42:BU:100:GLU:HB2 | 2.19 | 0.42 |
| 42:BU:86:PHE:HE1 | 42:BU:88:ASP:OD1 | 2.02 | 0.42 |
| 44:BX:1:MET:CB | 44:BX:4:LYS:HD3 | 2.47 | 0.42 |
| 45:BY:40:THR:HG22 | 45:BY:42:ALA:H | 1.84 | 0.42 |
| 1:CA:1058:G:H2' | 1:CA:1059:C:C6 | 2.55 | 0.42 |
| 1:CA:1078:U:H2' | 1:CA:1079:G:C8 | 2.54 | 0.42 |
| 1:CA:378:G:H2' | 1:CA:379:C:C6 | 2.54 | 0.42 |
| 1:CA:438:U:H4' | 3:CD:119:HIS:HD2 | 1.84 | 0.42 |
| 1:CA:848:C:H2' | 1:CA:849:G:O4' | 2.19 | 0.42 |
| 1:CA:974:A:H4' | 1:CA:975:A:C5' | 2.46 | 0.42 |
| 20:CB:55:GLU:O | 20:CB:58:LYS:HB2 | 2.19 | 0.42 |
| 2:CC:2:GLN:O | 2:CC:3:LYS:HB2 | 2.19 | 0.42 |
| 3:CD:24:VAL:HA | 3:CD:27:ILE:CD1 | 2.46 | 0.42 |
| 4:CE:106:ALA:HB1 | 4:CE:110:MET:CB | 2.49 | 0.42 |
| 4:CE:52:ALA:H | 4:CE:58:ALA:HB2 | 1.84 | 0.42 |
| 7:CH:125:ILE:HG22 | 7:CH:126:CYS:SG | 2.59 | 0.42 |
| 9:CJ:14:ASP:OD1 | 9:CJ:17:LEU:HB2 | 2.18 | 0.42 |
| 9:CJ:17:LEU:HD22 | 9:CJ:96:VAL:HG13 | 2.01 | 0.42 |
| 10:CK:42:GLY:HA3 | 10:CK:73:VAL:HG13 | 2.00 | 0.42 |
| 10:CK:57:SER:O | 10:CK:90:PRO:HG3 | 2.19 | 0.42 |
| 13:CN:69:PRO:HG2 | 13:CN:70:HIS:H | 1.83 | 0.42 |
| 14:CO:69:LEU:HD11 | 14:CO:76:ARG:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:CQ:32:ILE:HG23 | 16:CQ:33:TYR:CD2 | 2.54 | 0.42 |
| 16:CQ:40:THR:HG22 | 16:CQ:41:THR:N | 2.34 | 0.42 |
| 18:CS:2:ARG:HA | 18:CS:2:ARG:NE | 2.35 | 0.42 |
| 18:CS:39:ILE:HD13 | 18:CS:65:MET:HB3 | 2.01 | 0.42 |
| 23:DB:1028:A:N3 | 23:DB:2486:C:O2' | 2.41 | 0.42 |
| 23:DB:177:G:H3' | 23:DB:178:G:C8 | 2.54 | 0.42 |
| 23:DB:2026:U:H2' | 23:DB:2027:G:H8 | 1.84 | 0.42 |
| 23:DB:21:A:H2' | 23:DB:22:C:H6 | 1.83 | 0.42 |
| 23:DB:423:A:H5'' | 23:DB:424:G:H5' | 2.00 | 0.42 |
| 23:DB:80:G:HO2' | 23:DB:294:A:H2 | 1.65 | 0.42 |
| 25:DC:141:HIS:CG | 25:DC:142:ASN:N | 2.87 | 0.42 |
| 25:DC:92:LEU:HD12 | 25:DC:101:ARG:O | 2.19 | 0.42 |
| 26:DD:150:GLN:O | 26:DD:151:THR:C | 2.58 | 0.42 |
| 26:DD:3:GLY:HA2 | 26:DD:101:PHE:HZ | 1.83 | 0.42 |
| 28:DF:72:SER:CB | 28:DF:80:GLN:H | 2.32 | 0.42 |
| 29:DG:140:ILE:HD12 | 29:DG:141:GLY:N | 2.34 | 0.42 |
| 29:DG:175:LYS:HA | 29:DG:175:LYS:HD3 | 1.85 | 0.42 |
| 29:DG:1:SER:HA | 29:DG:61:TRP:CZ3 | 2.55 | 0.42 |
| 30:DH:133:GLN:HB2 | 30:DH:138:VAL:O | 2.19 | 0.42 |
| 52:DI:53:PRO:CG | 52:DI:77:VAL:HG11 | 2.49 | 0.42 |
| 23:DB:2898:U:O2 | 31:DJ:134:ALA:HB1 | 2.19 | 0.42 |
| 32:DK:71:ARG:HG3 | 32:DK:105:ARG:NH2 | 2.33 | 0.42 |
| 33:DL:29:LYS:C | 33:DL:31:GLY:N | 2.72 | 0.42 |
| 34:DM:10:ARG:HH11 | 34:DM:89:VAL:HG23 | 1.84 | 0.42 |
| 35:DN:98:LEU:O | 35:DN:112:TYR:HB2 | 2.19 | 0.42 |
| 38:DQ:112:ALA:O | 38:DQ:113:LYS:C | 2.57 | 0.42 |
| 38:DQ:91:ARG:HE | 38:DQ:94:LEU:CD2 | 2.32 | 0.42 |
| 41:DT:18:GLU:C | 41:DT:20:ALA:N | 2.71 | 0.42 |
| 42:DU:21:ARG:HG3 | 42:DU:21:ARG:NH1 | 2.34 | 0.42 |
| 23:DB:2365:G:C4' | 43:DW:59:PHE:HE1 | 2.17 | 0.42 |
| 45:DY:2:LYS:CD | 45:DY:2:LYS:H | 2.29 | 0.42 |
| 1:AA:1011:C:H2' | 1:AA:1012:A:C8 | 2.54 | 0.42 |
| 1:AA:1172:C:O2' | 1:AA:1173:U:H5' | 2.19 | 0.42 |
| 1:AA:1178:G:H3' | 8:AI:98:ARG:HH21 | 1.85 | 0.42 |
| 1:AA:1302:C:H6 | 12:AM:16:ILE:HG13 | 1.84 | 0.42 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:H6 | 1.84 | 0.42 |
| 1:AA:372:C:H1' | 1:AA:373:A:OP2 | 2.19 | 0.42 |
| 1:AA:602:A:H2' | 1:AA:603:U:H6 | 1.84 | 0.42 |
| 1:AA:292:G:O2' | 1:AA:609:A:N6 | 2.53 | 0.42 |
| 7:AH:108:GLY:O | 7:AH:110:MET:HG3 | 2.18 | 0.42 |
| 7:AH:6:ILE:CD1 | 7:AH:31:LEU:HD23 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AI:62:LEU:N | 8:AI:62:LEU:HD22 | 2.34 | 0.42 |
| 10:AK:14:GLN:HA | 10:AK:76:TYR:O | 2.19 | 0.42 |
| 11:AL:43:LYS:N | 11:AL:44:PRO:HD2 | 2.34 | 0.42 |
| 13:AN:16:ALA:O | 13:AN:20:PHE:HB3 | 2.19 | 0.42 |
| 13:AN:20:PHE:HB2 | 13:AN:54:SER:HG | 1.83 | 0.42 |
| 14:AO:69:LEU:HD11 | 14:AO:76:ARG:HB2 | 2.02 | 0.42 |
| 18:AS:40:PHE:HB2 | 18:AS:43:MET:CE | 2.49 | 0.42 |
| 48:B1:46:VAL:HG13 | 48:B1:47:ILE:N | 2.34 | 0.42 |
| 49:B2:26:ASN:HA | 49:B2:29:GLN:HB3 | 2.01 | 0.42 |
| 23:BB:80:G:N7 | 23:BB:102:U:O4 | 2.52 | 0.42 |
| 23:BB:1688:U:N3 | 23:BB:1698:A:C2 | 2.88 | 0.42 |
| 23:BB:1930:G:C2' | 23:BB:1931:U:OP2 | 2.67 | 0.42 |
| 23:BB:1931:U:H2' | 23:BB:1932:A:H8 | 1.84 | 0.42 |
| 23:BB:1:G:N3 | 23:BB:1:G:H2' | 2.35 | 0.42 |
| 23:BB:246:C:O2' | 23:BB:247:G:H5' | 2.20 | 0.42 |
| 23:BB:276:U:O2' | 23:BB:278:A:N7 | 2.51 | 0.42 |
| 23:BB:2885:G:H2' | 23:BB:2886:A:H4' | 2.02 | 0.42 |
| 23:BB:404:A:H4' | 23:BB:405:U:C5' | 2.45 | 0.42 |
| 23:BB:570:G:C4 | 23:BB:2030:A:N7 | 2.87 | 0.42 |
| 23:BB:750:A:H2' | 23:BB:751:A:H5" | 2.00 | 0.42 |
| 23:BB:912:C:H2' | 23:BB:913:U:C6 | 2.54 | 0.42 |
| 25:BC:138:SER:O | 25:BC:140:VAL:HG23 | 2.20 | 0.42 |
| 23:BB:2572:A:P | 26:BD:151:THR:HB | 2.59 | 0.42 |
| 27:BE:147:LEU:O | 27:BE:168:ASP:O | 2.37 | 0.42 |
| 28:BF:124:ARG:HH11 | 28:BF:124:ARG:HG2 | 1.84 | 0.42 |
| 28:BF:94:ARG:O | 28:BF:98:PHE:N | 2.45 | 0.42 |
| 29:BG:34:ARG:HD3 | 29:BG:34:ARG:N | 2.34 | 0.42 |
| 30:BH:122:LEU:CD1 | 30:BH:122:LEU:H | 2.31 | 0.42 |
| 30:BH:96:THR:OG1 | 30:BH:112:LYS:HD2 | 2.19 | 0.42 |
| 52:BI:103:ALA:O | 52:BI:107:GLU:HG3 | 2.20 | 0.42 |
| 52:BI:109:ALA:HB1 | 52:BI:124:MET:CG | 2.49 | 0.42 |
| 31:BJ:12:LYS:O | 31:BJ:13:ARG:HB2 | 2.19 | 0.42 |
| 32:BK:35:VAL:HG12 | 32:BK:69:VAL:HG22 | 2.01 | 0.42 |
| 23:BB:1666:G:H4' | 32:BK:6:THR:HG23 | 2.00 | 0.42 |
| 33:BL:138:ALA:O | 33:BL:139:GLY:C | 2.57 | 0.42 |
| 37:BP:113:LEU:C | 37:BP:114:ASN:HD22 | 2.22 | 0.42 |
| 24:BV:35:GLU:HG2 | 24:BV:93:ARG:NH1 | 2.35 | 0.42 |
| 24:BV:75:GLN:HA | 24:BV:75:GLN:OE1 | 2.18 | 0.42 |
| 46:BZ:76:GLU:HG3 | 46:BZ:77:LYS:N | 2.35 | 0.42 |
| 1:CA:1046:A:H2' | 1:CA:1047:G:O4' | 2.18 | 0.42 |
| 1:CA:1170:A:H3' | 1:CA:1171:A:H8 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1492:A:H2' | 23:DB:1913:A:C2 | 2.54 | 0.42 |
| 1:CA:256:U:H3' | 1:CA:257:G:H8 | 1.84 | 0.42 |
| 1:CA:260:G:H2' | 1:CA:261:U:C6 | 2.54 | 0.42 |
| 1:CA:263:A:H2' | 1:CA:264:C:C6 | 2.55 | 0.42 |
| 1:CA:458:U:H2' | 1:CA:459:A:C8 | 2.54 | 0.42 |
| 1:CA:477:C:H2' | 1:CA:478:A:C8 | 2.55 | 0.42 |
| 1:CA:602:A:H2' | 1:CA:603:U:H6 | 1.85 | 0.42 |
| 1:CA:808:C:O2' | 1:CA:809:G:H5' | 2.19 | 0.42 |
| 20:CB:82:ALA:HB3 | 20:CB:213:LEU:HD22 | 2.01 | 0.42 |
| 20:CB:96:LEU:HD23 | 20:CB:99:MET:CE | 2.49 | 0.42 |
| 2:CC:119:ILE:HD13 | 2:CC:136:ALA:HB2 | 2.01 | 0.42 |
| 3:CD:78:ALA:HA | 3:CD:81:LEU:HD12 | 2.02 | 0.42 |
| 5:CF:47:LEU:HB3 | 17:CR:65:SER:OG | 2.19 | 0.42 |
| 5:CF:66:ALA:HB1 | 5:CF:67:PRO:HD2 | 2.01 | 0.42 |
| 8:CI:36:GLN:N | 8:CI:36:GLN:HE21 | 2.17 | 0.42 |
| 1:CA:706:A:C4' | 10:CK:30:ILE:HD11 | 2.48 | 0.42 |
| 14:CO:73:ASP:OD1 | 14:CO:75:ALA:HB3 | 2.19 | 0.42 |
| 15:CP:40:ASN:ND2 | 15:CP:43:ALA:HB2 | 2.34 | 0.42 |
| 18:CS:10:ILE:CD1 | 18:CS:14:LEU:HD11 | 2.49 | 0.42 |
| 19:CT:49:ALA:CA | 19:CT:52:GLU:HB3 | 2.49 | 0.42 |
| 23:DB:1372:U:O2' | 23:DB:1373:A:H5' | 2.20 | 0.42 |
| 23:DB:1396:U:O2 | 23:DB:1396:U:H5' | 2.19 | 0.42 |
| 23:DB:2300:C:H2' | 23:DB:2301:C:C6 | 2.55 | 0.42 |
| 23:DB:2311:A:H3' | 23:DB:2312:U:C6 | 2.55 | 0.42 |
| 23:DB:2547:A:H2' | 23:DB:2548:U:H6 | 1.82 | 0.42 |
| 23:DB:583:G:H2' | 23:DB:584:C:H6 | 1.84 | 0.42 |
| 23:DB:643:A:C2 | 48:D1:43:ARG:HD2 | 2.54 | 0.42 |
| 23:DB:740:C:H5'' | 23:DB:1784:A:OP1 | 2.19 | 0.42 |
| 23:DB:974:G:H2' | 23:DB:974:G:N3 | 2.35 | 0.42 |
| 25:DC:255:LYS:C | 25:DC:256:THR:HG23 | 2.39 | 0.42 |
| 26:DD:101:PHE:HE1 | 26:DD:203:VAL:HG13 | 1.85 | 0.42 |
| 26:DD:109:VAL:HG11 | 26:DD:193:VAL:CB | 2.49 | 0.42 |
| 27:DE:148:ILE:HA | 27:DE:187:VAL:CG2 | 2.49 | 0.42 |
| 27:DE:21:ARG:NH2 | 27:DE:21:ARG:HB2 | 2.34 | 0.42 |
| 28:DF:7:TYR:O | 28:DF:11:VAL:HB | 2.19 | 0.42 |
| 28:DF:169:LEU:O | 28:DF:174:PHE:HB2 | 2.20 | 0.42 |
| 29:DG:107:GLY:HA3 | 29:DG:151:ARG:NH2 | 2.34 | 0.42 |
| 29:DG:9:VAL:HG12 | 29:DG:11:PRO:HD3 | 2.01 | 0.42 |
| 29:DG:154:GLU:O | 29:DG:156:TYR:N | 2.52 | 0.42 |
| 29:DG:84:LYS:HG3 | 29:DG:131:VAL:CB | 2.50 | 0.42 |
| 30:DH:83:LYS:N | 30:DH:83:LYS:HD2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:DI:101:SER:OG | 52:DI:104:GLN:HG3 | 2.19 | 0.42 |
| 52:DI:12:VAL:HG13 | 52:DI:41:PHE:CE2 | 2.55 | 0.42 |
| 23:DB:1098:A:C3' | 52:DI:3:LYS:C | 2.88 | 0.42 |
| 23:DB:636:G:P | 33:DL:128:THR:HG22 | 2.59 | 0.42 |
| 37:DP:89:GLY:N | 37:DP:112:ARG:NH1 | 2.67 | 0.42 |
| 38:DQ:60:TRP:O | 38:DQ:63:ARG:HG3 | 2.18 | 0.42 |
| 38:DQ:68:ALA:CA | 38:DQ:71:ASN:HB3 | 2.49 | 0.42 |
| 38:DQ:93:ILE:O | 38:DQ:96:ASP:HB3 | 2.19 | 0.42 |
| 39:DR:7:SER:CA | 39:DR:22:LEU:HD13 | 2.49 | 0.42 |
| 23:DB:814:C:OP1 | 39:DR:85:LYS:HA | 2.19 | 0.42 |
| 41:DT:30:ILE:O | 41:DT:85:VAL:HG23 | 2.20 | 0.42 |
| 42:DU:90:LYS:O | 42:DU:91:LYS:C | 2.58 | 0.42 |
| 24:DV:1:MET:HE3 | 24:DV:2:PHE:H | 1.83 | 0.42 |
| 43:DW:66:VAL:HG22 | 43:DW:81:ILE:HG22 | 2.01 | 0.42 |
| 1:AA:1077:G:N1 | 1:AA:1081:A:C6 | 2.88 | 0.42 |
| 1:AA:1330:U:H2' | 1:AA:1331:G:O4' | 2.19 | 0.42 |
| 1:AA:1305:G:O2' | 1:AA:1332:A:N6 | 2.53 | 0.42 |
| 1:AA:204:G:H2' | 1:AA:205:A:H8 | 1.81 | 0.42 |
| 1:AA:493:A:H3' | 1:AA:494:G:H8 | 1.83 | 0.42 |
| 1:AA:61:G:H2' | 1:AA:62:U:C6 | 2.54 | 0.42 |
| 1:AA:991:U:H2' | 1:AA:1212:U:O2 | 2.19 | 0.42 |
| 1:AA:9:G:H2' | 1:AA:10:A:C8 | 2.55 | 0.42 |
| 20:AB:134:LEU:HA | 20:AB:137:THR:CG2 | 2.49 | 0.42 |
| 20:AB:142:LYS:HA | 20:AB:145:ASN:CG | 2.40 | 0.42 |
| 2:AC:112:ALA:O | 2:AC:113:LYS:C | 2.58 | 0.42 |
| 2:AC:154:GLY:HA2 | 2:AC:163:ARG:N | 2.34 | 0.42 |
| 2:AC:99:GLN:O | 2:AC:100:ILE:HB | 2.19 | 0.42 |
| 6:AG:89:GLU:HG3 | 6:AG:89:GLU:H | 1.61 | 0.42 |
| 7:AH:49:LYS:HD2 | 7:AH:49:LYS:HA | 1.89 | 0.42 |
| 9:AJ:92:LEU:N | 9:AJ:92:LEU:HD22 | 2.34 | 0.42 |
| 10:AK:91:GLY:O | 10:AK:95:THR:HG22 | 2.20 | 0.42 |
| 11:AL:2:THR:HG22 | 11:AL:5:GLN:HE21 | 1.83 | 0.42 |
| 11:AL:31:GLY:HA3 | 11:AL:54:VAL:CG1 | 2.50 | 0.42 |
| 13:AN:15:LEU:HB3 | 13:AN:54:SER:CB | 2.44 | 0.42 |
| 15:AP:46:LYS:C | 15:AP:48:GLU:N | 2.73 | 0.42 |
| 1:AA:254:G:OP1 | 16:AQ:68:LYS:O | 2.38 | 0.42 |
| 16:AQ:80:LYS:NZ | 16:AQ:80:LYS:H | 2.17 | 0.42 |
| 17:AR:57:ALA:HA | 17:AR:60:ARG:HH11 | 1.84 | 0.42 |
| 19:AT:64:GLY:H | 19:AT:67:HIS:CD2 | 2.37 | 0.42 |
| 23:BB:2526:G:N3 | 51:B4:1:MET:N | 2.67 | 0.42 |
| 22:BA:75:G:H2' | 22:BA:76:G:C8 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:1296:G:O2' | 23:BB:1297:C:H5' | 2.20 | 0.42 |
| 23:BB:1633:G:O2' | 23:BB:1634:A:H5'' | 2.19 | 0.42 |
| 23:BB:1662:U:H2' | 23:BB:1663:G:O4' | 2.20 | 0.42 |
| 23:BB:1771:C:O2' | 23:BB:1772:A:H5' | 2.19 | 0.42 |
| 23:BB:1784:A:H4' | 23:BB:1785:A:O5' | 2.18 | 0.42 |
| 23:BB:179:C:H2' | 23:BB:180:G:O4' | 2.19 | 0.42 |
| 23:BB:1824:G:O2' | 23:BB:1825:U:H5' | 2.19 | 0.42 |
| 23:BB:2028:U:H2' | 23:BB:2029:G:C8 | 2.54 | 0.42 |
| 23:BB:2095:A:H2' | 23:BB:2096:C:C6 | 2.54 | 0.42 |
| 23:BB:2301:C:O2' | 23:BB:2302:U:H5' | 2.20 | 0.42 |
| 23:BB:2331:G:O2' | 23:BB:2332:C:H5' | 2.19 | 0.42 |
| 23:BB:2432:A:H2' | 23:BB:2433:A:C8 | 2.55 | 0.42 |
| 23:BB:2636:C:H2' | 23:BB:2637:U:H6 | 1.85 | 0.42 |
| 23:BB:2855:C:O2' | 23:BB:2856:A:H5' | 2.19 | 0.42 |
| 23:BB:307:G:H2' | 23:BB:309:A:OP2 | 2.19 | 0.42 |
| 23:BB:780:G:H2' | 23:BB:782:A:N7 | 2.34 | 0.42 |
| 25:BC:221:GLY:C | 25:BC:223:ALA:N | 2.72 | 0.42 |
| 25:BC:264:LYS:HG3 | 25:BC:265:PHE:HD2 | 1.84 | 0.42 |
| 26:BD:178:VAL:HB | 26:BD:188:LEU:CB | 2.47 | 0.42 |
| 26:BD:3:GLY:HA2 | 26:BD:101:PHE:HZ | 1.84 | 0.42 |
| 29:BG:9:VAL:HG12 | 29:BG:11:PRO:HD3 | 2.00 | 0.42 |
| 30:BH:73:ASN:HD22 | 30:BH:73:ASN:H | 1.67 | 0.42 |
| 34:BM:19:GLY:N | 34:BM:38:ARG:NH1 | 2.65 | 0.42 |
| 35:BN:75:ILE:O | 35:BN:79:LEU:HD12 | 2.19 | 0.42 |
| 37:BP:54:LEU:HA | 37:BP:76:HIS:CD2 | 2.55 | 0.42 |
| 38:BQ:109:VAL:HG12 | 38:BQ:113:LYS:HE3 | 2.02 | 0.42 |
| 39:BR:15:SER:O | 39:BR:16:GLU:C | 2.58 | 0.42 |
| 39:BR:72:VAL:CG2 | 39:BR:89:HIS:HB3 | 2.49 | 0.42 |
| 40:BS:76:VAL:HG12 | 40:BS:103:ILE:HA | 2.01 | 0.42 |
| 43:BW:19:ARG:H | 43:BW:19:ARG:NE | 2.17 | 0.42 |
| 44:BX:23:ARG:O | 44:BX:27:ASN:HB2 | 2.19 | 0.42 |
| 1:CA:1219:A:H2' | 1:CA:1220:G:H8 | 1.84 | 0.42 |
| 1:CA:1370:G:O2' | 1:CA:1371:G:H5' | 2.18 | 0.42 |
| 1:CA:372:C:H1' | 1:CA:373:A:OP2 | 2.20 | 0.42 |
| 1:CA:878:A:C5' | 7:CH:80:PRO:HG2 | 2.49 | 0.42 |
| 20:CB:16:GLY:HA2 | 20:CB:40:ILE:HD12 | 2.02 | 0.42 |
| 2:CC:52:SER:O | 2:CC:113:LYS:HG2 | 2.19 | 0.42 |
| 2:CC:166:TRP:HE3 | 2:CC:166:TRP:HA | 1.84 | 0.42 |
| 8:CI:62:LEU:HD22 | 8:CI:62:LEU:N | 2.34 | 0.42 |
| 1:CA:1152:A:H4' | 9:CJ:15:HIS:HD2 | 1.84 | 0.42 |
| 12:CM:13:HIS:HB2 | 12:CM:16:ILE:HG22 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:D0:41:HIS:O | 47:D0:42:ILE:O | 2.36 | 0.42 |
| 47:D0:53:VAL:O | 47:D0:54:ILE:CB | 2.67 | 0.42 |
| 50:D3:30:HIS:O | 50:D3:31:ILE:O | 2.38 | 0.42 |
| 51:D4:2:LYS:CE | 51:D4:4:ARG:HE | 2.33 | 0.42 |
| 22:DA:8:C:O2' | 36:DO:40:ILE:HD13 | 2.19 | 0.42 |
| 23:DB:1252:G:O4' | 38:DQ:32:ARG:HG2 | 2.20 | 0.42 |
| 23:DB:1496:A:H1' | 23:DB:1577:C:O2' | 2.19 | 0.42 |
| 23:DB:1591:A:O2' | 23:DB:1592:C:H5' | 2.19 | 0.42 |
| 23:DB:1640:A:O2' | 23:DB:1641:A:H5' | 2.19 | 0.42 |
| 23:DB:1745:A:H2' | 23:DB:1746:A:H8 | 1.85 | 0.42 |
| 23:DB:1937:A:N7 | 23:DB:1939:U:H2' | 2.34 | 0.42 |
| 23:DB:1984:G:O2' | 23:DB:1985:C:H5' | 2.18 | 0.42 |
| 23:DB:2012:G:OP1 | 40:DS:98:LYS:HG2 | 2.20 | 0.42 |
| 23:DB:2300:C:H2' | 23:DB:2301:C:H6 | 1.84 | 0.42 |
| 23:DB:2376:A:N6 | 36:DO:94:ARG:HD3 | 2.34 | 0.42 |
| 23:DB:2855:C:O2' | 23:DB:2856:A:H5' | 2.19 | 0.42 |
| 23:DB:2895:G:O2' | 23:DB:2896:C:H5' | 2.20 | 0.42 |
| 25:DC:208:GLY:O | 25:DC:209:ALA:C | 2.57 | 0.42 |
| 27:DE:150:THR:HG22 | 27:DE:170:ARG:O | 2.20 | 0.42 |
| 22:DA:57:A:O2' | 28:DF:26:GLN:NE2 | 2.53 | 0.42 |
| 28:DF:2:LYS:O | 28:DF:6:TYR:HB2 | 2.18 | 0.42 |
| 30:DH:115:VAL:HG23 | 30:DH:131:SER:O | 2.19 | 0.42 |
| 31:DJ:111:LYS:CB | 31:DJ:113:PRO:HD2 | 2.47 | 0.42 |
| 36:DO:78:VAL:HA | 36:DO:81:ARG:HB3 | 2.01 | 0.42 |
| 37:DP:109:ILE:HD12 | 37:DP:109:ILE:O | 2.19 | 0.42 |
| 32:DK:76:VAL:HB | 37:DP:72:VAL:CG2 | 2.50 | 0.42 |
| 23:DB:1248:G:C5 | 38:DQ:2:ARG:HD2 | 2.54 | 0.42 |
| 39:DR:66:HIS:CG | 39:DR:94:THR:HG22 | 2.54 | 0.42 |
| 44:DX:21:LEU:HD23 | 44:DX:21:LEU:N | 2.35 | 0.42 |
| 1:AA:1029:U:H2' | 1:AA:1031:C:C2 | 2.55 | 0.42 |
| 1:AA:1186:G:H4' | 8:AI:111:GLU:OE1 | 2.19 | 0.42 |
| 1:AA:795:C:H1' | 1:AA:1506:U:C5 | 2.54 | 0.42 |
| 1:AA:160:A:H2' | 1:AA:161:A:C8 | 2.55 | 0.42 |
| 1:AA:152:A:N6 | 1:AA:170:U:C2 | 2.88 | 0.42 |
| 1:AA:51:A:H61 | 1:AA:314:C:H1' | 1.85 | 0.42 |
| 1:AA:770:C:O2' | 1:AA:771:G:H5' | 2.19 | 0.42 |
| 1:AA:98:A:O2' | 1:AA:99:C:H5' | 2.19 | 0.42 |
| 20:AB:95:TRP:HZ3 | 20:AB:174:GLU:CD | 2.23 | 0.42 |
| 2:AC:42:LEU:O | 2:AC:46:LEU:HB2 | 2.20 | 0.42 |
| 4:AE:33:THR:HG22 | 4:AE:51:LYS:CB | 2.49 | 0.42 |
| 5:AF:53:LYS:NZ | 5:AF:53:LYS:N | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AF:36:ILE:HA | 5:AF:64:VAL:HG13 | 2.01 | 0.42 |
| 7:AH:54:THR:HG23 | 7:AH:55:LYS:HG2 | 2.01 | 0.42 |
| 8:AI:36:GLN:N | 8:AI:36:GLN:HE21 | 2.17 | 0.42 |
| 8:AI:35:GLU:HG3 | 8:AI:44:ARG:CD | 2.49 | 0.42 |
| 9:AJ:18:ILE:CG1 | 9:AJ:72:ARG:HG2 | 2.50 | 0.42 |
| 9:AJ:35:GLN:HG2 | 9:AJ:77:VAL:HG23 | 2.01 | 0.42 |
| 13:AN:12:ARG:NE | 13:AN:58:ARG:NH1 | 2.68 | 0.42 |
| 13:AN:97:LYS:HB3 | 13:AN:97:LYS:HZ2 | 1.84 | 0.42 |
| 15:AP:21:VAL:O | 15:AP:33:ILE:HB | 2.19 | 0.42 |
| 18:AS:61:VAL:HA | 18:AS:65:MET:SD | 2.59 | 0.42 |
| 12:AM:92:ARG:NH1 | 18:AS:79:TYR:HD2 | 2.10 | 0.42 |
| 47:B0:53:VAL:O | 47:B0:54:ILE:CB | 2.68 | 0.42 |
| 23:BB:125:A:H5' | 49:B2:19:ARG:CG | 2.49 | 0.42 |
| 23:BB:1479:G:O2' | 23:BB:1480:C:H5' | 2.20 | 0.42 |
| 23:BB:1552:A:H2' | 23:BB:1553:A:C5' | 2.49 | 0.42 |
| 23:BB:1789:A:H2' | 23:BB:1790:C:O4' | 2.19 | 0.42 |
| 23:BB:2314:A:H2' | 23:BB:2315:G:H8 | 1.85 | 0.42 |
| 23:BB:2751:G:OP1 | 23:BB:2751:G:H2' | 2.20 | 0.42 |
| 23:BB:2766:A:H2' | 23:BB:2766:A:N3 | 2.35 | 0.42 |
| 23:BB:282:A:O2' | 23:BB:283:G:H5' | 2.19 | 0.42 |
| 23:BB:335:C:O2' | 23:BB:336:C:H5' | 2.19 | 0.42 |
| 23:BB:786:C:O2' | 23:BB:787:C:H5' | 2.20 | 0.42 |
| 23:BB:827:U:H5' | 23:BB:828:U:O5' | 2.18 | 0.42 |
| 23:BB:929:U:O2 | 45:BY:25:GLY:HA2 | 2.20 | 0.42 |
| 25:BC:157:ALA:C | 25:BC:159:THR:H | 2.22 | 0.42 |
| 25:BC:245:THR:HG23 | 25:BC:249:VAL:O | 2.19 | 0.42 |
| 26:BD:150:GLN:O | 26:BD:151:THR:C | 2.58 | 0.42 |
| 27:BE:37:ALA:C | 27:BE:39:ALA:H | 2.20 | 0.42 |
| 30:BH:100:ALA:HA | 30:BH:110:VAL:CG2 | 2.39 | 0.42 |
| 52:BI:79:LEU:HD23 | 52:BI:108:ILE:CD1 | 2.50 | 0.42 |
| 32:BK:105:ARG:HH11 | 32:BK:122:VAL:CG1 | 2.33 | 0.42 |
| 33:BL:88:GLY:HA2 | 33:BL:120:VAL:HG13 | 2.02 | 0.42 |
| 33:BL:55:MET:HE2 | 33:BL:59:ARG:HB3 | 2.02 | 0.42 |
| 33:BL:4:ASN:HB2 | 33:BL:5:THR:H | 1.71 | 0.42 |
| 37:BP:46:VAL:HA | 37:BP:60:VAL:HG12 | 2.01 | 0.42 |
| 40:BS:6:LYS:HB3 | 40:BS:104:THR:HA | 2.02 | 0.42 |
| 42:BU:18:LYS:HB3 | 42:BU:19:GLY:H | 1.68 | 0.42 |
| 24:BV:42:LEU:HD23 | 24:BV:42:LEU:N | 2.34 | 0.42 |
| 23:BB:2352:A:N1 | 43:BW:30:VAL:HG11 | 2.34 | 0.42 |
| 43:BW:23:LYS:C | 43:BW:66:VAL:HB | 2.40 | 0.42 |
| 1:CA:1069:C:O4' | 1:CA:1191:A:H2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1374:A:H2' | 1:CA:1375:A:H8 | 1.85 | 0.42 |
| 1:CA:82:G:H21 | 1:CA:84:U:H3 | 1.67 | 0.42 |
| 1:CA:9:G:H2' | 1:CA:10:A:C8 | 2.55 | 0.42 |
| 20:CB:59:ILE:O | 20:CB:62:ARG:HD2 | 2.20 | 0.42 |
| 2:CC:184:ASN:HD22 | 2:CC:184:ASN:HA | 1.60 | 0.42 |
| 2:CC:31:ASN:ND2 | 2:CC:58:ARG:NE | 2.66 | 0.42 |
| 3:CD:115:GLN:HG3 | 3:CD:119:HIS:CE1 | 2.54 | 0.42 |
| 6:CG:125:ASP:HB3 | 6:CG:131:GLY:N | 2.34 | 0.42 |
| 8:CI:66:VAL:HG11 | 8:CI:78:ILE:HD11 | 2.02 | 0.42 |
| 9:CJ:55:PRO:O | 9:CJ:56:HIS:HB3 | 2.19 | 0.42 |
| 9:CJ:59:LYS:C | 9:CJ:61:ALA:H | 2.23 | 0.42 |
| 1:CA:972:C:P | 9:CJ:59:LYS:HD3 | 2.59 | 0.42 |
| 1:CA:36:C:H5'' | 11:CL:119:LYS:HD2 | 2.01 | 0.42 |
| 13:CN:46:LYS:NZ | 18:CS:10:ILE:HG13 | 2.34 | 0.42 |
| 23:DB:1055:G:H2' | 23:DB:1056:G:O4' | 2.20 | 0.42 |
| 23:DB:1405:U:H2' | 23:DB:1406:U:H6 | 1.84 | 0.42 |
| 23:DB:1539:U:H2' | 23:DB:1539:U:O2 | 2.19 | 0.42 |
| 23:DB:1670:C:H2' | 23:DB:1671:U:O4' | 2.19 | 0.42 |
| 23:DB:1707:G:O2' | 23:DB:1708:C:H5' | 2.19 | 0.42 |
| 23:DB:1870:C:H3' | 23:DB:1871:A:C8 | 2.54 | 0.42 |
| 23:DB:1916:A:H2' | 23:DB:1917:U:O4' | 2.20 | 0.42 |
| 23:DB:193:U:O3' | 23:DB:803:U:H4' | 2.20 | 0.42 |
| 23:DB:2389:G:H5'' | 23:DB:2390:U:O4' | 2.19 | 0.42 |
| 23:DB:2411:A:H2' | 23:DB:2412:A:H8 | 1.84 | 0.42 |
| 23:DB:2786:U:H2' | 23:DB:2787:C:H6 | 1.84 | 0.42 |
| 23:DB:2828:G:H2' | 23:DB:2829:A:H8 | 1.85 | 0.42 |
| 23:DB:2719:G:O2' | 23:DB:2846:G:H4' | 2.19 | 0.42 |
| 23:DB:416:U:H2' | 23:DB:417:C:H6 | 1.82 | 0.42 |
| 23:DB:518:G:H2' | 23:DB:519:U:C6 | 2.54 | 0.42 |
| 23:DB:599:A:O2' | 23:DB:600:G:H5' | 2.19 | 0.42 |
| 23:DB:629:G:O2' | 23:DB:630:G:H5' | 2.20 | 0.42 |
| 23:DB:659:G:N2 | 27:DE:30:GLN:NE2 | 2.67 | 0.42 |
| 23:DB:743:A:C2' | 23:DB:744:U:H5' | 2.49 | 0.42 |
| 23:DB:850:U:O2' | 45:DY:22:THR:HG22 | 2.18 | 0.42 |
| 25:DC:124:LYS:HG2 | 25:DC:125:PRO:N | 2.35 | 0.42 |
| 23:DB:784:G:H1 | 25:DC:227:VAL:HG11 | 1.80 | 0.42 |
| 26:DD:16:THR:HG22 | 26:DD:17:GLU:N | 2.35 | 0.42 |
| 27:DE:148:ILE:HB | 27:DE:169:VAL:HG12 | 2.00 | 0.42 |
| 27:DE:68:ALA:O | 27:DE:69:ARG:C | 2.58 | 0.42 |
| 28:DF:69:ALA:HB3 | 28:DF:80:GLN:O | 2.20 | 0.42 |
| 28:DF:94:ARG:O | 28:DF:98:PHE:N | 2.46 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DG:39:ALA:O | 29:DG:54:ARG:HB2 | 2.19 | 0.42 |
| 34:DM:32:GLY:HA3 | 34:DM:103:TYR:O | 2.19 | 0.42 |
| 35:DN:94:TYR:C | 35:DN:116:VAL:HG12 | 2.40 | 0.42 |
| 37:DP:62:LYS:O | 37:DP:63:ILE:HB | 2.19 | 0.42 |
| 45:DY:18:LYS:O | 45:DY:22:THR:HG23 | 2.20 | 0.42 |
| 46:DZ:30:LEU:CD2 | 46:DZ:30:LEU:H | 2.27 | 0.42 |
| 1:AA:141:G:H2' | 1:AA:142:G:O4' | 2.19 | 0.42 |
| 1:AA:1446:A:C2' | 1:AA:1447:A:H5'' | 2.50 | 0.42 |
| 1:AA:36:C:C2' | 1:AA:37:U:H5' | 2.50 | 0.42 |
| 1:AA:663:A:O3' | 17:AR:52:ARG:NH2 | 2.49 | 0.42 |
| 1:AA:696:A:O2' | 1:AA:697:U:H5' | 2.20 | 0.42 |
| 20:AB:83:ALA:HA | 20:AB:88:GLN:HE21 | 1.84 | 0.42 |
| 2:AC:52:SER:HA | 2:AC:113:LYS:HG2 | 2.01 | 0.42 |
| 2:AC:85:LYS:O | 2:AC:89:VAL:HG23 | 2.20 | 0.42 |
| 7:AH:5:PRO:HB2 | 7:AH:32:LYS:NZ | 2.34 | 0.42 |
| 10:AK:46:ALA:HA | 10:AK:65:ALA:HB2 | 2.00 | 0.42 |
| 1:AA:585:G:H4' | 11:AL:4:ASN:HD21 | 1.85 | 0.42 |
| 13:AN:70:HIS:O | 13:AN:71:GLY:C | 2.58 | 0.42 |
| 18:AS:52:ASN:HB2 | 18:AS:76:THR:HG22 | 2.02 | 0.42 |
| 48:B1:18:HIS:ND1 | 48:B1:19:PHE:N | 2.68 | 0.42 |
| 51:B4:7:VAL:HG23 | 51:B4:35:GLN:CB | 2.50 | 0.42 |
| 23:BB:1041:G:H2' | 23:BB:1042:G:H8 | 1.77 | 0.42 |
| 23:BB:1348:C:H2' | 23:BB:1349:C:H5' | 2.01 | 0.42 |
| 23:BB:1505:A:H2' | 23:BB:1506:U:H6 | 1.85 | 0.42 |
| 23:BB:1553:A:H2' | 23:BB:1555:G:N7 | 2.35 | 0.42 |
| 23:BB:1736:U:H2' | 23:BB:1737:G:O4' | 2.19 | 0.42 |
| 23:BB:2231:U:H2' | 23:BB:2232:C:H6 | 1.85 | 0.42 |
| 23:BB:2305:U:H5' | 28:BF:152:ASP:OD2 | 2.19 | 0.42 |
| 23:BB:2489:U:H2' | 23:BB:2490:G:O4' | 2.19 | 0.42 |
| 23:BB:2654:A:N6 | 23:BB:2666:C:OP2 | 2.51 | 0.42 |
| 23:BB:2699:C:H2' | 23:BB:2700:A:H8 | 1.85 | 0.42 |
| 23:BB:2742:G:OP2 | 51:B4:24:ARG:NH1 | 2.52 | 0.42 |
| 23:BB:2773:C:H5'' | 26:BD:169:ARG:HB3 | 2.01 | 0.42 |
| 23:BB:485:C:O2' | 23:BB:486:C:H5' | 2.20 | 0.42 |
| 23:BB:493:G:H2' | 23:BB:494:G:O4' | 2.19 | 0.42 |
| 23:BB:644:A:H2 | 23:BB:646:U:O4 | 2.03 | 0.42 |
| 25:BC:188:ARG:NH2 | 25:BC:188:ARG:HG2 | 2.35 | 0.42 |
| 25:BC:255:LYS:C | 25:BC:257:ARG:H | 2.23 | 0.42 |
| 26:BD:123:LYS:HD3 | 26:BD:165:MET:SD | 2.59 | 0.42 |
| 27:BE:3:LEU:O | 27:BE:12:LEU:N | 2.53 | 0.42 |
| 27:BE:187:VAL:HG12 | 27:BE:188:MET:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:37:C:H1' | 27:BE:45:ALA:HB2 | 2.02 | 0.42 |
| 28:BF:42:ALA:O | 28:BF:44:ALA:N | 2.53 | 0.42 |
| 28:BF:79:ARG:O | 28:BF:81:GLY:N | 2.53 | 0.42 |
| 30:BH:14:SER:HB2 | 30:BH:17:ASP:HB3 | 2.01 | 0.42 |
| 52:BI:78:LEU:HD13 | 52:BI:108:ILE:HG23 | 2.00 | 0.42 |
| 31:BJ:84:ILE:O | 31:BJ:84:ILE:HG13 | 2.19 | 0.42 |
| 26:BD:21:SER:HB2 | 32:BK:73:ASP:HA | 2.00 | 0.42 |
| 33:BL:75:ALA:HB3 | 33:BL:108:ALA:HB2 | 2.00 | 0.42 |
| 36:BO:8:ILE:HG13 | 36:BO:8:ILE:H | 1.70 | 0.42 |
| 26:BD:10:GLY:HA2 | 37:BP:4:ILE:HD11 | 2.01 | 0.42 |
| 37:BP:86:LYS:HB3 | 37:BP:87:ARG:H | 1.54 | 0.42 |
| 23:BB:814:C:OP1 | 39:BR:85:LYS:HA | 2.19 | 0.42 |
| 24:BV:28:ALA:HA | 24:BV:88:HIS:ND1 | 2.34 | 0.42 |
| 24:BV:1:MET:HG3 | 24:BV:2:PHE:CD2 | 2.54 | 0.42 |
| 43:BW:28:GLU:H | 43:BW:31:LEU:CD1 | 2.33 | 0.42 |
| 46:BZ:54:LYS:O | 46:BZ:57:ARG:HB2 | 2.20 | 0.42 |
| 1:CA:1355:G:O2' | 1:CA:1356:G:H5' | 2.19 | 0.42 |
| 1:CA:1426:G:H2' | 1:CA:1427:C:O4' | 2.20 | 0.42 |
| 1:CA:301:G:H2' | 1:CA:302:G:C8 | 2.53 | 0.42 |
| 1:CA:683:G:O2' | 1:CA:684:U:H5' | 2.20 | 0.42 |
| 1:CA:708:C:H2' | 1:CA:709:U:H6 | 1.84 | 0.42 |
| 1:CA:77:A:H2' | 1:CA:78:A:C8 | 2.55 | 0.42 |
| 1:CA:244:U:O4 | 1:CA:906:A:H1' | 2.20 | 0.42 |
| 20:CB:64:GLY:HA2 | 20:CB:158:ASP:OD1 | 2.20 | 0.42 |
| 20:CB:31:PHE:HB3 | 20:CB:39:ILE:HG22 | 2.01 | 0.42 |
| 8:CI:95:SER:O | 8:CI:99:LYS:HB2 | 2.19 | 0.42 |
| 12:CM:95:PRO:CA | 12:CM:108:ARG:HG2 | 2.50 | 0.42 |
| 15:CP:28:ARG:HD3 | 15:CP:29:ASN:ND2 | 2.35 | 0.42 |
| 16:CQ:39:ARG:HA | 16:CQ:39:ARG:CZ | 2.50 | 0.42 |
| 23:DB:1921:G:O2' | 23:DB:1922:G:H5' | 2.19 | 0.42 |
| 23:DB:2282:G:OP1 | 23:DB:2283:C:H1' | 2.20 | 0.42 |
| 23:DB:2349:G:OP2 | 50:D3:41:ARG:HD3 | 2.20 | 0.42 |
| 23:DB:2363:G:O2' | 23:DB:2364:C:H5' | 2.18 | 0.42 |
| 23:DB:2602:A:OP1 | 23:DB:2602:A:H3' | 2.20 | 0.42 |
| 23:DB:2757:A:N3 | 23:DB:2757:A:H2' | 2.34 | 0.42 |
| 23:DB:584:C:N4 | 23:DB:585:G:C6 | 2.87 | 0.42 |
| 23:DB:70:G:H3' | 23:DB:113:U:C4' | 2.49 | 0.42 |
| 25:DC:255:LYS:C | 25:DC:257:ARG:H | 2.23 | 0.42 |
| 26:DD:178:VAL:HG12 | 26:DD:179:ARG:N | 2.33 | 0.42 |
| 26:DD:186:LEU:HD21 | 37:DP:7:LEU:HD21 | 2.02 | 0.42 |
| 27:DE:109:LEU:HD13 | 27:DE:180:LEU:HD13 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DE:147:LEU:O | 27:DE:168:ASP:O | 2.38 | 0.42 |
| 28:DF:3:LEU:HB2 | 28:DF:100:GLU:OE1 | 2.19 | 0.42 |
| 29:DG:112:VAL:O | 29:DG:113:ASP:HB2 | 2.19 | 0.42 |
| 30:DH:117:LEU:HD13 | 30:DH:130:VAL:HA | 2.02 | 0.42 |
| 52:DI:27:LEU:HB2 | 52:DI:32:VAL:HG21 | 2.01 | 0.42 |
| 31:DJ:20:ALA:C | 31:DJ:22:GLY:N | 2.73 | 0.42 |
| 32:DK:87:LEU:HD12 | 32:DK:92:GLU:C | 2.40 | 0.42 |
| 33:DL:23:ILE:HD12 | 33:DL:23:ILE:H | 1.84 | 0.42 |
| 33:DL:95:LEU:HB2 | 33:DL:101:ILE:CG1 | 2.49 | 0.42 |
| 34:DM:33:LEU:HD22 | 34:DM:128:THR:HB | 2.02 | 0.42 |
| 35:DN:28:LEU:HD21 | 35:DN:113:ILE:HG23 | 2.02 | 0.42 |
| 37:DP:38:ARG:HB3 | 37:DP:38:ARG:NH2 | 2.35 | 0.42 |
| 37:DP:54:LEU:HA | 37:DP:76:HIS:HD2 | 1.85 | 0.42 |
| 38:DQ:24:TYR:CD1 | 38:DQ:25:GLY:N | 2.87 | 0.42 |
| 38:DQ:49:ARG:HG2 | 38:DQ:49:ARG:HH11 | 1.85 | 0.42 |
| 23:DB:1223:G:OP2 | 39:DR:90:ARG:NH1 | 2.53 | 0.42 |
| 43:DW:56:HIS:O | 43:DW:57:THR:C | 2.57 | 0.42 |
| 1:AA:126:G:H2' | 1:AA:127:G:O4' | 2.20 | 0.42 |
| 1:AA:1451:U:O5' | 1:AA:1452:C:H5 | 2.03 | 0.42 |
| 1:AA:277:C:O2' | 1:AA:278:G:H5' | 2.18 | 0.42 |
| 1:AA:301:G:H2' | 1:AA:302:G:C8 | 2.52 | 0.42 |
| 1:AA:36:C:H5'' | 11:AL:119:LYS:HD2 | 2.01 | 0.42 |
| 1:AA:64:G:H4' | 1:AA:65:A:H3' | 2.02 | 0.42 |
| 1:AA:939:G:H2' | 1:AA:940:C:C6 | 2.54 | 0.42 |
| 1:AA:993:G:O2' | 1:AA:994:A:N7 | 2.53 | 0.42 |
| 2:AC:154:GLY:HA2 | 2:AC:163:ARG:H | 1.84 | 0.42 |
| 3:AD:18:LEU:HG | 3:AD:63:ILE:HG12 | 2.02 | 0.42 |
| 3:AD:78:ALA:HB1 | 3:AD:85:THR:O | 2.19 | 0.42 |
| 4:AE:82:HIS:HE1 | 4:AE:147:ASN:H | 1.68 | 0.42 |
| 6:AG:49:LEU:HD21 | 6:AG:60:ALA:CB | 2.46 | 0.42 |
| 6:AG:67:ASN:O | 6:AG:134:VAL:HA | 2.19 | 0.42 |
| 8:AI:35:GLU:O | 8:AI:39:GLY:HA3 | 2.20 | 0.42 |
| 9:AJ:52:LEU:HB2 | 13:AN:80:ARG:NE | 2.35 | 0.42 |
| 9:AJ:6:ILE:HD12 | 9:AJ:76:ILE:HD11 | 2.01 | 0.42 |
| 15:AP:20:VAL:HG21 | 15:AP:32:PHE:CD2 | 2.54 | 0.42 |
| 16:AQ:30:HIS:CG | 16:AQ:33:TYR:HB2 | 2.54 | 0.42 |
| 16:AQ:60:ILE:HD13 | 16:AQ:60:ILE:N | 2.34 | 0.42 |
| 1:AA:1320:C:N4 | 18:AS:36:ARG:HA | 2.34 | 0.42 |
| 18:AS:39:ILE:HD13 | 18:AS:65:MET:HB3 | 2.01 | 0.42 |
| 21:AU:20:ARG:C | 21:AU:22:CYS:H | 2.21 | 0.42 |
| 50:B3:31:ILE:C | 50:B3:32:LEU:HG | 2.40 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1234:U:H2' | 23:BB:1235:G:O4' | 2.20 | 0.42 |
| 23:BB:170:U:O2' | 23:BB:171:U:H5' | 2.19 | 0.42 |
| 23:BB:183:C:O2 | 23:BB:432:A:H2 | 2.02 | 0.42 |
| 23:BB:2082:A:N6 | 23:BB:2237:G:H1' | 2.35 | 0.42 |
| 23:BB:19:A:H2' | 23:BB:20:C:H6 | 1.85 | 0.42 |
| 23:BB:230:G:H2' | 23:BB:231:A:C8 | 2.55 | 0.42 |
| 23:BB:2846:G:H2' | 23:BB:2847:U:O4' | 2.20 | 0.42 |
| 23:BB:625:G:O2' | 23:BB:626:A:H5' | 2.20 | 0.42 |
| 23:BB:68:G:H2' | 23:BB:69:C:H6 | 1.85 | 0.42 |
| 23:BB:708:G:N2 | 23:BB:724:U:H1' | 2.34 | 0.42 |
| 23:BB:924:G:H2' | 23:BB:925:A:C8 | 2.54 | 0.42 |
| 25:BC:141:HIS:CG | 25:BC:142:ASN:N | 2.87 | 0.42 |
| 27:BE:102:ARG:HG3 | 27:BE:102:ARG:HH21 | 1.84 | 0.42 |
| 27:BE:109:LEU:HD13 | 27:BE:180:LEU:HD13 | 2.02 | 0.42 |
| 27:BE:128:ALA:O | 27:BE:133:LEU:HD12 | 2.19 | 0.42 |
| 27:BE:200:LEU:HD22 | 27:BE:200:LEU:N | 2.35 | 0.42 |
| 28:BF:31:GLU:HB2 | 28:BF:158:THR:HG22 | 2.00 | 0.42 |
| 31:BJ:74:TYR:HE2 | 31:BJ:103:ILE:HD11 | 1.84 | 0.42 |
| 31:BJ:57:LEU:HD11 | 31:BJ:129:GLU:N | 2.29 | 0.42 |
| 31:BJ:77:HIS:HD2 | 31:BJ:84:ILE:N | 2.09 | 0.42 |
| 32:BK:111:LYS:HD3 | 32:BK:111:LYS:N | 2.35 | 0.42 |
| 35:BN:30:ARG:NH2 | 35:BN:72:ASP:OD1 | 2.53 | 0.42 |
| 38:BQ:83:LYS:HA | 38:BQ:87:VAL:O | 2.19 | 0.42 |
| 41:BT:22:THR:O | 41:BT:25:GLU:HB3 | 2.19 | 0.42 |
| 43:BW:59:PHE:CD2 | 43:BW:61:LYS:HG3 | 2.55 | 0.42 |
| 46:BZ:18:ARG:HA | 46:BZ:23:ASN:O | 2.19 | 0.42 |
| 1:CA:1007:U:H2' | 1:CA:1008:U:H6 | 1.84 | 0.42 |
| 1:CA:1033:G:H2' | 1:CA:1034:G:H5'' | 2.01 | 0.42 |
| 1:CA:1306:A:C2' | 1:CA:1307:U:H5' | 2.49 | 0.42 |
| 1:CA:1476:A:O2' | 1:CA:1477:U:H5' | 2.20 | 0.42 |
| 1:CA:279:A:H5' | 1:CA:281:G:O4' | 2.19 | 0.42 |
| 1:CA:523:A:H61 | 11:CL:88:ASP:HB2 | 1.85 | 0.42 |
| 1:CA:553:A:O2' | 11:CL:25:ALA:HB1 | 2.20 | 0.42 |
| 1:CA:688:G:O3' | 10:CK:45:THR:HG21 | 2.20 | 0.42 |
| 1:CA:87:C:H2' | 1:CA:88:U:C5 | 2.55 | 0.42 |
| 20:CB:83:ALA:C | 20:CB:85:SER:H | 2.23 | 0.42 |
| 10:CK:15:VAL:C | 10:CK:17:ASP:H | 2.23 | 0.42 |
| 19:CT:32:LYS:O | 19:CT:35:TYR:N | 2.52 | 0.42 |
| 48:D1:10:LEU:HB3 | 48:D1:48:TYR:HB3 | 2.02 | 0.42 |
| 23:DB:1131:G:O2' | 23:DB:1133:A:N7 | 2.52 | 0.42 |
| 23:DB:1891:G:H2' | 23:DB:1892:C:H6 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:215:G:C4' | 23:DB:216:A:H4' | 2.47 | 0.42 |
| 23:DB:2215:C:H2' | 23:DB:2216:G:C8 | 2.55 | 0.42 |
| 23:DB:2283:C:H2' | 23:DB:2284:A:H5' | 2.01 | 0.42 |
| 23:DB:2721:A:H2' | 23:DB:2722:G:H8 | 1.84 | 0.42 |
| 23:DB:2838:G:C4 | 23:DB:2839:G:C8 | 3.07 | 0.42 |
| 23:DB:329:G:H1 | 42:DU:16:LYS:HE3 | 1.84 | 0.42 |
| 23:DB:346:A:H3' | 23:DB:347:A:H8 | 1.84 | 0.42 |
| 23:DB:374:A:N6 | 23:DB:400:G:H1' | 2.35 | 0.42 |
| 23:DB:26:G:H1' | 23:DB:514:A:N6 | 2.34 | 0.42 |
| 23:DB:548:G:O2' | 23:DB:549:G:H5'' | 2.20 | 0.42 |
| 23:DB:912:C:H2' | 23:DB:913:U:C6 | 2.54 | 0.42 |
| 23:DB:981:A:H4' | 23:DB:2037:A:H5' | 2.02 | 0.42 |
| 25:DC:119:VAL:HG13 | 25:DC:133:ASN:HD21 | 1.84 | 0.42 |
| 25:DC:153:LEU:HD22 | 25:DC:175:LEU:HD22 | 2.01 | 0.42 |
| 28:DF:109:ARG:HB3 | 28:DF:135:ILE:HD12 | 2.00 | 0.42 |
| 28:DF:11:VAL:HG13 | 28:DF:171:ALA:HB1 | 2.01 | 0.42 |
| 28:DF:33:ILE:HB | 28:DF:90:LEU:CG | 2.49 | 0.42 |
| 28:DF:90:LEU:HB3 | 28:DF:95:MET:HB2 | 2.02 | 0.42 |
| 31:DJ:6:ALA:HB3 | 31:DJ:45:THR:CG2 | 2.44 | 0.42 |
| 33:DL:138:ALA:O | 33:DL:139:GLY:C | 2.58 | 0.42 |
| 34:DM:66:ARG:HB3 | 34:DM:101:VAL:HG13 | 2.01 | 0.42 |
| 34:DM:108:VAL:CG1 | 34:DM:112:LEU:HD12 | 2.49 | 0.42 |
| 35:DN:33:ILE:HG22 | 35:DN:114:GLU:CB | 2.44 | 0.42 |
| 35:DN:47:VAL:O | 35:DN:51:LEU:HD13 | 2.20 | 0.42 |
| 36:DO:100:HIS:ND1 | 36:DO:101:GLY:N | 2.68 | 0.42 |
| 37:DP:89:GLY:N | 37:DP:112:ARG:HH12 | 2.17 | 0.42 |
| 23:DB:2847:U:OP1 | 37:DP:95:LYS:HD3 | 2.19 | 0.42 |
| 39:DR:19:THR:HG22 | 39:DR:97:LYS:HD2 | 2.01 | 0.42 |
| 40:DS:2:GLU:O | 40:DS:3:THR:C | 2.58 | 0.42 |
| 42:DU:85:ARG:O | 42:DU:92:VAL:HB | 2.20 | 0.42 |
| 44:DX:35:GLY:O | 44:DX:36:GLN:C | 2.57 | 0.42 |
| 46:DZ:21:ALA:C | 46:DZ:22:LEU:HG | 2.39 | 0.42 |
| 46:DZ:38:PHE:CE2 | 46:DZ:51:VAL:HG21 | 2.55 | 0.42 |
| 1:AA:1036:A:H2' | 1:AA:1037:C:O4' | 2.19 | 0.42 |
| 1:AA:1136:C:H2' | 1:AA:1136:C:O2 | 2.19 | 0.42 |
| 1:AA:1202:U:H2' | 1:AA:1203:C:H5' | 2.02 | 0.42 |
| 1:AA:300:A:H2' | 1:AA:301:G:O4' | 2.19 | 0.42 |
| 1:AA:438:U:H4' | 3:AD:119:HIS:HD2 | 1.85 | 0.42 |
| 1:AA:614:C:O2' | 1:AA:615:G:H5' | 2.20 | 0.42 |
| 1:AA:821:G:O2' | 1:AA:822:U:H5' | 2.20 | 0.42 |
| 1:AA:958:A:N1 | 18:AS:53:GLY:C | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:984:C:H2' | 1:AA:985:C:H6 | 1.85 | 0.42 |
| 20:AB:137:THR:O | 20:AB:141:GLU:HG3 | 2.20 | 0.42 |
| 2:AC:78:LYS:HE3 | 2:AC:79:LYS:HZ3 | 1.84 | 0.42 |
| 5:AF:47:LEU:HD13 | 5:AF:51:ILE:CG2 | 2.50 | 0.42 |
| 5:AF:44:ARG:HA | 5:AF:57:ALA:O | 2.20 | 0.42 |
| 5:AF:51:ILE:CD1 | 5:AF:86:ARG:HG3 | 2.50 | 0.42 |
| 6:AG:129:ASN:CA | 6:AG:134:VAL:HG21 | 2.49 | 0.42 |
| 8:AI:93:LEU:HD13 | 8:AI:97:LEU:CD1 | 2.47 | 0.42 |
| 10:AK:124:LYS:HA | 21:AU:34:ARG:CG | 2.49 | 0.42 |
| 1:AA:706:A:C4' | 10:AK:30:ILE:HD11 | 2.48 | 0.42 |
| 11:AL:79:ILE:C | 11:AL:101:LEU:HD12 | 2.40 | 0.42 |
| 11:AL:82:ARG:HG2 | 11:AL:82:ARG:NH1 | 2.35 | 0.42 |
| 14:AO:49:HIS:O | 14:AO:52:ARG:HB3 | 2.20 | 0.42 |
| 1:AA:564:C:C4 | 16:AQ:32:ILE:HD11 | 2.55 | 0.42 |
| 19:AT:54:GLN:O | 19:AT:57:VAL:HG23 | 2.20 | 0.42 |
| 49:B2:9:VAL:HG13 | 49:B2:10:LEU:N | 2.34 | 0.42 |
| 23:BB:104:A:H2' | 23:BB:105:C:O4' | 2.19 | 0.42 |
| 23:BB:1060:U:C1' | 23:BB:1062:G:H5' | 2.50 | 0.42 |
| 23:BB:106:C:H2' | 23:BB:107:G:C8 | 2.54 | 0.42 |
| 23:BB:1161:C:H2' | 23:BB:1162:G:H8 | 1.85 | 0.42 |
| 23:BB:1214:A:H2' | 23:BB:1215:G:H8 | 1.85 | 0.42 |
| 23:BB:1344:U:O2' | 23:BB:1385:A:H2' | 2.20 | 0.42 |
| 23:BB:1714:U:HO2' | 23:BB:1715:G:P | 2.43 | 0.42 |
| 23:BB:1910:G:H2' | 23:BB:1911:U:O4' | 2.19 | 0.42 |
| 23:BB:2081:U:H2' | 23:BB:2082:A:C8 | 2.55 | 0.42 |
| 23:BB:20:C:H2' | 23:BB:21:A:C8 | 2.54 | 0.42 |
| 23:BB:212:G:H2' | 23:BB:213:A:C8 | 2.54 | 0.42 |
| 23:BB:2409:G:H2' | 23:BB:2410:G:O4' | 2.19 | 0.42 |
| 23:BB:2676:C:O2' | 23:BB:2677:G:H5' | 2.20 | 0.42 |
| 23:BB:2733:A:H3' | 23:BB:2733:A:C8 | 2.54 | 0.42 |
| 23:BB:2795:C:O5' | 23:BB:2795:C:H6 | 2.03 | 0.42 |
| 23:BB:335:C:H2' | 23:BB:336:C:H6 | 1.85 | 0.42 |
| 23:BB:560:C:H3' | 23:BB:561:G:C8 | 2.55 | 0.42 |
| 23:BB:717:C:C3' | 23:BB:718:A:H5'' | 2.48 | 0.42 |
| 27:BE:150:THR:HG22 | 27:BE:170:ARG:O | 2.20 | 0.42 |
| 28:BF:137:PHE:O | 28:BF:139:GLU:N | 2.53 | 0.42 |
| 28:BF:1:ALA:HB1 | 28:BF:4:HIS:HB3 | 2.01 | 0.42 |
| 28:BF:83:PRO:O | 28:BF:84:ILE:HD12 | 2.20 | 0.42 |
| 28:BF:33:ILE:HB | 28:BF:90:LEU:CG | 2.50 | 0.42 |
| 29:BG:33:THR:HB | 29:BG:74:MET:HG2 | 2.02 | 0.42 |
| 30:BH:68:ARG:HB2 | 30:BH:134:VAL:HG23 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:BI:11:GLN:NE2 | 52:BI:74:PRO:HG2 | 2.35 | 0.42 |
| 31:BJ:30:THR:N | 31:BJ:108:MET:HE3 | 2.35 | 0.42 |
| 31:BJ:14:ASP:O | 31:BJ:53:TYR:N | 2.51 | 0.42 |
| 31:BJ:38:GLY:O | 31:BJ:43:GLU:HB2 | 2.20 | 0.42 |
| 33:BL:75:ALA:HB2 | 33:BL:101:ILE:HG23 | 2.02 | 0.42 |
| 23:BB:670:A:H5' | 33:BL:42:SER:HB2 | 2.01 | 0.42 |
| 34:BM:18:ARG:C | 34:BM:38:ARG:HH22 | 2.23 | 0.42 |
| 35:BN:87:PHE:C | 35:BN:89:SER:H | 2.23 | 0.42 |
| 37:BP:50:ARG:O | 37:BP:51:ASN:HB2 | 2.19 | 0.42 |
| 39:BR:86:GLN:HE21 | 39:BR:86:GLN:HB2 | 1.54 | 0.42 |
| 40:BS:60:HIS:O | 40:BS:61:ASN:HB2 | 2.19 | 0.42 |
| 40:BS:85:ILE:N | 40:BS:85:ILE:HD12 | 2.34 | 0.42 |
| 41:BT:62:VAL:HG12 | 41:BT:63:VAL:N | 2.34 | 0.42 |
| 41:BT:66:LYS:N | 41:BT:76:ARG:HH21 | 2.18 | 0.42 |
| 42:BU:14:THR:HG23 | 42:BU:15:GLY:N | 2.35 | 0.42 |
| 42:BU:43:LYS:HD3 | 42:BU:44:HIS:N | 2.33 | 0.42 |
| 43:BW:35:ILE:O | 43:BW:37:VAL:N | 2.53 | 0.42 |
| 44:BX:23:ARG:HD2 | 44:BX:27:ASN:ND2 | 2.32 | 0.42 |
| 46:BZ:58:VAL:O | 46:BZ:62:LYS:N | 2.43 | 0.42 |
| 1:CA:152:A:H3' | 1:CA:153:C:H6 | 1.85 | 0.42 |
| 1:CA:430:A:C2' | 1:CA:431:A:H5' | 2.50 | 0.42 |
| 30:BH:8:LYS:HE3 | 1:CA:495:A:OP1 | 2.19 | 0.42 |
| 20:CB:127:LYS:CD | 20:CB:128:LEU:HD13 | 2.50 | 0.42 |
| 4:CE:71:ILE:HG21 | 4:CE:144:GLU:OE2 | 2.20 | 0.42 |
| 4:CE:25:LYS:HG3 | 4:CE:26:GLY:H | 1.85 | 0.42 |
| 7:CH:24:VAL:CG1 | 7:CH:60:LEU:HB3 | 2.49 | 0.42 |
| 1:CA:586:C:O2' | 7:CH:3:GLN:NE2 | 2.53 | 0.42 |
| 8:CI:19:PHE:HB2 | 8:CI:63:TYR:O | 2.19 | 0.42 |
| 12:CM:72:ILE:O | 12:CM:76:ILE:HG13 | 2.19 | 0.42 |
| 14:CO:8:ALA:O | 14:CO:11:VAL:HB | 2.20 | 0.42 |
| 19:CT:75:LYS:O | 19:CT:76:ALA:C | 2.59 | 0.42 |
| 51:D4:3:VAL:O | 51:D4:4:ARG:HB2 | 2.19 | 0.42 |
| 23:DB:1028:A:N6 | 23:DB:1125:G:H2' | 2.35 | 0.42 |
| 23:DB:1210:G:H5' | 23:DB:1212:G:C4' | 2.49 | 0.42 |
| 23:DB:1280:G:C2' | 23:DB:1281:G:H5' | 2.49 | 0.42 |
| 23:DB:1401:G:H2' | 23:DB:1402:U:H6 | 1.85 | 0.42 |
| 23:DB:1441:G:H2' | 23:DB:1442:U:H6 | 1.83 | 0.42 |
| 23:DB:1662:U:H2' | 23:DB:1663:G:O4' | 2.20 | 0.42 |
| 23:DB:169:G:O2' | 23:DB:170:U:H5' | 2.19 | 0.42 |
| 23:DB:1831:G:C6 | 23:DB:1832:C:N4 | 2.88 | 0.42 |
| 23:DB:1847:A:H1' | 23:DB:1848:A:N7 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1914:C:O2' | 23:DB:1915:U:C5' | 2.68 | 0.42 |
| 23:DB:2260:C:O2' | 23:DB:2261:C:H5' | 2.20 | 0.42 |
| 23:DB:2419:U:H2' | 23:DB:2420:C:C6 | 2.55 | 0.42 |
| 23:DB:26:G:H2' | 23:DB:27:G:C1' | 2.50 | 0.42 |
| 23:DB:2622:U:O2' | 23:DB:2825:G:N7 | 2.53 | 0.42 |
| 23:DB:1:G:H2' | 23:DB:2:G:C8 | 2.54 | 0.42 |
| 23:DB:321:U:O4' | 27:DE:159:LEU:HG | 2.19 | 0.42 |
| 23:DB:227:A:H61 | 23:DB:410:G:H1' | 1.84 | 0.42 |
| 23:DB:504:A:HO2' | 23:DB:505:A:P | 2.42 | 0.42 |
| 23:DB:55:G:H2' | 23:DB:56:A:C8 | 2.55 | 0.42 |
| 23:DB:850:U:O3' | 45:DY:22:THR:HG22 | 2.19 | 0.42 |
| 23:DB:969:G:H2' | 23:DB:970:U:H6 | 1.85 | 0.42 |
| 23:DB:1490:A:H2' | 25:DC:97:ASP:CG | 2.41 | 0.42 |
| 26:DD:121:THR:C | 26:DD:123:LYS:N | 2.72 | 0.42 |
| 26:DD:26:VAL:HG13 | 26:DD:188:LEU:CD2 | 2.50 | 0.42 |
| 26:DD:27:ILE:HG23 | 26:DD:201:LEU:HD12 | 2.02 | 0.42 |
| 27:DE:147:LEU:O | 27:DE:147:LEU:HD13 | 2.20 | 0.42 |
| 23:DB:2667:C:HO2' | 29:DG:108:PHE:HD2 | 1.68 | 0.42 |
| 29:DG:89:VAL:HG21 | 29:DG:162:ARG:HH11 | 1.84 | 0.42 |
| 23:DB:1099:G:C8 | 52:DI:3:LYS:CB | 3.03 | 0.42 |
| 32:DK:41:ILE:CG1 | 32:DK:42:THR:N | 2.82 | 0.42 |
| 33:DL:98:ALA:O | 33:DL:99:ASN:C | 2.59 | 0.42 |
| 34:DM:124:LEU:HA | 34:DM:125:PRO:HD3 | 1.87 | 0.42 |
| 34:DM:18:ARG:C | 34:DM:38:ARG:HH22 | 2.23 | 0.42 |
| 36:DO:36:TYR:N | 36:DO:36:TYR:CD2 | 2.87 | 0.42 |
| 37:DP:4:ILE:O | 37:DP:5:LYS:HB2 | 2.20 | 0.42 |
| 38:DQ:71:ASN:ND2 | 38:DQ:72:GLY:N | 2.68 | 0.42 |
| 38:DQ:87:VAL:HB | 39:DR:52:PRO:HG3 | 2.02 | 0.42 |
| 40:DS:57:ASN:HD22 | 40:DS:57:ASN:HA | 1.59 | 0.42 |
| 43:DW:18:LYS:HG3 | 43:DW:19:ARG:CZ | 2.49 | 0.42 |
| 1:AA:1013:G:H2' | 1:AA:1015:G:OP2 | 2.20 | 0.42 |
| 1:AA:1046:A:H2' | 1:AA:1047:G:O4' | 2.20 | 0.42 |
| 1:AA:1194:U:H5' | 4:AE:26:GLY:O | 2.20 | 0.42 |
| 1:AA:1225:A:H5'' | 1:AA:1226:C:C5 | 2.55 | 0.42 |
| 1:AA:317:U:H2' | 1:AA:318:G:C8 | 2.54 | 0.42 |
| 1:AA:450:G:N7 | 1:AA:481:G:O6 | 2.52 | 0.42 |
| 1:AA:564:C:H1' | 16:AQ:32:ILE:O | 2.19 | 0.42 |
| 1:AA:647:C:H2' | 1:AA:648:A:H8 | 1.85 | 0.42 |
| 1:AA:828:U:H2' | 1:AA:829:G:O5' | 2.20 | 0.42 |
| 1:AA:978:A:H5' | 1:AA:1362:A:H62 | 1.84 | 0.42 |
| 20:AB:8:MET:O | 20:AB:11:ALA:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AB:164:ASP:OD1 | 20:AB:186:VAL:HA | 2.20 | 0.42 |
| 20:AB:68:PHE:CE1 | 20:AB:88:GLN:HB3 | 2.55 | 0.42 |
| 2:AC:38:VAL:HG23 | 2:AC:39:ARG:N | 2.34 | 0.42 |
| 6:AG:70:PRO:HD2 | 6:AG:95:ARG:O | 2.20 | 0.42 |
| 8:AI:19:PHE:HB2 | 8:AI:63:TYR:O | 2.20 | 0.42 |
| 9:AJ:26:VAL:HG12 | 9:AJ:30:LYS:HG3 | 2.02 | 0.42 |
| 10:AK:125:LYS:O | 21:AU:33:ARG:NH2 | 2.53 | 0.42 |
| 21:AU:36:PHE:CE1 | 21:AU:44:ARG:HD3 | 2.55 | 0.42 |
| 51:B4:11:CYS:HB3 | 51:B4:33:HIS:HE1 | 1.84 | 0.42 |
| 23:BB:1028:A:N3 | 23:BB:2486:C:O2' | 2.39 | 0.42 |
| 23:BB:1116:G:H2' | 23:BB:1117:C:H6 | 1.85 | 0.42 |
| 23:BB:1795:C:H2' | 23:BB:1796:U:C6 | 2.55 | 0.42 |
| 23:BB:1936:A:H2 | 23:BB:1943:U:O4 | 2.03 | 0.42 |
| 23:BB:2000:C:O2' | 23:BB:2001:C:H5' | 2.19 | 0.42 |
| 23:BB:2069:G:O2' | 23:BB:2070:A:H5' | 2.20 | 0.42 |
| 23:BB:2669:G:O2' | 23:BB:2670:A:H5' | 2.20 | 0.42 |
| 23:BB:279:A:H8 | 23:BB:279:A:P | 2.43 | 0.42 |
| 23:BB:2840:C:H5'' | 35:BN:53:THR:CG2 | 2.50 | 0.42 |
| 23:BB:2899:A:H2' | 23:BB:2900:A:H8 | 1.84 | 0.42 |
| 23:BB:616:A:H3' | 23:BB:617:G:C8 | 2.43 | 0.42 |
| 23:BB:709:U:H2' | 23:BB:710:U:H6 | 1.85 | 0.42 |
| 23:BB:727:A:H2' | 23:BB:728:G:C8 | 2.55 | 0.42 |
| 23:BB:995:C:H42 | 31:BJ:2:LYS:HB2 | 1.84 | 0.42 |
| 25:BC:245:THR:O | 25:BC:247:TRP:N | 2.53 | 0.42 |
| 27:BE:118:LEU:HA | 27:BE:186:VAL:HG13 | 2.02 | 0.42 |
| 27:BE:31:VAL:O | 27:BE:34:ALA:HB3 | 2.20 | 0.42 |
| 27:BE:38:GLY:C | 27:BE:40:ARG:H | 2.22 | 0.42 |
| 27:BE:61:ARG:O | 27:BE:62:GLN:C | 2.58 | 0.42 |
| 28:BF:37:MET:HG3 | 28:BF:52:ALA:HB1 | 2.01 | 0.42 |
| 30:BH:69:ALA:C | 30:BH:71:LYS:N | 2.73 | 0.42 |
| 31:BJ:36:LEU:HD11 | 31:BJ:121:LYS:HB2 | 2.02 | 0.42 |
| 23:BB:7:G:OP1 | 31:BJ:132:HIS:HE1 | 2.02 | 0.42 |
| 33:BL:123:ARG:HD2 | 33:BL:123:ARG:C | 2.40 | 0.42 |
| 33:BL:81:ASP:HA | 33:BL:84:LYS:CD | 2.49 | 0.42 |
| 33:BL:98:ALA:O | 33:BL:99:ASN:C | 2.58 | 0.42 |
| 34:BM:126:ILE:HG22 | 34:BM:127:LYS:N | 2.35 | 0.42 |
| 38:BQ:107:ALA:C | 39:BR:48:LYS:HD3 | 2.40 | 0.42 |
| 39:BR:71:LYS:HG2 | 39:BR:73:LYS:HZ1 | 1.81 | 0.42 |
| 40:BS:33:LEU:HD23 | 40:BS:51:LEU:HD23 | 2.01 | 0.42 |
| 40:BS:55:ILE:HD12 | 40:BS:69:LEU:HD23 | 2.00 | 0.42 |
| 42:BU:96:LYS:C | 42:BU:98:ASN:H | 2.23 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:BW:15:SER:O | 43:BW:16:GLU:C | 2.58 | 0.42 |
| 46:BZ:53:ALA:O | 46:BZ:54:LYS:HB3 | 2.19 | 0.42 |
| 1:CA:1229:A:H2' | 1:CA:1230:C:H6 | 1.83 | 0.42 |
| 1:CA:1346:A:H61 | 1:CA:1374:A:H3' | 1.84 | 0.42 |
| 1:CA:1499:A:H1' | 1:CA:1520:C:OP1 | 2.20 | 0.42 |
| 1:CA:152:A:H3' | 1:CA:153:C:C6 | 2.55 | 0.42 |
| 1:CA:277:C:O2' | 1:CA:278:G:H5' | 2.19 | 0.42 |
| 1:CA:499:A:C2 | 1:CA:546:A:N3 | 2.88 | 0.42 |
| 1:CA:58:C:C2' | 1:CA:59:A:H5' | 2.50 | 0.42 |
| 1:CA:704:A:C2 | 1:CA:705:G:H1' | 2.54 | 0.42 |
| 1:CA:711:G:O2' | 1:CA:712:A:H5' | 2.20 | 0.42 |
| 1:CA:822:U:H2' | 1:CA:823:C:C6 | 2.54 | 0.42 |
| 1:CA:853:C:O2' | 1:CA:854:U:H5' | 2.19 | 0.42 |
| 2:CC:111:ASP:HB3 | 2:CC:114:LEU:HD12 | 2.02 | 0.42 |
| 2:CC:38:VAL:HG23 | 2:CC:39:ARG:N | 2.35 | 0.42 |
| 2:CC:76:ILE:O | 2:CC:82:ASP:N | 2.53 | 0.42 |
| 3:CD:48:SER:O | 3:CD:52:VAL:HG23 | 2.19 | 0.42 |
| 6:CG:130:LYS:N | 6:CG:134:VAL:HG21 | 2.35 | 0.42 |
| 8:CI:32:ARG:HD3 | 8:CI:37:TYR:HD1 | 1.85 | 0.42 |
| 9:CJ:92:LEU:HD22 | 9:CJ:92:LEU:N | 2.35 | 0.42 |
| 16:CQ:52:CYS:SG | 16:CQ:77:VAL:HG22 | 2.60 | 0.42 |
| 22:DA:32:U:H2' | 22:DA:33:G:H8 | 1.85 | 0.42 |
| 23:DB:1207:C:H2' | 23:DB:1208:C:C6 | 2.55 | 0.42 |
| 23:DB:1448:G:H2' | 23:DB:1449:G:H8 | 1.85 | 0.42 |
| 23:DB:1637:A:H2' | 23:DB:1638:C:C6 | 2.55 | 0.42 |
| 23:DB:776:G:N1 | 23:DB:2072:C:OP1 | 2.41 | 0.42 |
| 23:DB:2301:C:H2' | 23:DB:2302:U:C6 | 2.55 | 0.42 |
| 23:DB:234:U:H2' | 23:DB:235:U:H6 | 1.85 | 0.42 |
| 23:DB:256:A:O2' | 23:DB:257:C:H5' | 2.19 | 0.42 |
| 23:DB:404:A:H4' | 23:DB:405:U:C5' | 2.44 | 0.42 |
| 23:DB:441:U:O2' | 23:DB:442:G:H5' | 2.20 | 0.42 |
| 23:DB:68:G:O2' | 23:DB:69:C:H5' | 2.19 | 0.42 |
| 23:DB:841:G:O2' | 23:DB:842:U:H5' | 2.20 | 0.42 |
| 23:DB:924:G:H2' | 23:DB:925:A:C8 | 2.54 | 0.42 |
| 23:DB:936:A:O2' | 23:DB:937:C:H5' | 2.20 | 0.42 |
| 25:DC:128:THR:HG22 | 25:DC:188:ARG:HB3 | 2.02 | 0.42 |
| 25:DC:67:LYS:O | 25:DC:188:ARG:HD3 | 2.20 | 0.42 |
| 26:DD:35:THR:N | 26:DD:49:GLN:O | 2.51 | 0.42 |
| 28:DF:134:GLN:HE21 | 28:DF:134:GLN:HB3 | 1.62 | 0.42 |
| 29:DG:18:ILE:HA | 29:DG:22:VAL:O | 2.20 | 0.42 |
| 31:DJ:75:TYR:O | 31:DJ:76:HIS:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DK:99:ILE:HG12 | 32:DK:115:ILE:HG13 | 2.01 | 0.42 |
| 33:DL:61:LEU:HD23 | 50:D3:23:HIS:CG | 2.55 | 0.42 |
| 36:DO:7:ARG:HH11 | 36:DO:7:ARG:CG | 2.33 | 0.42 |
| 38:DQ:93:ILE:HG23 | 38:DQ:94:LEU:N | 2.35 | 0.42 |
| 39:DR:79:ARG:HD2 | 39:DR:80:ARG:HH21 | 1.84 | 0.42 |
| 40:DS:24:ILE:O | 40:DS:25:ARG:C | 2.58 | 0.42 |
| 1:AA:1386:G:H2' | 1:AA:1387:G:H8 | 1.85 | 0.41 |
| 1:AA:1504:G:H3' | 56:AA:2144:HOH:O | 2.20 | 0.41 |
| 1:AA:33:A:O2' | 1:AA:34:C:H5' | 2.20 | 0.41 |
| 1:AA:35:G:H2' | 1:AA:36:C:H6 | 1.80 | 0.41 |
| 1:AA:560:A:H5' | 1:AA:566:G:N2 | 2.35 | 0.41 |
| 1:AA:742:G:H2' | 1:AA:743:A:C8 | 2.53 | 0.41 |
| 1:AA:817:C:C2 | 1:AA:819:A:O4' | 2.73 | 0.41 |
| 1:AA:878:A:H5'' | 7:AH:80:PRO:HG2 | 2.02 | 0.41 |
| 20:AB:165:ALA:H | 20:AB:186:VAL:HG12 | 1.85 | 0.41 |
| 20:AB:25:LYS:HD3 | 20:AB:193:ASP:OD2 | 2.20 | 0.41 |
| 20:AB:46:VAL:CG1 | 20:AB:47:PRO:HD3 | 2.34 | 0.41 |
| 5:AF:6:ILE:HD12 | 5:AF:7:VAL:N | 2.34 | 0.41 |
| 7:AH:118:ALA:HB3 | 7:AH:120:LEU:CD2 | 2.50 | 0.41 |
| 1:AA:1152:A:H4' | 9:AJ:15:HIS:HD2 | 1.85 | 0.41 |
| 9:AJ:42:LEU:CD1 | 9:AJ:73:LEU:HB2 | 2.39 | 0.41 |
| 11:AL:53:ARG:HG2 | 11:AL:61:GLU:OE1 | 2.20 | 0.41 |
| 11:AL:56:LEU:HG | 11:AL:60:PHE:O | 2.20 | 0.41 |
| 12:AM:26:LYS:O | 12:AM:30:LYS:HB2 | 2.20 | 0.41 |
| 13:AN:53:ASP:HA | 13:AN:58:ARG:NE | 2.35 | 0.41 |
| 18:AS:42:ASN:H | 18:AS:42:ASN:HD22 | 1.67 | 0.41 |
| 48:B1:38:PHE:O | 48:B1:40:PRO:HD3 | 2.20 | 0.41 |
| 49:B2:19:ARG:NH2 | 49:B2:19:ARG:HG2 | 2.34 | 0.41 |
| 33:BL:61:LEU:HD23 | 50:B3:23:HIS:CG | 2.55 | 0.41 |
| 23:BB:2349:G:OP2 | 50:B3:41:ARG:HD3 | 2.19 | 0.41 |
| 23:BB:100:U:H2' | 23:BB:101:A:C8 | 2.55 | 0.41 |
| 23:BB:1046:A:H3' | 23:BB:1047:G:C5' | 2.49 | 0.41 |
| 23:BB:116:C:H2' | 23:BB:117:G:C8 | 2.55 | 0.41 |
| 23:BB:1306:C:O2' | 23:BB:1307:A:H5' | 2.19 | 0.41 |
| 23:BB:135:U:H2' | 23:BB:136:G:C8 | 2.55 | 0.41 |
| 23:BB:1409:U:O2' | 23:BB:1410:G:H5' | 2.19 | 0.41 |
| 23:BB:1681:G:N3 | 23:BB:1762:A:H2' | 2.34 | 0.41 |
| 23:BB:1827:U:C2' | 23:BB:1828:G:H5' | 2.50 | 0.41 |
| 1:AA:1408:A:HO2' | 23:BB:1916:A:H61 | 1.67 | 0.41 |
| 23:BB:2335:A:H2' | 23:BB:2336:A:H5'' | 2.02 | 0.41 |
| 23:BB:235:U:H2' | 23:BB:236:C:H6 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:2655:G:H1' | 23:BB:2656:U:H5 | 1.84 | 0.41 |
| 23:BB:2745:C:H3' | 23:BB:2746:U:C5 | 2.54 | 0.41 |
| 23:BB:445:C:H4' | 23:BB:1248:G:O6 | 2.20 | 0.41 |
| 22:BA:97:C:O2 | 23:BB:918:A:H4' | 2.20 | 0.41 |
| 23:BB:96:C:H2' | 23:BB:97:C:H6 | 1.85 | 0.41 |
| 26:BD:121:THR:C | 26:BD:123:LYS:N | 2.73 | 0.41 |
| 26:BD:61:THR:OG1 | 26:BD:64:GLU:HB2 | 2.19 | 0.41 |
| 27:BE:48:THR:C | 27:BE:50:ALA:N | 2.73 | 0.41 |
| 27:BE:34:ALA:CB | 27:BE:96:VAL:HG21 | 2.50 | 0.41 |
| 28:BF:105:ILE:O | 28:BF:109:ARG:HB2 | 2.20 | 0.41 |
| 28:BF:29:ARG:H | 28:BF:29:ARG:HD3 | 1.85 | 0.41 |
| 30:BH:129:GLU:C | 30:BH:131:SER:H | 2.24 | 0.41 |
| 30:BH:4:ILE:HG23 | 30:BH:17:ASP:N | 2.35 | 0.41 |
| 52:BI:38:CYS:O | 52:BI:42:ASN:ND2 | 2.53 | 0.41 |
| 32:BK:13:ASN:HD21 | 32:BK:98:ARG:N | 2.07 | 0.41 |
| 34:BM:59:ARG:CZ | 34:BM:60:GLN:HB3 | 2.49 | 0.41 |
| 35:BN:65:LEU:HD11 | 35:BN:69:ARG:NH2 | 2.35 | 0.41 |
| 36:BO:35:ILE:HG21 | 36:BO:71:ALA:HB1 | 2.02 | 0.41 |
| 37:BP:91:VAL:HG23 | 37:BP:92:ARG:N | 2.26 | 0.41 |
| 38:BQ:112:ALA:O | 38:BQ:113:LYS:C | 2.58 | 0.41 |
| 38:BQ:93:ILE:HG23 | 38:BQ:94:LEU:H | 1.85 | 0.41 |
| 38:BQ:92:LYS:O | 38:BQ:95:ALA:HB3 | 2.20 | 0.41 |
| 40:BS:24:ILE:O | 40:BS:25:ARG:C | 2.58 | 0.41 |
| 45:BY:6:ILE:HD13 | 45:BY:56:VAL:CG1 | 2.50 | 0.41 |
| 1:CA:1162:C:H2' | 1:CA:1163:A:O4' | 2.20 | 0.41 |
| 1:CA:222:C:H2' | 1:CA:223:A:C8 | 2.55 | 0.41 |
| 1:CA:54:C:N4 | 1:CA:352:C:H2' | 2.35 | 0.41 |
| 1:CA:43:C:H2' | 1:CA:44:A:O4' | 2.20 | 0.41 |
| 1:CA:635:A:H2' | 1:CA:636:U:C6 | 2.54 | 0.41 |
| 1:CA:67:C:H2' | 1:CA:68:G:H8 | 1.84 | 0.41 |
| 1:CA:926:G:N2 | 1:CA:1505:G:H2' | 2.35 | 0.41 |
| 1:CA:998:C:H2' | 1:CA:999:C:C6 | 2.56 | 0.41 |
| 20:CB:25:LYS:HD3 | 20:CB:193:ASP:OD2 | 2.20 | 0.41 |
| 3:CD:155:LYS:HG3 | 3:CD:156:ALA:N | 2.35 | 0.41 |
| 3:CD:159:GLU:C | 3:CD:161:ALA:H | 2.24 | 0.41 |
| 9:CJ:80:THR:CG2 | 9:CJ:82:LYS:HZ2 | 2.33 | 0.41 |
| 12:CM:43:LYS:C | 12:CM:45:SER:N | 2.74 | 0.41 |
| 49:D2:21:ARG:CD | 49:D2:43:THR:HG21 | 2.50 | 0.41 |
| 50:D3:14:LYS:O | 50:D3:15:LYS:C | 2.58 | 0.41 |
| 50:D3:49:VAL:HG11 | 50:D3:54:LEU:HA | 2.02 | 0.41 |
| 51:D4:11:CYS:HB3 | 51:D4:33:HIS:HE1 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:1180:U:H2' | 23:DB:1181:U:O4' | 2.20 | 0.41 |
| 23:DB:1187:G:H5'' | 39:DR:83:TYR:CE2 | 2.55 | 0.41 |
| 23:DB:1334:G:O2' | 23:DB:1335:C:H5' | 2.20 | 0.41 |
| 23:DB:1706:C:H2' | 23:DB:1757:A:OP2 | 2.19 | 0.41 |
| 23:DB:1727:C:H2' | 23:DB:1728:C:O4' | 2.20 | 0.41 |
| 23:DB:1998:A:H2' | 23:DB:1999:C:H6 | 1.84 | 0.41 |
| 23:DB:2219:U:H2' | 23:DB:2220:U:H6 | 1.85 | 0.41 |
| 23:DB:2314:A:H2' | 23:DB:2315:G:H8 | 1.84 | 0.41 |
| 23:DB:2478:A:H2' | 23:DB:2479:U:O4' | 2.20 | 0.41 |
| 23:DB:2586:U:H2' | 23:DB:2587:A:C8 | 2.54 | 0.41 |
| 23:DB:2743:U:H2' | 23:DB:2744:G:C5' | 2.41 | 0.41 |
| 23:DB:451:U:C2 | 23:DB:453:A:N7 | 2.88 | 0.41 |
| 23:DB:612:G:H2' | 23:DB:614:A:H5'' | 2.01 | 0.41 |
| 23:DB:649:G:H2' | 23:DB:650:C:C6 | 2.55 | 0.41 |
| 23:DB:811:U:O2 | 23:DB:1250:G:H3' | 2.19 | 0.41 |
| 25:DC:115:ILE:HA | 25:DC:124:LYS:HZ1 | 1.84 | 0.41 |
| 23:DB:1801:A:P | 25:DC:149:LYS:HZ3 | 2.43 | 0.41 |
| 26:DD:110:THR:O | 26:DD:201:LEU:HA | 2.20 | 0.41 |
| 27:DE:150:THR:OG1 | 27:DE:151:GLY:N | 2.52 | 0.41 |
| 27:DE:59:PRO:O | 27:DE:67:ARG:NH2 | 2.53 | 0.41 |
| 28:DF:65:LEU:HD23 | 28:DF:87:LYS:CD | 2.45 | 0.41 |
| 28:DF:8:LYS:HA | 28:DF:12:VAL:CG2 | 2.45 | 0.41 |
| 30:DH:90:LEU:HD12 | 30:DH:90:LEU:N | 2.35 | 0.41 |
| 31:DJ:35:ARG:HG3 | 31:DJ:40:HIS:HE2 | 1.85 | 0.41 |
| 32:DK:105:ARG:HH11 | 32:DK:122:VAL:CG1 | 2.33 | 0.41 |
| 32:DK:6:THR:HG22 | 32:DK:7:MET:H | 1.84 | 0.41 |
| 33:DL:118:THR:HA | 33:DL:119:PRO:HD3 | 1.91 | 0.41 |
| 34:DM:26:VAL:CG2 | 34:DM:133:LYS:HA | 2.50 | 0.41 |
| 36:DO:19:GLN:HB3 | 36:DO:19:GLN:HE21 | 1.62 | 0.41 |
| 36:DO:49:VAL:HG11 | 36:DO:82:ALA:CA | 2.44 | 0.41 |
| 37:DP:86:LYS:HB3 | 37:DP:87:ARG:H | 1.54 | 0.41 |
| 39:DR:39:LEU:HD22 | 39:DR:53:PHE:CD1 | 2.55 | 0.41 |
| 41:DT:45:ALA:HA | 41:DT:48:GLN:CG | 2.50 | 0.41 |
| 42:DU:71:ILE:HD11 | 42:DU:81:ARG:O | 2.19 | 0.41 |
| 45:DY:51:SER:HA | 45:DY:54:VAL:CG2 | 2.50 | 0.41 |
| 1:AA:1170:A:H3' | 1:AA:1171:A:H8 | 1.85 | 0.41 |
| 1:AA:1201:A:H4' | 1:AA:1202:U:O5' | 2.20 | 0.41 |
| 1:AA:1258:G:C2 | 1:AA:1278:G:N2 | 2.88 | 0.41 |
| 1:AA:1269:A:N6 | 1:AA:1313:U:H5' | 2.35 | 0.41 |
| 1:AA:1355:G:O2' | 1:AA:1356:G:H5' | 2.20 | 0.41 |
| 1:AA:285:C:O2' | 1:AA:286:C:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:621:A:H2' | 1:AA:622:A:H8 | 1.83 | 0.41 |
| 1:AA:697:U:O2 | 1:AA:798:U:H1' | 2.20 | 0.41 |
| 1:AA:857:C:H2' | 1:AA:858:G:O4' | 2.21 | 0.41 |
| 1:AA:91:U:H2' | 1:AA:92:U:O4' | 2.20 | 0.41 |
| 20:AB:75:ALA:O | 20:AB:76:SER:C | 2.59 | 0.41 |
| 20:AB:95:TRP:HH2 | 20:AB:100:LEU:HD22 | 1.86 | 0.41 |
| 2:AC:87:ARG:HB2 | 2:AC:100:ILE:HG22 | 2.02 | 0.41 |
| 2:AC:78:LYS:C | 2:AC:80:GLY:N | 2.73 | 0.41 |
| 4:AE:104:ILE:HG13 | 4:AE:122:VAL:HG23 | 2.02 | 0.41 |
| 4:AE:20:VAL:HG12 | 4:AE:21:SER:N | 2.35 | 0.41 |
| 5:AF:42:TRP:HE1 | 5:AF:61:LEU:CD2 | 2.33 | 0.41 |
| 5:AF:81:ASN:OD1 | 5:AF:83:ALA:HB3 | 2.20 | 0.41 |
| 7:AH:10:LEU:CD2 | 7:AH:74:ILE:HD11 | 2.49 | 0.41 |
| 8:AI:123:ARG:NH1 | 8:AI:123:ARG:HB3 | 2.34 | 0.41 |
| 8:AI:30:ASN:ND2 | 8:AI:65:THR:HA | 2.35 | 0.41 |
| 11:AL:43:LYS:HG3 | 11:AL:43:LYS:H | 1.65 | 0.41 |
| 13:AN:55:SER:HB2 | 13:AN:58:ARG:HD2 | 2.02 | 0.41 |
| 16:AQ:39:ARG:CZ | 16:AQ:39:ARG:HA | 2.50 | 0.41 |
| 18:AS:35:ARG:HB3 | 18:AS:50:VAL:CG1 | 2.49 | 0.41 |
| 47:B0:41:HIS:O | 47:B0:42:ILE:O | 2.38 | 0.41 |
| 22:BA:65:U:C2' | 22:BA:66:A:H5' | 2.49 | 0.41 |
| 23:BB:1184:U:O2' | 23:BB:1185:G:H5' | 2.20 | 0.41 |
| 23:BB:1210:G:H4' | 23:BB:1211:C:OP2 | 2.21 | 0.41 |
| 23:BB:1222:U:OP2 | 39:BR:90:ARG:NH2 | 2.53 | 0.41 |
| 23:BB:1248:G:C5 | 38:BQ:2:ARG:HD2 | 2.54 | 0.41 |
| 23:BB:1904:G:O2' | 23:BB:1905:C:H5' | 2.20 | 0.41 |
| 23:BB:191:A:O2' | 23:BB:192:C:H5' | 2.20 | 0.41 |
| 23:BB:2218:G:O2' | 23:BB:2219:U:H5' | 2.20 | 0.41 |
| 23:BB:2223:G:C2' | 23:BB:2224:G:H5' | 2.49 | 0.41 |
| 23:BB:250:G:H2' | 23:BB:251:A:C8 | 2.55 | 0.41 |
| 23:BB:2857:G:N2 | 23:BB:2859:G:H3' | 2.34 | 0.41 |
| 23:BB:288:U:O2' | 23:BB:289:G:H5' | 2.19 | 0.41 |
| 23:BB:317:G:H2' | 23:BB:318:C:H6 | 1.85 | 0.41 |
| 23:BB:829:A:H5' | 23:BB:831:G:N7 | 2.34 | 0.41 |
| 23:BB:993:G:H1' | 39:BR:91:GLN:NE2 | 2.35 | 0.41 |
| 25:BC:189:ALA:C | 25:BC:190:THR:HG23 | 2.40 | 0.41 |
| 26:BD:110:THR:O | 26:BD:201:LEU:HA | 2.19 | 0.41 |
| 26:BD:38:LYS:HD3 | 26:BD:45:TYR:OH | 2.20 | 0.41 |
| 27:BE:68:ALA:O | 27:BE:69:ARG:C | 2.58 | 0.41 |
| 29:BG:84:LYS:HG3 | 29:BG:131:VAL:CB | 2.50 | 0.41 |
| 29:BG:175:LYS:HD3 | 29:BG:175:LYS:HA | 1.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BI:37:PHE:HZ | 52:BI:56:VAL:HG11 | 1.85 | 0.41 |
| 52:BI:63:ASP:C | 52:BI:65:SER:N | 2.73 | 0.41 |
| 34:BM:135:VAL:HG12 | 34:BM:135:VAL:O | 2.20 | 0.41 |
| 35:BN:49:GLU:N | 35:BN:50:PRO:CD | 2.83 | 0.41 |
| 35:BN:51:LEU:O | 35:BN:54:LEU:HB3 | 2.20 | 0.41 |
| 35:BN:65:LEU:O | 35:BN:68:ALA:HB3 | 2.21 | 0.41 |
| 39:BR:79:ARG:O | 39:BR:81:LYS:HG2 | 2.20 | 0.41 |
| 24:BV:42:LEU:HB2 | 24:BV:47:VAL:HG21 | 2.02 | 0.41 |
| 45:BY:7:THR:O | 45:BY:54:VAL:HG12 | 2.19 | 0.41 |
| 1:CA:1029:U:H2' | 1:CA:1031:C:C2 | 2.55 | 0.41 |
| 1:CA:1148:U:H2' | 1:CA:1149:C:O4' | 2.20 | 0.41 |
| 1:CA:551:U:H2' | 1:CA:552:U:C6 | 2.54 | 0.41 |
| 1:CA:921:U:O2 | 4:CE:23:THR:HG23 | 2.20 | 0.41 |
| 1:CA:977:A:H1' | 1:CA:982:U:O4 | 2.20 | 0.41 |
| 20:CB:22:TRP:CZ3 | 20:CB:24:PRO:HA | 2.55 | 0.41 |
| 20:CB:93:HIS:O | 20:CB:94:ARG:HG2 | 2.19 | 0.41 |
| 2:CC:154:GLY:HA2 | 2:CC:163:ARG:O | 2.20 | 0.41 |
| 2:CC:75:VAL:O | 2:CC:82:ASP:HB2 | 2.20 | 0.41 |
| 4:CE:19:ARG:NH1 | 4:CE:28:ARG:HH12 | 2.18 | 0.41 |
| 7:CH:124:ILE:O | 7:CH:125:ILE:HG13 | 2.20 | 0.41 |
| 8:CI:35:GLU:O | 8:CI:39:GLY:HA3 | 2.20 | 0.41 |
| 9:CJ:18:ILE:CG1 | 9:CJ:72:ARG:HG2 | 2.50 | 0.41 |
| 9:CJ:53:ILE:HG13 | 13:CN:84:ARG:CZ | 2.49 | 0.41 |
| 10:CK:46:ALA:HA | 10:CK:65:ALA:HB2 | 2.01 | 0.41 |
| 47:D0:29:VAL:HG22 | 47:D0:30:ASP:N | 2.35 | 0.41 |
| 49:D2:6:GLN:HA | 49:D2:7:PRO:HD2 | 1.89 | 0.41 |
| 23:DB:1098:A:H3' | 52:DI:3:LYS:HB3 | 2.00 | 0.41 |
| 23:DB:1173:U:H2' | 23:DB:1174:U:C6 | 2.56 | 0.41 |
| 23:DB:1207:C:H2' | 23:DB:1208:C:H6 | 1.85 | 0.41 |
| 23:DB:1552:A:H2' | 23:DB:1553:A:C5' | 2.49 | 0.41 |
| 23:DB:1637:A:H5' | 23:DB:1760:C:O2' | 2.20 | 0.41 |
| 23:DB:2013:A:H2' | 23:DB:2014:A:H5' | 2.02 | 0.41 |
| 23:DB:2018:G:H2' | 23:DB:2019:A:H8 | 1.85 | 0.41 |
| 23:DB:2191:A:H2' | 23:DB:2192:U:O4' | 2.20 | 0.41 |
| 23:DB:268:C:O2 | 23:DB:268:C:H2' | 2.19 | 0.41 |
| 23:DB:459:U:O2' | 23:DB:460:A:H5' | 2.20 | 0.41 |
| 23:DB:499:U:H5' | 42:DU:44:HIS:CE1 | 2.46 | 0.41 |
| 23:DB:68:G:H2' | 23:DB:69:C:H6 | 1.85 | 0.41 |
| 25:DC:166:ARG:HG3 | 25:DC:166:ARG:HH21 | 1.85 | 0.41 |
| 28:DF:124:ARG:HH11 | 28:DF:124:ARG:HG2 | 1.85 | 0.41 |
| 28:DF:35:LEU:HD13 | 28:DF:56:LEU:HD13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:DG:84:LYS:CB | 29:DG:132:LEU:H | 2.33 | 0.41 |
| 29:DG:91:VAL:HG23 | 29:DG:92:GLY:N | 2.36 | 0.41 |
| 30:DH:86:ASP:HB2 | 30:DH:89:LYS:CD | 2.42 | 0.41 |
| 31:DJ:38:GLY:O | 31:DJ:43:GLU:HB2 | 2.21 | 0.41 |
| 34:DM:40:ARG:HD3 | 34:DM:93:VAL:CG2 | 2.33 | 0.41 |
| 35:DN:79:LEU:C | 35:DN:81:ASN:H | 2.22 | 0.41 |
| 36:DO:56:LYS:O | 36:DO:60:GLU:HG2 | 2.20 | 0.41 |
| 37:DP:21:PRO:O | 37:DP:96:LEU:HD22 | 2.20 | 0.41 |
| 37:DP:4:ILE:HA | 37:DP:7:LEU:CD1 | 2.50 | 0.41 |
| 37:DP:20:ARG:HG3 | 37:DP:91:VAL:HG11 | 2.01 | 0.41 |
| 37:DP:98:TYR:CE2 | 37:DP:99:LEU:HD23 | 2.55 | 0.41 |
| 39:DR:6:GLN:HE21 | 39:DR:6:GLN:C | 2.23 | 0.41 |
| 41:DT:18:GLU:O | 41:DT:20:ALA:N | 2.53 | 0.41 |
| 41:DT:17:SER:N | 41:DT:21:SER:OG | 2.52 | 0.41 |
| 41:DT:29:THR:HB | 41:DT:86:THR:HG22 | 2.03 | 0.41 |
| 42:DU:78:LYS:HD3 | 42:DU:79:ALA:H | 1.85 | 0.41 |
| 43:DW:18:LYS:HE3 | 43:DW:19:ARG:CD | 2.51 | 0.41 |
| 44:DX:25:GLN:HB3 | 44:DX:25:GLN:HE21 | 1.53 | 0.41 |
| 45:DY:35:VAL:HG21 | 45:DY:37:ARG:NH2 | 2.34 | 0.41 |
| 46:DZ:53:ALA:C | 46:DZ:55:GLY:H | 2.19 | 0.41 |
| 1:AA:1058:G:H2' | 1:AA:1059:C:C6 | 2.56 | 0.41 |
| 1:AA:1256:A:O4' | 1:AA:1278:G:N2 | 2.54 | 0.41 |
| 1:AA:1238:A:H5' | 1:AA:1336:C:N4 | 2.30 | 0.41 |
| 1:AA:637:C:H2' | 1:AA:638:U:C6 | 2.55 | 0.41 |
| 1:AA:692:U:H2' | 1:AA:694:A:OP2 | 2.20 | 0.41 |
| 1:AA:708:C:H2' | 1:AA:709:U:H6 | 1.84 | 0.41 |
| 1:AA:720:C:O5' | 1:AA:720:C:H6 | 2.03 | 0.41 |
| 1:AA:775:G:H2' | 1:AA:776:G:C8 | 2.55 | 0.41 |
| 20:AB:114:LYS:O | 20:AB:117:GLU:HB3 | 2.21 | 0.41 |
| 20:AB:187:ASP:O | 20:AB:189:ASN:N | 2.53 | 0.41 |
| 20:AB:218:ALA:C | 20:AB:220:VAL:H | 2.24 | 0.41 |
| 3:AD:25:ARG:O | 3:AD:27:ILE:N | 2.53 | 0.41 |
| 3:AD:55:ARG:NE | 3:AD:55:ARG:HA | 2.36 | 0.41 |
| 3:AD:95:GLY:O | 3:AD:136:VAL:HG22 | 2.20 | 0.41 |
| 4:AE:48:GLY:H | 4:AE:66:ALA:CB | 2.34 | 0.41 |
| 7:AH:63:LYS:HG2 | 7:AH:64:TYR:N | 2.35 | 0.41 |
| 8:AI:98:ARG:HG3 | 8:AI:103:VAL:HG22 | 2.01 | 0.41 |
| 11:AL:54:VAL:HG12 | 11:AL:55:ARG:H | 1.85 | 0.41 |
| 14:AO:8:ALA:O | 14:AO:11:VAL:HB | 2.21 | 0.41 |
| 50:B3:14:LYS:O | 50:B3:15:LYS:C | 2.58 | 0.41 |
| 23:BB:1370:C:H2' | 23:BB:1371:G:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:1408:G:H2' | 23:BB:1409:U:C6 | 2.55 | 0.41 |
| 23:BB:177:G:H3' | 23:BB:178:G:C8 | 2.55 | 0.41 |
| 23:BB:2353:G:H1' | 43:BW:30:VAL:HG13 | 2.01 | 0.41 |
| 23:BB:484:C:H2' | 23:BB:485:C:H6 | 1.84 | 0.41 |
| 23:BB:550:C:H2' | 23:BB:550:C:O2 | 2.20 | 0.41 |
| 23:BB:567:U:H2' | 23:BB:568:U:O4' | 2.20 | 0.41 |
| 23:BB:600:G:H1' | 27:BE:100:MET:CG | 2.50 | 0.41 |
| 23:BB:619:G:H2' | 23:BB:620:G:H5'' | 2.02 | 0.41 |
| 23:BB:675:A:C6 | 23:BB:676:A:C6 | 3.08 | 0.41 |
| 23:BB:85:G:OP1 | 42:BU:6:ARG:N | 2.53 | 0.41 |
| 23:BB:922:C:H2' | 23:BB:923:G:H8 | 1.85 | 0.41 |
| 23:BB:939:G:C2' | 23:BB:940:G:H5' | 2.50 | 0.41 |
| 28:BF:121:PHE:HB2 | 28:BF:126:ASN:O | 2.20 | 0.41 |
| 30:BH:14:SER:HB2 | 30:BH:17:ASP:CB | 2.50 | 0.41 |
| 30:BH:58:LEU:O | 30:BH:60:GLU:N | 2.53 | 0.41 |
| 30:BH:63:ALA:HA | 30:BH:66:ASN:HD21 | 1.85 | 0.41 |
| 31:BJ:18:VAL:CG1 | 31:BJ:54:ILE:HD11 | 2.50 | 0.41 |
| 31:BJ:20:ALA:HA | 31:BJ:23:LYS:CG | 2.51 | 0.41 |
| 31:BJ:58:ASN:O | 31:BJ:59:ALA:HB3 | 2.20 | 0.41 |
| 31:BJ:72:LYS:HB3 | 31:BJ:73:VAL:H | 1.52 | 0.41 |
| 33:BL:61:LEU:N | 33:BL:61:LEU:CD1 | 2.82 | 0.41 |
| 33:BL:89:VAL:HA | 33:BL:121:THR:OG1 | 2.21 | 0.41 |
| 34:BM:53:MET:O | 34:BM:56:ALA:HB3 | 2.21 | 0.41 |
| 34:BM:69:PRO:HA | 34:BM:94:ALA:CA | 2.49 | 0.41 |
| 35:BN:10:LEU:HD21 | 35:BN:43:GLU:HG3 | 2.01 | 0.41 |
| 35:BN:31:HIS:C | 35:BN:33:ILE:H | 2.22 | 0.41 |
| 38:BQ:93:ILE:HG23 | 38:BQ:94:LEU:N | 2.35 | 0.41 |
| 38:BQ:91:ARG:NH1 | 39:BR:10:LYS:HB3 | 2.33 | 0.41 |
| 41:BT:65:GLY:HA3 | 41:BT:76:ARG:NH2 | 2.34 | 0.41 |
| 42:BU:26:ASN:O | 42:BU:26:ASN:ND2 | 2.54 | 0.41 |
| 24:BV:48:MET:SD | 24:BV:85:LYS:HA | 2.60 | 0.41 |
| 44:BX:39:GLN:HB2 | 44:BX:42:LEU:HD22 | 2.02 | 0.41 |
| 45:BY:3:THR:HB | 45:BY:36:GLU:CG | 2.51 | 0.41 |
| 46:BZ:38:PHE:CE2 | 46:BZ:51:VAL:HG21 | 2.56 | 0.41 |
| 1:CA:1015:G:H2' | 1:CA:1016:A:C8 | 2.56 | 0.41 |
| 1:CA:1127:G:C2' | 1:CA:1128:C:H5' | 2.50 | 0.41 |
| 1:CA:1503:A:H5' | 1:CA:1531:A:H1' | 2.02 | 0.41 |
| 1:CA:298:A:H8 | 1:CA:298:A:OP1 | 2.02 | 0.41 |
| 1:CA:301:G:O2' | 1:CA:302:G:H5' | 2.19 | 0.41 |
| 1:CA:371:A:O2' | 1:CA:372:C:H5' | 2.20 | 0.41 |
| 1:CA:448:A:H2' | 1:CA:449:G:H8 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:681:A:H2' | 1:CA:682:G:C8 | 2.56 | 0.41 |
| 1:CA:824:G:C6 | 1:CA:877:G:C6 | 3.08 | 0.41 |
| 1:CA:991:U:H2' | 1:CA:1212:U:O2 | 2.20 | 0.41 |
| 1:CA:6:G:C8 | 4:CE:123:LEU:HD21 | 2.55 | 0.41 |
| 6:CG:70:PRO:HD2 | 6:CG:95:ARG:O | 2.20 | 0.41 |
| 12:CM:43:LYS:O | 12:CM:47:LEU:HD23 | 2.20 | 0.41 |
| 2:CC:17:TRP:HZ2 | 13:CN:95:LEU:O | 2.03 | 0.41 |
| 15:CP:20:VAL:HG21 | 15:CP:32:PHE:CD2 | 2.56 | 0.41 |
| 21:CU:24:LYS:HZ3 | 21:CU:25:ALA:N | 2.00 | 0.41 |
| 23:DB:1040:A:O2' | 23:DB:1041:G:H5' | 2.20 | 0.41 |
| 23:DB:1161:C:H2' | 23:DB:1162:G:H8 | 1.85 | 0.41 |
| 23:DB:1168:G:C6 | 23:DB:1182:G:C6 | 3.08 | 0.41 |
| 23:DB:1430:G:H2' | 23:DB:1431:A:C8 | 2.55 | 0.41 |
| 23:DB:1723:G:H2' | 23:DB:1724:G:H5' | 2.02 | 0.41 |
| 23:DB:1951:U:H2' | 23:DB:1953:A:OP2 | 2.19 | 0.41 |
| 23:DB:2019:A:H4' | 38:DQ:33:VAL:HG11 | 2.02 | 0.41 |
| 23:DB:574:A:H1' | 23:DB:2055:C:C5 | 2.55 | 0.41 |
| 23:DB:2733:A:H3' | 23:DB:2733:A:C8 | 2.55 | 0.41 |
| 23:DB:2889:C:O2' | 23:DB:2890:G:H5' | 2.20 | 0.41 |
| 23:DB:921:C:H2' | 23:DB:922:C:H6 | 1.83 | 0.41 |
| 23:DB:937:C:H2' | 23:DB:938:G:C8 | 2.55 | 0.41 |
| 25:DC:131:MET:HE3 | 25:DC:187:CYS:O | 2.19 | 0.41 |
| 25:DC:149:LYS:HD3 | 25:DC:152:GLN:NE2 | 2.35 | 0.41 |
| 26:DD:150:GLN:O | 26:DD:153:GLY:N | 2.53 | 0.41 |
| 27:DE:59:PRO:HB2 | 27:DE:67:ARG:NH2 | 2.35 | 0.41 |
| 27:DE:9:GLN:O | 27:DE:9:GLN:HG3 | 2.21 | 0.41 |
| 23:DB:2305:U:C1' | 28:DF:132:ARG:HA | 2.50 | 0.41 |
| 28:DF:42:ALA:O | 28:DF:43:ILE:C | 2.58 | 0.41 |
| 29:DG:94:ARG:HH21 | 29:DG:105:SER:H | 1.68 | 0.41 |
| 31:DJ:54:ILE:HD12 | 31:DJ:55:ILE:H | 1.84 | 0.41 |
| 33:DL:80:SER:HB3 | 33:DL:115:GLU:CD | 2.41 | 0.41 |
| 33:DL:40:SER:C | 33:DL:41:ARG:HG3 | 2.39 | 0.41 |
| 23:DB:833:A:H1' | 33:DL:52:GLY:N | 2.35 | 0.41 |
| 35:DN:60:VAL:O | 35:DN:63:ARG:HB3 | 2.20 | 0.41 |
| 35:DN:9:GLN:O | 35:DN:17:ARG:HD3 | 2.20 | 0.41 |
| 36:DO:52:SER:HA | 36:DO:74:VAL:CG1 | 2.50 | 0.41 |
| 38:DQ:38:VAL:O | 38:DQ:39:ILE:C | 2.56 | 0.41 |
| 41:DT:25:GLU:HA | 41:DT:28:ASN:O | 2.20 | 0.41 |
| 42:DU:23:LYS:H | 42:DU:23:LYS:HD2 | 1.86 | 0.41 |
| 42:DU:41:VAL:N | 42:DU:60:LYS:O | 2.53 | 0.41 |
| 44:DX:46:VAL:O | 44:DX:50:VAL:HG23 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:125:U:H2' | 1:AA:126:G:C8 | 2.56 | 0.41 |
| 1:AA:1314:C:N4 | 18:AS:3:SER:HB3 | 2.35 | 0.41 |
| 1:AA:1329:A:H5'' | 12:AM:24:VAL:HA | 2.02 | 0.41 |
| 1:AA:1394:A:C5 | 1:AA:1501:C:H4' | 2.55 | 0.41 |
| 1:AA:282:A:N3 | 1:AA:282:A:H2' | 2.35 | 0.41 |
| 1:AA:526:C:OP2 | 11:AL:87:LYS:HE3 | 2.20 | 0.41 |
| 1:AA:54:C:N4 | 1:AA:352:C:H2' | 2.35 | 0.41 |
| 1:AA:766:A:H2' | 1:AA:767:A:C8 | 2.55 | 0.41 |
| 1:AA:902:G:H2' | 1:AA:903:G:H8 | 1.85 | 0.41 |
| 20:AB:112:ARG:O | 20:AB:116:LEU:HB2 | 2.20 | 0.41 |
| 20:AB:59:ILE:O | 20:AB:62:ARG:HD2 | 2.21 | 0.41 |
| 2:AC:154:GLY:HA2 | 2:AC:163:ARG:O | 2.20 | 0.41 |
| 3:AD:79:ALA:N | 3:AD:85:THR:HG23 | 2.35 | 0.41 |
| 1:AA:8:A:H1' | 4:AE:106:ALA:O | 2.20 | 0.41 |
| 4:AE:19:ARG:HH12 | 4:AE:28:ARG:HH12 | 1.67 | 0.41 |
| 4:AE:52:ALA:H | 4:AE:58:ALA:HB2 | 1.85 | 0.41 |
| 5:AF:79:ARG:HD3 | 5:AF:79:ARG:HA | 1.89 | 0.41 |
| 6:AG:57:GLU:H | 6:AG:57:GLU:CD | 2.24 | 0.41 |
| 7:AH:12:ARG:NH1 | 7:AH:12:ARG:HG3 | 2.35 | 0.41 |
| 8:AI:53:LEU:N | 8:AI:53:LEU:HD22 | 2.34 | 0.41 |
| 12:AM:63:VAL:CG1 | 12:AM:67:ASP:HB2 | 2.49 | 0.41 |
| 14:AO:87:ARG:NE | 14:AO:87:ARG:HA | 2.35 | 0.41 |
| 16:AQ:80:LYS:O | 16:AQ:80:LYS:HD2 | 2.21 | 0.41 |
| 50:B3:30:HIS:O | 50:B3:31:ILE:O | 2.38 | 0.41 |
| 23:BB:1283:G:H22 | 23:BB:1286:A:C5' | 2.15 | 0.41 |
| 23:BB:1547:C:H2' | 23:BB:1548:A:H8 | 1.86 | 0.41 |
| 23:BB:1848:A:H2' | 23:BB:1849:G:H8 | 1.84 | 0.41 |
| 23:BB:214:G:N2 | 23:BB:216:A:N3 | 2.64 | 0.41 |
| 23:BB:2562:U:H2' | 23:BB:2563:U:H5' | 2.03 | 0.41 |
| 23:BB:2617:U:H2' | 23:BB:2618:G:H5' | 2.02 | 0.41 |
| 23:BB:269:C:H2' | 23:BB:270:A:H8 | 1.86 | 0.41 |
| 23:BB:2787:C:O2' | 23:BB:2788:C:H5' | 2.20 | 0.41 |
| 23:BB:518:G:H2' | 23:BB:519:U:C6 | 2.56 | 0.41 |
| 23:BB:548:G:H4' | 23:BB:549:G:N1 | 2.35 | 0.41 |
| 23:BB:583:G:H2' | 23:BB:584:C:C6 | 2.55 | 0.41 |
| 23:BB:866:A:H61 | 23:BB:913:U:C1' | 2.34 | 0.41 |
| 25:BC:203:VAL:O | 25:BC:204:LEU:HB2 | 2.20 | 0.41 |
| 26:BD:113:SER:HB3 | 26:BD:167:ASN:CA | 2.51 | 0.41 |
| 27:BE:9:GLN:HG3 | 27:BE:9:GLN:O | 2.20 | 0.41 |
| 28:BF:134:GLN:HE22 | 28:BF:136:ILE:HD13 | 1.81 | 0.41 |
| 28:BF:31:GLU:HB2 | 28:BF:158:THR:CG2 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:BG:112:VAL:O | 29:BG:113:ASP:HB2 | 2.19 | 0.41 |
| 29:BG:43:LYS:CB | 29:BG:50:THR:HB | 2.46 | 0.41 |
| 34:BM:108:VAL:CG1 | 34:BM:112:LEU:HD12 | 2.51 | 0.41 |
| 34:BM:29:GLY:O | 34:BM:133:LYS:HD2 | 2.21 | 0.41 |
| 34:BM:41:LEU:CD2 | 34:BM:124:LEU:HD22 | 2.50 | 0.41 |
| 35:BN:12:ARG:HG2 | 35:BN:16:HIS:ND1 | 2.36 | 0.41 |
| 36:BO:16:ARG:C | 36:BO:18:LEU:N | 2.74 | 0.41 |
| 37:BP:89:GLY:N | 37:BP:112:ARG:NH1 | 2.67 | 0.41 |
| 40:BS:57:ASN:HA | 40:BS:57:ASN:HD22 | 1.59 | 0.41 |
| 42:BU:39:ASN:HB3 | 42:BU:62:ALA:HB3 | 2.02 | 0.41 |
| 46:BZ:27:ARG:CG | 46:BZ:28:ARG:N | 2.82 | 0.41 |
| 46:BZ:71:LEU:HA | 46:BZ:74:ARG:HE | 1.85 | 0.41 |
| 1:CA:100:G:N7 | 1:CA:101:A:C5 | 2.88 | 0.41 |
| 1:CA:1200:C:H4' | 1:CA:1201:A:H3' | 2.03 | 0.41 |
| 1:CA:1202:U:H2' | 1:CA:1203:C:H5' | 2.02 | 0.41 |
| 1:CA:1337:G:H5'' | 1:CA:1338:G:OP1 | 2.20 | 0.41 |
| 1:CA:1531:A:H2' | 1:CA:1532:U:H5' | 2.02 | 0.41 |
| 1:CA:154:U:H2' | 1:CA:155:A:H8 | 1.80 | 0.41 |
| 1:CA:261:U:H2' | 1:CA:263:A:OP2 | 2.19 | 0.41 |
| 1:CA:493:A:H5' | 1:CA:494:G:OP2 | 2.19 | 0.41 |
| 1:CA:956:U:O2' | 1:CA:957:U:H5' | 2.20 | 0.41 |
| 11:CL:30:ARG:HA | 11:CL:80:LEU:HD12 | 2.02 | 0.41 |
| 12:CM:3:ILE:HA | 12:CM:56:ARG:HB2 | 2.01 | 0.41 |
| 15:CP:12:LYS:O | 15:CP:13:LYS:HB2 | 2.20 | 0.41 |
| 15:CP:12:LYS:C | 15:CP:14:ARG:H | 2.24 | 0.41 |
| 16:CQ:23:ALA:HA | 16:CQ:41:THR:O | 2.19 | 0.41 |
| 18:CS:43:MET:C | 18:CS:46:LEU:HD23 | 2.40 | 0.41 |
| 1:CA:1313:U:OP1 | 18:CS:6:LYS:HD3 | 2.20 | 0.41 |
| 48:D1:18:HIS:ND1 | 48:D1:19:PHE:N | 2.68 | 0.41 |
| 23:DB:460:A:P | 49:D2:41:ARG:HH12 | 2.44 | 0.41 |
| 22:DA:32:U:H1' | 22:DA:52:A:N7 | 2.35 | 0.41 |
| 23:DB:1716:U:H2' | 23:DB:1717:A:C8 | 2.56 | 0.41 |
| 23:DB:1789:A:H2' | 23:DB:1790:C:O4' | 2.20 | 0.41 |
| 23:DB:570:G:C4 | 23:DB:2030:A:N7 | 2.88 | 0.41 |
| 23:DB:2219:U:O2' | 23:DB:2220:U:H5' | 2.20 | 0.41 |
| 23:DB:230:G:H2' | 23:DB:231:A:C8 | 2.55 | 0.41 |
| 23:DB:235:U:H2' | 23:DB:236:C:H6 | 1.85 | 0.41 |
| 23:DB:2437:G:H2' | 23:DB:2438:U:C6 | 2.56 | 0.41 |
| 23:DB:2607:G:O2' | 23:DB:2608:G:H5' | 2.20 | 0.41 |
| 23:DB:2769:U:O2' | 23:DB:2770:G:H5' | 2.20 | 0.41 |
| 23:DB:325:G:O2' | 23:DB:326:G:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DB:341:C:O2' | 23:DB:342:A:H5' | 2.21 | 0.41 |
| 23:DB:506:G:H1' | 23:DB:507:A:C8 | 2.55 | 0.41 |
| 23:DB:532:A:N3 | 23:DB:532:A:H2' | 2.34 | 0.41 |
| 23:DB:686:U:O4 | 49:D2:12:ARG:HB2 | 2.20 | 0.41 |
| 25:DC:144:GLU:CA | 25:DC:151:GLY:HA2 | 2.40 | 0.41 |
| 23:DB:1798:U:H5'' | 25:DC:257:ARG:HB2 | 2.02 | 0.41 |
| 25:DC:29:PHE:CE2 | 25:DC:31:PRO:HG2 | 2.55 | 0.41 |
| 26:DD:201:LEU:C | 26:DD:202:ILE:HD12 | 2.41 | 0.41 |
| 26:DD:15:PHE:HA | 26:DD:20:VAL:O | 2.21 | 0.41 |
| 26:DD:62:LYS:N | 26:DD:63:PRO:CD | 2.84 | 0.41 |
| 27:DE:194:LYS:O | 27:DE:197:GLU:HB3 | 2.21 | 0.41 |
| 28:DF:148:VAL:O | 28:DF:149:ARG:HG2 | 2.20 | 0.41 |
| 29:DG:148:ARG:HA | 29:DG:161:VAL:CB | 2.45 | 0.41 |
| 30:DH:54:LEU:CD2 | 30:DH:58:LEU:HD12 | 2.46 | 0.41 |
| 30:DH:58:LEU:O | 30:DH:61:VAL:HG12 | 2.20 | 0.41 |
| 52:DI:99:LYS:HB2 | 52:DI:140:GLU:OE1 | 2.20 | 0.41 |
| 31:DJ:140:LEU:HD23 | 31:DJ:141:ASP:N | 2.34 | 0.41 |
| 34:DM:100:LYS:HD3 | 34:DM:100:LYS:HA | 1.87 | 0.41 |
| 34:DM:26:VAL:HB | 34:DM:104:GLU:OE2 | 2.19 | 0.41 |
| 35:DN:12:ARG:HA | 35:DN:12:ARG:HD2 | 1.72 | 0.41 |
| 36:DO:36:TYR:HA | 36:DO:52:SER:CB | 2.50 | 0.41 |
| 38:DQ:48:ASP:HA | 38:DQ:51:GLN:HG3 | 2.03 | 0.41 |
| 31:DJ:44:TYR:HB2 | 38:DQ:63:ARG:HD2 | 2.01 | 0.41 |
| 38:DQ:108:LEU:HA | 39:DR:48:LYS:HD3 | 2.01 | 0.41 |
| 40:DS:55:ILE:HD12 | 40:DS:69:LEU:HD23 | 2.02 | 0.41 |
| 41:DT:22:THR:O | 41:DT:26:LYS:N | 2.44 | 0.41 |
| 41:DT:5:GLU:N | 41:DT:8:LEU:HD12 | 2.35 | 0.41 |
| 41:DT:68:LYS:HE3 | 41:DT:68:LYS:HB2 | 1.81 | 0.41 |
| 42:DU:32:LYS:N | 42:DU:32:LYS:HD3 | 2.34 | 0.41 |
| 42:DU:88:ASP:CG | 42:DU:89:GLY:N | 2.73 | 0.41 |
| 44:DX:23:ARG:O | 44:DX:27:ASN:HB2 | 2.20 | 0.41 |
| 46:DZ:11:ARG:HB3 | 46:DZ:12:PRO:HD2 | 2.01 | 0.41 |
| 46:DZ:27:ARG:HD2 | 46:DZ:29:PHE:CE1 | 2.55 | 0.41 |
| 46:DZ:7:VAL:CG2 | 46:DZ:67:VAL:HG11 | 2.50 | 0.41 |
| 1:AA:1285:A:HO2' | 1:AA:1286:U:P | 2.44 | 0.41 |
| 1:AA:1269:A:H2 | 1:AA:1312:G:H21 | 1.67 | 0.41 |
| 1:AA:1436:U:H2' | 1:AA:1437:A:C8 | 2.55 | 0.41 |
| 1:AA:298:A:OP1 | 1:AA:298:A:H8 | 2.03 | 0.41 |
| 1:AA:356:A:H1' | 1:AA:368:U:O2' | 2.20 | 0.41 |
| 1:AA:415:A:N1 | 1:AA:428:G:O6 | 2.54 | 0.41 |
| 1:AA:493:A:H5' | 1:AA:494:G:OP2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:856:C:O2' | 1:AA:857:C:H5' | 2.20 | 0.41 |
| 20:AB:104:LYS:NZ | 20:AB:104:LYS:HB2 | 2.35 | 0.41 |
| 20:AB:85:SER:O | 20:AB:86:CYS:HB2 | 2.21 | 0.41 |
| 2:AC:133:MET:O | 2:AC:137:VAL:HG23 | 2.20 | 0.41 |
| 2:AC:134:LYS:HE3 | 2:AC:138:GLN:HG2 | 2.03 | 0.41 |
| 5:AF:66:ALA:HB1 | 5:AF:67:PRO:HD2 | 2.03 | 0.41 |
| 5:AF:66:ALA:HB1 | 5:AF:70:VAL:HG21 | 2.01 | 0.41 |
| 6:AG:80:GLY:C | 6:AG:82:SER:H | 2.24 | 0.41 |
| 10:AK:15:VAL:C | 10:AK:17:ASP:H | 2.24 | 0.41 |
| 10:AK:35:ASP:OD1 | 10:AK:37:GLN:HB2 | 2.20 | 0.41 |
| 1:AA:553:A:O2' | 11:AL:25:ALA:HB1 | 2.20 | 0.41 |
| 12:AM:43:LYS:C | 12:AM:45:SER:N | 2.73 | 0.41 |
| 13:AN:73:LEU:HD12 | 13:AN:83:VAL:HG21 | 2.03 | 0.41 |
| 19:AT:69:ASN:O | 19:AT:70:LYS:C | 2.58 | 0.41 |
| 50:B3:18:LYS:HE3 | 50:B3:20:GLY:H | 1.85 | 0.41 |
| 23:BB:1054:A:H2' | 23:BB:1055:G:H8 | 1.82 | 0.41 |
| 23:BB:1266:G:N2 | 23:BB:2012:G:H2' | 2.36 | 0.41 |
| 23:BB:1389:G:O2' | 23:BB:1390:U:H5' | 2.21 | 0.41 |
| 23:BB:1806:C:O2' | 23:BB:1807:G:H5' | 2.20 | 0.41 |
| 23:BB:215:G:C4' | 23:BB:216:A:H4' | 2.47 | 0.41 |
| 23:BB:2496:C:C2' | 23:BB:2497:A:H5' | 2.50 | 0.41 |
| 23:BB:2518:A:N3 | 23:BB:2518:A:H5' | 2.35 | 0.41 |
| 23:BB:2685:G:O2' | 23:BB:2686:G:H5' | 2.20 | 0.41 |
| 23:BB:2751:G:OP2 | 29:BG:2:ARG:HD2 | 2.20 | 0.41 |
| 23:BB:2794:C:H2' | 23:BB:2795:C:C5 | 2.55 | 0.41 |
| 23:BB:522:A:H2' | 23:BB:523:C:H6 | 1.84 | 0.41 |
| 23:BB:935:C:H2' | 23:BB:936:A:H8 | 1.85 | 0.41 |
| 23:BB:973:A:O4' | 23:BB:1188:U:C6 | 2.74 | 0.41 |
| 25:BC:146:LYS:HB2 | 25:BC:149:LYS:HB2 | 2.02 | 0.41 |
| 25:BC:107:LYS:N | 25:BC:193:GLU:O | 2.51 | 0.41 |
| 28:BF:4:HIS:O | 28:BF:7:TYR:HB3 | 2.21 | 0.41 |
| 30:BH:132:PHE:O | 30:BH:140:ALA:HB3 | 2.20 | 0.41 |
| 30:BH:90:LEU:CD1 | 30:BH:146:VAL:HG11 | 2.45 | 0.41 |
| 30:BH:77:THR:CG2 | 30:BH:79:THR:HG23 | 2.49 | 0.41 |
| 52:BI:126:ARG:HA | 52:BI:129:GLU:OE2 | 2.20 | 0.41 |
| 37:BP:38:ARG:NH2 | 37:BP:38:ARG:HB3 | 2.35 | 0.41 |
| 37:BP:4:ILE:O | 37:BP:5:LYS:HB2 | 2.20 | 0.41 |
| 37:BP:89:GLY:N | 37:BP:112:ARG:HH12 | 2.18 | 0.41 |
| 38:BQ:94:LEU:O | 38:BQ:97:ILE:HG23 | 2.20 | 0.41 |
| 38:BQ:9:ALA:O | 38:BQ:12:ARG:N | 2.53 | 0.41 |
| 41:BT:1:MET:C | 41:BT:2:ILE:HD13 | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:13:ALA:O | 41:BT:33:LYS:N | 2.54 | 0.41 |
| 24:BV:24:ASN:O | 24:BV:26:PHE:N | 2.54 | 0.41 |
| 46:BZ:2:SER:O | 46:BZ:3:ARG:C | 2.58 | 0.41 |
| 46:BZ:64:ILE:HG22 | 46:BZ:68:LEU:HD11 | 2.01 | 0.41 |
| 1:CA:1140:C:O2' | 1:CA:1141:C:H5' | 2.20 | 0.41 |
| 1:CA:1261:A:N7 | 1:CA:1274:A:H2 | 2.17 | 0.41 |
| 1:CA:1314:C:H2' | 1:CA:1315:U:H6 | 1.86 | 0.41 |
| 1:CA:1320:C:N4 | 18:CS:36:ARG:HA | 2.36 | 0.41 |
| 1:CA:1330:U:H4' | 12:CM:69:ARG:NH1 | 2.33 | 0.41 |
| 1:CA:355:C:O2' | 1:CA:356:A:H5' | 2.21 | 0.41 |
| 1:CA:975:A:H61 | 9:CJ:50:THR:HG21 | 1.85 | 0.41 |
| 20:CB:127:LYS:HD2 | 20:CB:127:LYS:C | 2.40 | 0.41 |
| 20:CB:62:ARG:HG3 | 20:CB:62:ARG:HH11 | 1.86 | 0.41 |
| 4:CE:143:LEU:C | 4:CE:145:ASN:H | 2.23 | 0.41 |
| 5:CF:48:ALA:N | 17:CR:65:SER:OG | 2.54 | 0.41 |
| 6:CG:46:LEU:O | 6:CG:57:GLU:HG3 | 2.20 | 0.41 |
| 7:CH:29:SER:OG | 7:CH:32:LYS:HG3 | 2.20 | 0.41 |
| 7:CH:49:LYS:HA | 7:CH:49:LYS:HD2 | 1.88 | 0.41 |
| 8:CI:18:VAL:HG12 | 8:CI:19:PHE:N | 2.36 | 0.41 |
| 11:CL:43:LYS:N | 11:CL:44:PRO:HD2 | 2.34 | 0.41 |
| 12:CM:26:LYS:O | 12:CM:30:LYS:HB2 | 2.20 | 0.41 |
| 16:CQ:7:LEU:HD21 | 16:CQ:24:ILE:HG21 | 2.01 | 0.41 |
| 1:CA:1315:U:H5 | 18:CS:5:LYS:HZ1 | 1.69 | 0.41 |
| 21:CU:33:ARG:NE | 21:CU:34:ARG:HG3 | 2.36 | 0.41 |
| 50:D3:26:ALA:O | 50:D3:27:ASN:C | 2.59 | 0.41 |
| 51:D4:22:VAL:O | 51:D4:24:ARG:N | 2.54 | 0.41 |
| 22:DA:25:U:OP1 | 22:DA:25:U:H3' | 2.20 | 0.41 |
| 22:DA:27:C:H2' | 22:DA:28:C:H5' | 2.02 | 0.41 |
| 23:DB:1369:G:H2' | 23:DB:1370:C:O4' | 2.20 | 0.41 |
| 23:DB:1423:G:H2' | 23:DB:1424:G:H8 | 1.85 | 0.41 |
| 1:CA:702:A:N6 | 23:DB:1848:A:C6 | 2.88 | 0.41 |
| 23:DB:20:C:H2' | 23:DB:21:A:C8 | 2.55 | 0.41 |
| 23:DB:2327:A:H2' | 23:DB:2328:A:C8 | 2.56 | 0.41 |
| 23:DB:2335:A:H2' | 23:DB:2336:A:H5'' | 2.02 | 0.41 |
| 23:DB:2386:A:H4' | 43:DW:54:ARG:O | 2.19 | 0.41 |
| 23:DB:2407:A:H2' | 23:DB:2408:U:C6 | 2.56 | 0.41 |
| 23:DB:2800:A:H2' | 23:DB:2801:G:C1' | 2.50 | 0.41 |
| 23:DB:346:A:O4' | 23:DB:346:A:N3 | 2.54 | 0.41 |
| 23:DB:828:U:H2' | 23:DB:829:A:C8 | 2.54 | 0.41 |
| 25:DC:124:LYS:CG | 25:DC:125:PRO:HD2 | 2.50 | 0.41 |
| 25:DC:58:LYS:HD2 | 25:DC:58:LYS:HA | 1.95 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:DF:102:LEU:C | 28:DF:102:LEU:HD13 | 2.41 | 0.41 |
| 28:DF:107:VAL:O | 28:DF:110:ILE:HG22 | 2.21 | 0.41 |
| 28:DF:82:TYR:O | 28:DF:84:ILE:HD13 | 2.21 | 0.41 |
| 29:DG:94:ARG:HB2 | 29:DG:127:GLN:HG2 | 2.01 | 0.41 |
| 29:DG:50:THR:HG22 | 29:DG:51:PHE:N | 2.36 | 0.41 |
| 52:DI:108:ILE:CG2 | 52:DI:128:ILE:HD13 | 2.50 | 0.41 |
| 31:DJ:84:ILE:HG13 | 31:DJ:84:ILE:O | 2.21 | 0.41 |
| 32:DK:117:SER:C | 32:DK:118:LEU:HD12 | 2.41 | 0.41 |
| 23:DB:661:A:H1' | 33:DL:12:SER:O | 2.21 | 0.41 |
| 24:DV:77:VAL:HG12 | 34:DM:136:MET:CE | 2.50 | 0.41 |
| 34:DM:21:ALA:HB3 | 34:DM:99:GLY:O | 2.21 | 0.41 |
| 34:DM:43:ALA:O | 34:DM:47:GLU:HB2 | 2.21 | 0.41 |
| 38:DQ:63:ARG:HH12 | 38:DQ:96:ASP:CA | 2.32 | 0.41 |
| 40:DS:73:LYS:HA | 40:DS:73:LYS:HD2 | 1.66 | 0.41 |
| 42:DU:43:LYS:HD3 | 42:DU:44:HIS:N | 2.35 | 0.41 |
| 42:DU:73:ASN:HD21 | 42:DU:76:THR:H | 1.67 | 0.41 |
| 42:DU:96:LYS:C | 42:DU:98:ASN:H | 2.23 | 0.41 |
| 24:DV:2:PHE:HD1 | 24:DV:50:MET:HE2 | 1.86 | 0.41 |
| 43:DW:49:ASN:CA | 43:DW:61:LYS:HB2 | 2.50 | 0.41 |
| 45:DY:55:LYS:O | 45:DY:56:VAL:C | 2.59 | 0.41 |
| 46:DZ:51:VAL:HG12 | 46:DZ:52:SER:N | 2.36 | 0.41 |
| 1:AA:1291:U:H2' | 1:AA:1292:G:H8 | 1.84 | 0.41 |
| 1:AA:1320:C:N3 | 18:AS:35:ARG:NH1 | 2.69 | 0.41 |
| 1:AA:1370:G:O2' | 1:AA:1371:G:H5' | 2.21 | 0.41 |
| 1:AA:360:G:O2' | 1:AA:361:G:H5' | 2.20 | 0.41 |
| 1:AA:38:G:O2' | 1:AA:39:G:H5' | 2.21 | 0.41 |
| 1:AA:648:A:O2' | 1:AA:649:A:H5' | 2.21 | 0.41 |
| 1:AA:80:A:C4 | 1:AA:81:A:H1' | 2.56 | 0.41 |
| 1:AA:865:A:H2' | 1:AA:866:C:C6 | 2.55 | 0.41 |
| 20:AB:185:ILE:HA | 20:AB:199:ILE:O | 2.20 | 0.41 |
| 2:AC:120:THR:CG2 | 2:AC:188:ALA:HB2 | 2.51 | 0.41 |
| 2:AC:76:ILE:O | 2:AC:82:ASP:N | 2.53 | 0.41 |
| 3:AD:115:GLN:HE21 | 3:AD:119:HIS:CE1 | 2.37 | 0.41 |
| 3:AD:20:LEU:C | 3:AD:21:LYS:HD2 | 2.41 | 0.41 |
| 3:AD:48:SER:O | 3:AD:49:ASP:C | 2.59 | 0.41 |
| 3:AD:13:ARG:HG3 | 3:AD:55:ARG:NH1 | 2.36 | 0.41 |
| 4:AE:87:VAL:HG23 | 4:AE:91:SER:O | 2.20 | 0.41 |
| 12:AM:15:VAL:N | 12:AM:33:LEU:HD11 | 2.36 | 0.41 |
| 12:AM:43:LYS:C | 12:AM:45:SER:H | 2.24 | 0.41 |
| 16:AQ:65:PRO:HA | 16:AQ:71:SER:OG | 2.20 | 0.41 |
| 21:AU:39:LYS:HD3 | 21:AU:39:LYS:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:29:A:H3' | 22:BA:30:C:C6 | 2.47 | 0.41 |
| 22:BA:32:U:H2' | 22:BA:33:G:C8 | 2.55 | 0.41 |
| 22:BA:64:G:O2' | 22:BA:65:U:H5' | 2.21 | 0.41 |
| 22:BA:8:C:O2' | 36:BO:40:ILE:HD13 | 2.20 | 0.41 |
| 23:BB:1259:G:O2' | 23:BB:1260:A:H5' | 2.21 | 0.41 |
| 23:BB:1481:U:H2' | 23:BB:1482:G:H4' | 2.03 | 0.41 |
| 23:BB:1870:C:H2' | 23:BB:1871:A:C8 | 2.56 | 0.41 |
| 23:BB:1979:U:C2' | 23:BB:1980:G:H5' | 2.51 | 0.41 |
| 23:BB:245:G:H2' | 23:BB:246:C:C6 | 2.56 | 0.41 |
| 23:BB:2734:A:C2' | 23:BB:2735:G:H5' | 2.43 | 0.41 |
| 23:BB:2747:G:H1 | 23:BB:2754:U:H2' | 1.86 | 0.41 |
| 23:BB:426:C:O2' | 23:BB:427:U:H5' | 2.20 | 0.41 |
| 23:BB:493:G:O2' | 40:BS:7:HIS:HA | 2.21 | 0.41 |
| 23:BB:755:U:H2' | 23:BB:756:A:C8 | 2.56 | 0.41 |
| 23:BB:757:G:C2' | 23:BB:758:C:H5' | 2.51 | 0.41 |
| 23:BB:910:A:C6 | 23:BB:911:A:C6 | 3.09 | 0.41 |
| 23:BB:963:U:H2' | 23:BB:964:C:C6 | 2.55 | 0.41 |
| 26:BD:2:ILE:O | 26:BD:2:ILE:HD12 | 2.21 | 0.41 |
| 26:BD:51:THR:HG21 | 26:BD:75:ALA:O | 2.20 | 0.41 |
| 27:BE:112:LEU:C | 27:BE:114:ARG:N | 2.74 | 0.41 |
| 27:BE:137:LYS:HG3 | 27:BE:141:MET:SD | 2.60 | 0.41 |
| 27:BE:198:GLU:O | 27:BE:199:MET:C | 2.59 | 0.41 |
| 32:BK:15:GLY:HA3 | 32:BK:52:VAL:CG2 | 2.47 | 0.41 |
| 35:BN:114:GLU:HG2 | 35:BN:115:LEU:N | 2.34 | 0.41 |
| 35:BN:47:VAL:O | 35:BN:51:LEU:HD13 | 2.21 | 0.41 |
| 36:BO:116:GLN:O | 36:BO:117:PHE:HB3 | 2.19 | 0.41 |
| 36:BO:67:ASN:H | 36:BO:70:ALA:CB | 2.29 | 0.41 |
| 36:BO:67:ASN:N | 36:BO:70:ALA:HB3 | 2.32 | 0.41 |
| 37:BP:62:LYS:O | 37:BP:63:ILE:HB | 2.20 | 0.41 |
| 39:BR:2:TYR:N | 39:BR:42:ALA:HB2 | 2.35 | 0.41 |
| 40:BS:46:LEU:O | 40:BS:50:VAL:HG23 | 2.20 | 0.41 |
| 42:BU:78:LYS:HD3 | 42:BU:79:ALA:H | 1.85 | 0.41 |
| 1:CA:1087:G:O2' | 1:CA:1088:G:H5' | 2.20 | 0.41 |
| 1:CA:1096:C:O2' | 1:CA:1097:C:H5' | 2.21 | 0.41 |
| 1:CA:1258:G:C4 | 1:CA:1278:G:N2 | 2.89 | 0.41 |
| 1:CA:1320:C:N3 | 18:CS:35:ARG:NH1 | 2.69 | 0.41 |
| 1:CA:1320:C:H2' | 1:CA:1321:U:O4' | 2.20 | 0.41 |
| 1:CA:1325:C:H2' | 1:CA:1326:U:H6 | 1.84 | 0.41 |
| 1:CA:1483:A:H2' | 1:CA:1484:C:O4' | 2.20 | 0.41 |
| 1:CA:152:A:N6 | 1:CA:170:U:C2 | 2.88 | 0.41 |
| 1:CA:203:G:H1' | 1:CA:465:A:N6 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:CA:501:C:OP1 | 11:CL:113:ARG:NH2 | 2.54 | 0.41 |
| 1:CA:577:G:O2' | 1:CA:578:C:H5' | 2.21 | 0.41 |
| 1:CA:613:C:H2' | 1:CA:614:C:H6 | 1.82 | 0.41 |
| 1:CA:832:G:H2' | 1:CA:833:G:H8 | 1.86 | 0.41 |
| 20:CB:204:ASP:O | 20:CB:209:VAL:HG13 | 2.21 | 0.41 |
| 20:CB:57:ASN:HA | 20:CB:60:ALA:HB3 | 2.02 | 0.41 |
| 2:CC:112:ALA:O | 2:CC:113:LYS:C | 2.58 | 0.41 |
| 2:CC:179:ALA:O | 2:CC:180:ASP:O | 2.39 | 0.41 |
| 3:CD:89:LEU:HD22 | 3:CD:199:ILE:HD11 | 2.03 | 0.41 |
| 6:CG:45:ALA:CB | 6:CG:120:ALA:HB2 | 2.49 | 0.41 |
| 6:CG:3:ARG:HB3 | 6:CG:4:ARG:H | 1.71 | 0.41 |
| 4:CE:156:ARG:HB3 | 7:CH:43:GLY:O | 2.21 | 0.41 |
| 7:CH:88:LYS:CG | 7:CH:89:ASP:H | 2.33 | 0.41 |
| 8:CI:18:VAL:CG1 | 8:CI:82:ILE:HG12 | 2.48 | 0.41 |
| 10:CK:47:GLY:C | 10:CK:49:SER:H | 2.24 | 0.41 |
| 11:CL:71:HIS:HD2 | 11:CL:73:LEU:HG | 1.86 | 0.41 |
| 14:CO:44:GLU:O | 14:CO:46:LYS:N | 2.51 | 0.41 |
| 18:CS:51:HIS:HB2 | 18:CS:56:HIS:NE2 | 2.35 | 0.41 |
| 48:D1:8:ILE:HG21 | 48:D1:51:ALA:CB | 2.51 | 0.41 |
| 49:D2:19:ARG:HG2 | 49:D2:19:ARG:NH2 | 2.35 | 0.41 |
| 50:D3:31:ILE:C | 50:D3:32:LEU:HG | 2.41 | 0.41 |
| 22:DA:112:G:O2' | 22:DA:113:C:H5' | 2.19 | 0.41 |
| 22:DA:61:G:H2' | 22:DA:62:C:H6 | 1.84 | 0.41 |
| 23:DB:1060:U:C1' | 23:DB:1062:G:H5' | 2.50 | 0.41 |
| 23:DB:1161:C:O2' | 23:DB:1162:G:H5' | 2.20 | 0.41 |
| 23:DB:1295:C:H2' | 23:DB:1296:G:C8 | 2.55 | 0.41 |
| 23:DB:1446:C:H2' | 23:DB:1447:C:C6 | 2.55 | 0.41 |
| 23:DB:1654:A:O2' | 23:DB:1655:A:H5' | 2.21 | 0.41 |
| 23:DB:182:A:O2' | 23:DB:183:C:H5' | 2.20 | 0.41 |
| 23:DB:2052:A:C4 | 26:DD:155:VAL:HG23 | 2.56 | 0.41 |
| 23:DB:2069:G:O2' | 23:DB:2070:A:H5' | 2.20 | 0.41 |
| 23:DB:2526:G:H2' | 23:DB:2527:C:C6 | 2.55 | 0.41 |
| 23:DB:289:G:H3' | 23:DB:289:G:OP2 | 2.20 | 0.41 |
| 23:DB:319:G:H2' | 23:DB:320:A:O4' | 2.21 | 0.41 |
| 23:DB:183:C:O2 | 23:DB:432:A:H2 | 2.04 | 0.41 |
| 23:DB:480:A:H2 | 23:DB:499:U:O2 | 2.03 | 0.41 |
| 23:DB:547:A:OP1 | 23:DB:548:G:OP2 | 2.39 | 0.41 |
| 23:DB:697:G:H2' | 23:DB:698:C:C6 | 2.56 | 0.41 |
| 23:DB:780:G:H2' | 23:DB:782:A:N7 | 2.35 | 0.41 |
| 23:DB:866:A:O2' | 23:DB:867:C:H5' | 2.20 | 0.41 |
| 27:DE:109:LEU:O | 27:DE:113:VAL:HG23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DE:155:GLU:O | 27:DE:159:LEU:HB2 | 2.20 | 0.41 |
| 27:DE:154:ASP:C | 27:DE:156:ASN:H | 2.23 | 0.41 |
| 27:DE:3:LEU:H | 27:DE:13:THR:N | 2.18 | 0.41 |
| 27:DE:62:GLN:HE21 | 27:DE:62:GLN:HB2 | 1.60 | 0.41 |
| 28:DF:133:GLU:HA | 28:DF:150:GLY:CA | 2.51 | 0.41 |
| 28:DF:74:ALA:C | 28:DF:76:PHE:H | 2.23 | 0.41 |
| 29:DG:71:LEU:O | 29:DG:75:VAL:HG23 | 2.21 | 0.41 |
| 52:DI:54:ILE:O | 52:DI:54:ILE:HG23 | 2.19 | 0.41 |
| 32:DK:13:ASN:HD21 | 32:DK:98:ARG:N | 2.08 | 0.41 |
| 32:DK:33:ALA:CB | 32:DK:39:ILE:HD11 | 2.50 | 0.41 |
| 32:DK:47:ILE:HG23 | 32:DK:48:PRO:CD | 2.51 | 0.41 |
| 34:DM:40:ARG:NH2 | 34:DM:73:ILE:HD12 | 2.35 | 0.41 |
| 35:DN:27:SER:O | 35:DN:30:ARG:HB2 | 2.20 | 0.41 |
| 36:DO:16:ARG:C | 36:DO:18:LEU:N | 2.74 | 0.41 |
| 38:DQ:77:LYS:O | 38:DQ:80:ASN:HB3 | 2.20 | 0.41 |
| 40:DS:24:ILE:CG2 | 40:DS:71:VAL:HG11 | 2.44 | 0.41 |
| 24:DV:24:ASN:O | 24:DV:26:PHE:N | 2.54 | 0.41 |
| 43:DW:18:LYS:CA | 43:DW:36:ILE:HG12 | 2.40 | 0.41 |
| 45:DY:40:THR:HG22 | 45:DY:42:ALA:H | 1.86 | 0.41 |
| 46:DZ:2:SER:O | 46:DZ:3:ARG:C | 2.58 | 0.41 |
| 1:AA:1119:C:O2' | 1:AA:1120:C:H5' | 2.21 | 0.41 |
| 1:AA:112:G:O2' | 1:AA:113:G:H5' | 2.20 | 0.41 |
| 1:AA:1230:C:H2' | 1:AA:1231:G:H8 | 1.86 | 0.41 |
| 1:AA:1313:U:O2' | 1:AA:1314:C:H5' | 2.20 | 0.41 |
| 1:AA:1320:C:H2' | 1:AA:1321:U:O4' | 2.21 | 0.41 |
| 1:AA:173:U:H5' | 1:AA:197:A:O4' | 2.21 | 0.41 |
| 1:AA:237:G:H2' | 1:AA:238:A:H8 | 1.85 | 0.41 |
| 1:AA:324:G:N1 | 1:AA:327:A:OP2 | 2.50 | 0.41 |
| 1:AA:618:C:H3' | 1:AA:620:C:OP2 | 2.21 | 0.41 |
| 1:AA:635:A:H2' | 1:AA:636:U:C6 | 2.56 | 0.41 |
| 1:AA:711:G:O2' | 1:AA:712:A:H5' | 2.20 | 0.41 |
| 1:AA:751:U:H2' | 1:AA:752:G:O4' | 2.21 | 0.41 |
| 1:AA:796:C:H5' | 10:AK:128:VAL:HG13 | 2.03 | 0.41 |
| 20:AB:85:SER:CB | 20:AB:221:ARG:HD3 | 2.38 | 0.41 |
| 20:AB:16:GLY:HA2 | 20:AB:40:ILE:HD12 | 2.02 | 0.41 |
| 2:AC:59:PRO:HB2 | 2:AC:60:ALA:H | 1.74 | 0.41 |
| 4:AE:93:VAL:HG22 | 4:AE:126:ALA:CB | 2.51 | 0.41 |
| 6:AG:64:ALA:O | 6:AG:68:VAL:HG23 | 2.21 | 0.41 |
| 8:AI:44:ARG:HB3 | 8:AI:48:ARG:NH2 | 2.35 | 0.41 |
| 8:AI:18:VAL:CG1 | 8:AI:82:ILE:HG12 | 2.51 | 0.41 |
| 10:AK:59:PRO:HA | 10:AK:90:PRO:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AM:7:ASN:N | 12:AM:7:ASN:HD22 | 2.18 | 0.41 |
| 15:AP:67:ILE:HD11 | 15:AP:75:ILE:HD11 | 2.02 | 0.41 |
| 18:AS:12:LEU:HA | 18:AS:15:LEU:HD12 | 2.02 | 0.41 |
| 49:B2:13:ASN:O | 49:B2:17:GLY:HA3 | 2.20 | 0.41 |
| 23:BB:839:U:O2' | 23:BB:1191:G:H1' | 2.20 | 0.41 |
| 23:BB:1577:C:H2' | 23:BB:1578:U:C6 | 2.55 | 0.41 |
| 23:BB:1716:U:H2' | 23:BB:1717:A:C8 | 2.55 | 0.41 |
| 23:BB:1829:A:N6 | 23:BB:1977:A:N6 | 2.68 | 0.41 |
| 23:BB:2018:G:O2' | 23:BB:2019:A:H5' | 2.21 | 0.41 |
| 23:BB:2076:U:O4' | 23:BB:2076:U:O2 | 2.39 | 0.41 |
| 23:BB:2356:U:H2' | 23:BB:2357:G:O4' | 2.21 | 0.41 |
| 23:BB:2671:G:H2' | 23:BB:2672:U:C6 | 2.56 | 0.41 |
| 23:BB:2720:U:H2' | 23:BB:2721:A:H8 | 1.86 | 0.41 |
| 23:BB:327:G:H2' | 23:BB:328:U:C6 | 2.56 | 0.41 |
| 23:BB:704:G:O2' | 23:BB:727:A:N6 | 2.53 | 0.41 |
| 23:BB:765:C:H2' | 23:BB:766:U:C6 | 2.55 | 0.41 |
| 23:BB:820:A:H2' | 23:BB:821:A:O4' | 2.20 | 0.41 |
| 25:BC:20:ASN:O | 25:BC:23:LEU:HB2 | 2.21 | 0.41 |
| 25:BC:90:ILE:HD13 | 25:BC:90:ILE:HA | 1.93 | 0.41 |
| 27:BE:46:GLN:HB2 | 27:BE:87:ALA:O | 2.20 | 0.41 |
| 29:BG:18:ILE:HA | 29:BG:22:VAL:O | 2.21 | 0.41 |
| 30:BH:5:LEU:HD12 | 30:BH:17:ASP:HB3 | 2.03 | 0.41 |
| 30:BH:70:GLU:O | 30:BH:72:ILE:N | 2.54 | 0.41 |
| 31:BJ:58:ASN:CA | 31:BJ:127:GLY:HA2 | 2.26 | 0.41 |
| 31:BJ:55:ILE:HG13 | 31:BJ:55:ILE:O | 2.19 | 0.41 |
| 32:BK:99:ILE:CB | 32:BK:118:LEU:HD22 | 2.47 | 0.41 |
| 33:BL:23:ILE:HD12 | 33:BL:23:ILE:H | 1.84 | 0.41 |
| 35:BN:28:LEU:HD21 | 35:BN:113:ILE:HG23 | 2.01 | 0.41 |
| 35:BN:94:TYR:C | 35:BN:116:VAL:HG12 | 2.41 | 0.41 |
| 35:BN:61:ALA:C | 35:BN:63:ARG:H | 2.22 | 0.41 |
| 35:BN:79:LEU:C | 35:BN:81:ASN:H | 2.24 | 0.41 |
| 36:BO:56:LYS:O | 36:BO:60:GLU:HG2 | 2.19 | 0.41 |
| 36:BO:79:ALA:O | 36:BO:83:LEU:HD13 | 2.20 | 0.41 |
| 37:BP:50:ARG:HB3 | 37:BP:57:ALA:N | 2.36 | 0.41 |
| 38:BQ:4:LYS:HE3 | 38:BQ:8:ILE:CD1 | 2.49 | 0.41 |
| 41:BT:50:LEU:O | 41:BT:51:PHE:HB2 | 2.21 | 0.41 |
| 42:BU:25:LYS:N | 42:BU:34:ILE:O | 2.54 | 0.41 |
| 23:BB:2336:A:H61 | 43:BW:40:ARG:CD | 2.34 | 0.41 |
| 43:BW:66:VAL:HG22 | 43:BW:81:ILE:HG22 | 2.03 | 0.41 |
| 45:BY:18:LYS:O | 45:BY:22:THR:HG23 | 2.21 | 0.41 |
| 1:CA:1036:A:H2' | 1:CA:1037:C:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1120:C:H2' | 1:CA:1121:U:H6 | 1.84 | 0.41 |
| 1:CA:1125:U:H1' | 1:CA:1126:U:H6 | 1.86 | 0.41 |
| 1:CA:1336:C:O4' | 1:CA:1337:G:C2 | 2.74 | 0.41 |
| 1:CA:187:G:N2 | 1:CA:189:A:H3' | 2.36 | 0.41 |
| 1:CA:245:U:H2' | 1:CA:246:A:H5' | 2.03 | 0.41 |
| 1:CA:409:U:H2' | 1:CA:410:G:C8 | 2.55 | 0.41 |
| 1:CA:486:U:O2' | 1:CA:487:A:H5' | 2.21 | 0.41 |
| 1:CA:516:U:O2' | 1:CA:517:G:H5' | 2.20 | 0.41 |
| 1:CA:126:G:H4' | 1:CA:634:C:O2 | 2.21 | 0.41 |
| 1:CA:637:C:H2' | 1:CA:638:U:C6 | 2.56 | 0.41 |
| 1:CA:746:A:N1 | 1:CA:747:A:N6 | 2.68 | 0.41 |
| 1:CA:572:A:N3 | 1:CA:917:G:H1' | 2.35 | 0.41 |
| 20:CB:164:ASP:OD1 | 20:CB:186:VAL:HA | 2.20 | 0.41 |
| 20:CB:75:ALA:O | 20:CB:78:ALA:N | 2.53 | 0.41 |
| 20:CB:77:GLU:O | 20:CB:77:GLU:HG2 | 2.21 | 0.41 |
| 2:CC:149:LYS:CB | 2:CC:168:ARG:HG3 | 2.51 | 0.41 |
| 2:CC:188:ALA:HB3 | 2:CC:195:ILE:HB | 2.02 | 0.41 |
| 2:CC:63:ILE:HD12 | 2:CC:98:ALA:CB | 2.48 | 0.41 |
| 2:CC:87:ARG:HB2 | 2:CC:100:ILE:CG2 | 2.51 | 0.41 |
| 3:CD:84:ASN:OD1 | 3:CD:87:GLU:HB2 | 2.20 | 0.41 |
| 6:CG:132:THR:HA | 6:CG:135:LYS:HB3 | 2.03 | 0.41 |
| 1:CA:1240:U:H3 | 6:CG:29:LEU:HD23 | 1.85 | 0.41 |
| 7:CH:12:ARG:NH1 | 7:CH:26:MET:HB3 | 2.35 | 0.41 |
| 10:CK:70:ALA:O | 10:CK:72:ALA:N | 2.53 | 0.41 |
| 1:CA:1226:C:H5' | 12:CM:94:LEU:HD11 | 2.03 | 0.41 |
| 8:CI:112:ARG:HD2 | 13:CN:100:TRP:OXT | 2.21 | 0.41 |
| 13:CN:15:LEU:HB3 | 13:CN:54:SER:CB | 2.44 | 0.41 |
| 14:CO:10:ILE:O | 14:CO:14:PHE:HD1 | 2.03 | 0.41 |
| 16:CQ:22:VAL:O | 16:CQ:42:LYS:HA | 2.21 | 0.41 |
| 16:CQ:18:LYS:H | 16:CQ:50:ASN:HD21 | 1.69 | 0.41 |
| 16:CQ:80:LYS:H | 16:CQ:80:LYS:NZ | 2.18 | 0.41 |
| 21:CU:44:ARG:NH1 | 21:CU:44:ARG:HG3 | 2.35 | 0.41 |
| 47:D0:25:THR:O | 47:D0:39:ARG:NH2 | 2.53 | 0.41 |
| 23:DB:1243:C:O2' | 23:DB:1244:A:H5' | 2.21 | 0.41 |
| 23:DB:1248:G:C4 | 38:DQ:2:ARG:HD2 | 2.56 | 0.41 |
| 23:DB:1258:U:H2' | 23:DB:1259:G:H8 | 1.85 | 0.41 |
| 23:DB:116:C:O2' | 23:DB:126:A:C8 | 2.69 | 0.41 |
| 23:DB:1280:G:H2' | 23:DB:1281:G:H5' | 2.02 | 0.41 |
| 23:DB:1572:A:O2' | 23:DB:1573:G:H5' | 2.21 | 0.41 |
| 23:DB:1704:C:H2' | 23:DB:1705:A:C8 | 2.56 | 0.41 |
| 23:DB:1889:A:H2' | 23:DB:1890:A:C8 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1901:A:OP2 | 25:DC:252:LYS:NZ | 2.53 | 0.41 |
| 23:DB:2143:C:H5'' | 23:DB:2144:G:C8 | 2.55 | 0.41 |
| 23:DB:2186:G:H2' | 23:DB:2187:U:O4' | 2.21 | 0.41 |
| 23:DB:2208:C:O2' | 23:DB:2209:G:H5' | 2.21 | 0.41 |
| 23:DB:2301:C:O2' | 23:DB:2302:U:H5' | 2.20 | 0.41 |
| 23:DB:2352:A:H8 | 23:DB:2352:A:O5' | 2.04 | 0.41 |
| 23:DB:246:C:H2' | 23:DB:247:G:C5' | 2.50 | 0.41 |
| 23:DB:2671:G:H2' | 23:DB:2672:U:C6 | 2.56 | 0.41 |
| 23:DB:2694:G:H2' | 23:DB:2695:U:C6 | 2.55 | 0.41 |
| 23:DB:2623:G:O5' | 23:DB:2826:A:H1' | 2.20 | 0.41 |
| 23:DB:324:A:H61 | 23:DB:338:G:C2' | 2.33 | 0.41 |
| 23:DB:453:A:N3 | 23:DB:457:A:O2' | 2.53 | 0.41 |
| 23:DB:810:U:O2' | 33:DL:20:GLY:HA3 | 2.21 | 0.41 |
| 25:DC:107:LYS:HB3 | 25:DC:108:GLY:H | 1.68 | 0.41 |
| 25:DC:156:SER:HB3 | 25:DC:159:THR:HG21 | 2.02 | 0.41 |
| 23:DB:764:A:H5'' | 25:DC:208:GLY:HA2 | 2.02 | 0.41 |
| 25:DC:245:THR:O | 25:DC:247:TRP:N | 2.53 | 0.41 |
| 27:DE:21:ARG:HG3 | 27:DE:22:ASP:O | 2.21 | 0.41 |
| 27:DE:61:ARG:O | 27:DE:62:GLN:C | 2.58 | 0.41 |
| 28:DF:105:ILE:O | 28:DF:109:ARG:HB2 | 2.20 | 0.41 |
| 28:DF:11:VAL:CG1 | 28:DF:12:VAL:H | 2.18 | 0.41 |
| 28:DF:37:MET:SD | 28:DF:52:ALA:HB1 | 2.60 | 0.41 |
| 29:DG:34:ARG:HD3 | 29:DG:34:ARG:N | 2.35 | 0.41 |
| 30:DH:5:LEU:HD12 | 30:DH:17:ASP:HB3 | 2.03 | 0.41 |
| 30:DH:83:LYS:HD2 | 30:DH:83:LYS:H | 1.85 | 0.41 |
| 23:DB:995:C:H42 | 31:DJ:2:LYS:HB2 | 1.86 | 0.41 |
| 23:DB:1666:G:O3' | 32:DK:6:THR:HG23 | 2.21 | 0.41 |
| 33:DL:61:LEU:HA | 33:DL:62:PRO:HD3 | 1.92 | 0.41 |
| 34:DM:73:ILE:HG21 | 34:DM:91:TYR:CE2 | 2.56 | 0.41 |
| 38:DQ:73:ILE:HD11 | 38:DQ:77:LYS:HB3 | 2.03 | 0.41 |
| 40:DS:3:THR:O | 40:DS:3:THR:HG23 | 2.21 | 0.41 |
| 40:DS:61:ASN:HD22 | 40:DS:61:ASN:HA | 1.55 | 0.41 |
| 40:DS:66:ILE:CG1 | 40:DS:67:ASP:N | 2.84 | 0.41 |
| 42:DU:25:LYS:N | 42:DU:34:ILE:O | 2.54 | 0.41 |
| 24:DV:1:MET:HE3 | 24:DV:2:PHE:HA | 2.02 | 0.41 |
| 24:DV:62:THR:CG2 | 24:DV:71:LYS:HG2 | 2.46 | 0.41 |
| 43:DW:15:SER:O | 43:DW:16:GLU:C | 2.58 | 0.41 |
| 43:DW:24:ARG:HH11 | 43:DW:65:LYS:HA | 1.86 | 0.41 |
| 43:DW:28:GLU:H | 43:DW:31:LEU:CD1 | 2.34 | 0.41 |
| 43:DW:35:ILE:O | 43:DW:37:VAL:N | 2.53 | 0.41 |
| 1:AA:1220:G:H2' | 1:AA:1221:G:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1258:G:C4 | 1:AA:1278:G:N2 | 2.89 | 0.41 |
| 1:AA:1473:G:O2' | 1:AA:1474:U:H5' | 2.21 | 0.41 |
| 1:AA:1514:G:H2' | 1:AA:1515:G:C8 | 2.55 | 0.41 |
| 1:AA:998:C:H2' | 1:AA:999:C:C6 | 2.56 | 0.41 |
| 20:AB:31:PHE:HB3 | 20:AB:39:ILE:HG22 | 2.03 | 0.41 |
| 20:AB:83:ALA:C | 20:AB:85:SER:H | 2.24 | 0.41 |
| 2:AC:87:ARG:HB2 | 2:AC:100:ILE:CG2 | 2.50 | 0.41 |
| 3:AD:191:SER:O | 3:AD:192:ALA:HB2 | 2.20 | 0.41 |
| 3:AD:197:HIS:CE1 | 3:AD:198:LEU:HG | 2.56 | 0.41 |
| 4:AE:107:GLY:C | 4:AE:109:ALA:H | 2.24 | 0.41 |
| 5:AF:47:LEU:HD21 | 5:AF:57:ALA:CB | 2.48 | 0.41 |
| 5:AF:90:MET:HE3 | 17:AR:60:ARG:HE | 1.84 | 0.41 |
| 1:AA:1348:U:C4' | 8:AI:121:ARG:HG3 | 2.46 | 0.41 |
| 10:AK:23:HIS:HB3 | 10:AK:30:ILE:HG12 | 2.03 | 0.41 |
| 12:AM:18:LEU:C | 12:AM:20:SER:N | 2.74 | 0.41 |
| 1:AA:1226:C:H5'' | 12:AM:94:LEU:HD11 | 2.02 | 0.41 |
| 14:AO:77:TYR:CZ | 14:AO:81:ILE:HD11 | 2.54 | 0.41 |
| 15:AP:28:ARG:HD3 | 15:AP:29:ASN:ND2 | 2.36 | 0.41 |
| 1:AA:1220:G:O3' | 18:AS:35:ARG:HD2 | 2.19 | 0.41 |
| 18:AS:44:ILE:HD12 | 18:AS:63:ASP:HA | 2.03 | 0.41 |
| 48:B1:22:THR:OG1 | 48:B1:23:THR:N | 2.53 | 0.41 |
| 49:B2:21:ARG:HG2 | 49:B2:31:LEU:HD21 | 2.02 | 0.41 |
| 50:B3:44:ARG:N | 50:B3:45:PRO:CD | 2.82 | 0.41 |
| 22:BA:113:C:H2' | 22:BA:114:C:C6 | 2.56 | 0.41 |
| 23:BB:1423:G:H2' | 23:BB:1424:G:H8 | 1.86 | 0.41 |
| 23:BB:164:C:H2' | 23:BB:165:A:H5' | 2.03 | 0.41 |
| 23:BB:181:A:H1' | 23:BB:435:C:H5' | 2.03 | 0.41 |
| 23:BB:776:G:N1 | 23:BB:2072:C:OP1 | 2.43 | 0.41 |
| 23:BB:2391:G:O6 | 23:BB:2427:C:H1' | 2.21 | 0.41 |
| 23:BB:2465:C:O2' | 23:BB:2466:C:H5' | 2.19 | 0.41 |
| 23:BB:2526:G:O2' | 51:B4:34:LYS:HE3 | 2.21 | 0.41 |
| 23:BB:2693:G:H2' | 23:BB:2694:G:C8 | 2.50 | 0.41 |
| 23:BB:2786:U:H2' | 23:BB:2787:C:H6 | 1.85 | 0.41 |
| 23:BB:528:A:H3' | 23:BB:528:A:H8 | 1.85 | 0.41 |
| 23:BB:689:A:H2' | 23:BB:690:G:H8 | 1.86 | 0.41 |
| 23:BB:705:A:H8 | 23:BB:705:A:O5' | 2.02 | 0.41 |
| 23:BB:833:A:H1' | 33:BL:52:GLY:N | 2.35 | 0.41 |
| 23:BB:974:G:H2' | 23:BB:974:G:N3 | 2.35 | 0.41 |
| 23:BB:988:A:H5'' | 45:BY:11:SER:HB3 | 2.02 | 0.41 |
| 25:BC:153:LEU:HD22 | 25:BC:175:LEU:HD22 | 2.02 | 0.41 |
| 26:BD:24:VAL:HG23 | 26:BD:189:VAL:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BE:154:ASP:C | 27:BE:156:ASN:H | 2.24 | 0.41 |
| 28:BF:163:GLU:HA | 28:BF:166:ARG:NH1 | 2.36 | 0.41 |
| 29:BG:40:VAL:CG2 | 29:BG:64:ALA:HA | 2.45 | 0.41 |
| 29:BG:89:VAL:CG1 | 29:BG:90:GLY:H | 2.27 | 0.41 |
| 52:BI:91:LYS:O | 52:BI:94:LYS:HB2 | 2.21 | 0.41 |
| 23:BB:7:G:H4' | 31:BJ:15:TRP:HZ2 | 1.85 | 0.41 |
| 32:BK:6:THR:HG22 | 32:BK:7:MET:H | 1.85 | 0.41 |
| 34:BM:73:ILE:HG21 | 34:BM:91:TYR:CE2 | 2.55 | 0.41 |
| 36:BO:15:ARG:HH21 | 36:BO:95:SER:HB3 | 1.85 | 0.41 |
| 36:BO:63:LYS:HD2 | 36:BO:64:TYR:HB2 | 2.03 | 0.41 |
| 38:BQ:111:LYS:NZ | 38:BQ:111:LYS:HB2 | 2.34 | 0.41 |
| 38:BQ:81:GLY:O | 38:BQ:85:ALA:N | 2.52 | 0.41 |
| 40:BS:3:THR:O | 40:BS:3:THR:HG23 | 2.21 | 0.41 |
| 41:BT:17:SER:N | 41:BT:21:SER:OG | 2.53 | 0.41 |
| 41:BT:53:VAL:HG12 | 41:BT:54:GLU:N | 2.36 | 0.41 |
| 24:BV:75:GLN:HG2 | 24:BV:92:VAL:CG2 | 2.44 | 0.41 |
| 24:BV:32:GLY:O | 24:BV:93:ARG:HB2 | 2.21 | 0.41 |
| 1:CA:1053:G:C6 | 1:CA:1199:U:H2' | 2.56 | 0.41 |
| 1:CA:1178:G:H2' | 1:CA:1180:A:OP2 | 2.20 | 0.41 |
| 1:CA:1366:C:H2' | 1:CA:1367:C:C6 | 2.55 | 0.41 |
| 1:CA:259:G:O2' | 1:CA:260:G:H5' | 2.20 | 0.41 |
| 1:CA:415:A:N1 | 1:CA:428:G:O6 | 2.54 | 0.41 |
| 1:CA:585:G:H4' | 11:CL:4:ASN:HD21 | 1.86 | 0.41 |
| 1:CA:599:C:H2' | 1:CA:600:A:H8 | 1.85 | 0.41 |
| 1:CA:621:A:H2' | 1:CA:622:A:H8 | 1.84 | 0.41 |
| 1:CA:987:G:H2' | 1:CA:988:G:H8 | 1.85 | 0.41 |
| 20:CB:18:GLN:C | 20:CB:37:VAL:HG23 | 2.41 | 0.41 |
| 2:CC:134:LYS:HE3 | 2:CC:138:GLN:HG2 | 2.02 | 0.41 |
| 2:CC:123:LEU:HD12 | 2:CC:188:ALA:CB | 2.51 | 0.41 |
| 3:CD:116:LEU:O | 3:CD:121:ALA:HB3 | 2.20 | 0.41 |
| 5:CF:6:ILE:HD12 | 5:CF:7:VAL:N | 2.35 | 0.41 |
| 1:CA:1375:A:P | 6:CG:24:LYS:HZ3 | 2.43 | 0.41 |
| 1:CA:600:A:OP1 | 7:CH:87:ARG:HB3 | 2.21 | 0.41 |
| 9:CJ:17:LEU:HD13 | 9:CJ:96:VAL:HG13 | 2.01 | 0.41 |
| 10:CK:92:ARG:HH11 | 10:CK:92:ARG:HG2 | 1.84 | 0.41 |
| 12:CM:80:MET:C | 12:CM:82:LEU:H | 2.24 | 0.41 |
| 16:CQ:52:CYS:SG | 16:CQ:74:LEU:HG | 2.61 | 0.41 |
| 18:CS:20:LYS:NZ | 18:CS:24:SER:HB3 | 2.36 | 0.41 |
| 19:CT:38:ILE:HD11 | 19:CT:82:ILE:HA | 2.03 | 0.41 |
| 21:CU:36:PHE:CD1 | 21:CU:44:ARG:HD3 | 2.56 | 0.41 |
| 49:D2:39:ARG:HG3 | 49:D2:39:ARG:NH1 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:1099:G:N7 | 52:DI:3:LYS:CD | 2.84 | 0.41 |
| 23:DB:1126:A:H4' | 23:DB:1127:A:C5' | 2.50 | 0.41 |
| 23:DB:1174:U:O2 | 23:DB:1174:U:H2' | 2.20 | 0.41 |
| 23:DB:1187:G:H5'' | 39:DR:83:TYR:CZ | 2.55 | 0.41 |
| 23:DB:1322:A:C5 | 23:DB:1323:C:C5 | 3.09 | 0.41 |
| 23:DB:1475:G:OP1 | 23:DB:1475:G:H3' | 2.21 | 0.41 |
| 23:DB:1577:C:H2' | 23:DB:1578:U:C6 | 2.55 | 0.41 |
| 23:DB:1636:U:H2' | 23:DB:1637:A:C8 | 2.56 | 0.41 |
| 23:DB:191:A:O2' | 23:DB:192:C:H5' | 2.21 | 0.41 |
| 23:DB:2039:U:O2' | 23:DB:2040:G:H5' | 2.21 | 0.41 |
| 23:DB:2262:U:H2' | 23:DB:2263:C:H6 | 1.86 | 0.41 |
| 23:DB:2336:A:N6 | 43:DW:40:ARG:CG | 2.81 | 0.41 |
| 23:DB:2369:A:H2' | 23:DB:2370:G:C8 | 2.55 | 0.41 |
| 23:DB:2393:U:H5' | 33:DL:60:ARG:O | 2.21 | 0.41 |
| 23:DB:2623:G:O2' | 23:DB:2624:G:H5' | 2.21 | 0.41 |
| 23:DB:2675:A:H4' | 32:DK:29:HIS:HB2 | 2.02 | 0.41 |
| 23:DB:2721:A:H2' | 23:DB:2722:G:C8 | 2.55 | 0.41 |
| 23:DB:2751:G:N3 | 23:DB:2751:G:H2' | 2.35 | 0.41 |
| 23:DB:275:C:H2' | 23:DB:276:U:O4' | 2.20 | 0.41 |
| 23:DB:316:C:O2' | 23:DB:317:G:H5' | 2.20 | 0.41 |
| 23:DB:379:G:N1 | 23:DB:396:G:C6 | 2.89 | 0.41 |
| 23:DB:466:A:N3 | 23:DB:683:U:H1' | 2.36 | 0.41 |
| 23:DB:514:A:N6 | 23:DB:515:A:N6 | 2.68 | 0.41 |
| 23:DB:667:U:H2' | 23:DB:668:A:O4' | 2.21 | 0.41 |
| 25:DC:132:ARG:HG3 | 25:DC:132:ARG:O | 2.20 | 0.41 |
| 25:DC:203:VAL:O | 25:DC:204:LEU:HB2 | 2.21 | 0.41 |
| 25:DC:221:GLY:C | 25:DC:223:ALA:N | 2.73 | 0.41 |
| 26:DD:38:LYS:HD3 | 26:DD:45:TYR:OH | 2.21 | 0.41 |
| 29:DG:33:THR:HA | 29:DG:34:ARG:NH1 | 2.36 | 0.41 |
| 29:DG:67:ALA:O | 29:DG:71:LEU:HD23 | 2.21 | 0.41 |
| 30:DH:14:SER:HB2 | 30:DH:17:ASP:HB3 | 2.03 | 0.41 |
| 52:DI:91:LYS:HD2 | 52:DI:91:LYS:N | 2.35 | 0.41 |
| 31:DJ:20:ALA:HA | 31:DJ:23:LYS:CG | 2.50 | 0.41 |
| 31:DJ:24:THR:O | 31:DJ:25:LEU:HB3 | 2.20 | 0.41 |
| 31:DJ:45:THR:H | 31:DJ:46:PRO:CD | 2.28 | 0.41 |
| 32:DK:109:SER:O | 32:DK:111:LYS:N | 2.54 | 0.41 |
| 23:DB:1243:C:O2 | 33:DL:4:ASN:HA | 2.20 | 0.41 |
| 23:DB:2358:A:H61 | 33:DL:54:GLN:HE22 | 1.68 | 0.41 |
| 35:DN:82:GLU:HB3 | 35:DN:83:LEU:H | 1.63 | 0.41 |
| 36:DO:88:LYS:HA | 36:DO:115:LEU:HD13 | 2.03 | 0.41 |
| 36:DO:63:LYS:HD2 | 36:DO:64:TYR:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DQ:109:VAL:CG1 | 38:DQ:113:LYS:HE3 | 2.50 | 0.41 |
| 41:DT:72:GLN:HG2 | 41:DT:72:GLN:H | 1.68 | 0.41 |
| 24:DV:2:PHE:HD2 | 24:DV:59:GLU:OE1 | 2.03 | 0.41 |
| 43:DW:44:PHE:CE2 | 43:DW:76:ARG:HD3 | 2.56 | 0.41 |
| 45:DY:6:ILE:HB | 45:DY:35:VAL:HG12 | 2.03 | 0.41 |
| 1:AA:1073:U:O2' | 1:AA:1074:G:H5' | 2.21 | 0.41 |
| 1:AA:1098:C:O2' | 1:AA:1099:G:H5' | 2.20 | 0.41 |
| 1:AA:1162:C:H2' | 1:AA:1163:A:O4' | 2.21 | 0.41 |
| 1:AA:1170:A:H2' | 1:AA:1171:A:O4' | 2.21 | 0.41 |
| 1:AA:1325:C:H2' | 1:AA:1326:U:H6 | 1.85 | 0.41 |
| 1:AA:237:G:H5'' | 16:AQ:26:ARG:NH2 | 2.36 | 0.41 |
| 1:AA:397:A:N3 | 1:AA:397:A:H3' | 2.36 | 0.41 |
| 1:AA:509:A:H5' | 3:AD:51:GLY:HA2 | 2.02 | 0.41 |
| 1:AA:51:A:H4' | 1:AA:52:C:C5' | 2.51 | 0.41 |
| 1:AA:641:U:H1' | 1:AA:642:A:N7 | 2.35 | 0.41 |
| 1:AA:984:C:H2' | 1:AA:985:C:C6 | 2.55 | 0.41 |
| 2:AC:63:ILE:CD1 | 2:AC:98:ALA:HB2 | 2.46 | 0.41 |
| 3:AD:155:LYS:HG3 | 3:AD:156:ALA:N | 2.36 | 0.41 |
| 3:AD:31:CYS:O | 3:AD:32:LYS:HB2 | 2.20 | 0.41 |
| 4:AE:11:GLN:HB2 | 4:AE:116:VAL:HB | 2.03 | 0.41 |
| 6:AG:148:LYS:HG3 | 6:AG:151:ALA:HB3 | 2.02 | 0.41 |
| 1:AA:586:C:O2' | 7:AH:3:GLN:NE2 | 2.54 | 0.41 |
| 8:AI:64:ILE:HD12 | 8:AI:64:ILE:N | 2.31 | 0.41 |
| 1:AA:975:A:N1 | 9:AJ:50:THR:HB | 2.36 | 0.41 |
| 10:AK:51:PHE:O | 10:AK:51:PHE:HD1 | 2.03 | 0.41 |
| 11:AL:66:ILE:HG22 | 11:AL:66:ILE:O | 2.21 | 0.41 |
| 13:AN:27:LYS:HA | 13:AN:31:SER:HB2 | 2.03 | 0.41 |
| 13:AN:78:LEU:HD23 | 13:AN:82:LYS:HB3 | 2.03 | 0.41 |
| 16:AQ:25:GLU:HA | 16:AQ:39:ARG:O | 2.21 | 0.41 |
| 18:AS:13:HIS:HD2 | 18:AS:34:SER:HB3 | 1.86 | 0.41 |
| 19:AT:27:MET:O | 19:AT:31:ILE:HG13 | 2.20 | 0.41 |
| 23:BB:1562:U:H2' | 23:BB:1563:U:C6 | 2.55 | 0.41 |
| 23:BB:1831:G:C6 | 23:BB:1832:C:N4 | 2.89 | 0.41 |
| 23:BB:1859:U:H2' | 23:BB:1860:G:H8 | 1.86 | 0.41 |
| 23:BB:227:A:H61 | 23:BB:410:G:H1' | 1.85 | 0.41 |
| 23:BB:2471:A:O2' | 23:BB:2472:G:C8 | 2.60 | 0.41 |
| 23:BB:2531:A:H5'' | 29:BG:156:TYR:CE2 | 2.56 | 0.41 |
| 23:BB:2835:A:H61 | 23:BB:2878:U:H2' | 1.86 | 0.41 |
| 23:BB:2848:G:N3 | 23:BB:2849:U:H5 | 2.18 | 0.41 |
| 23:BB:319:G:H2' | 23:BB:320:A:O4' | 2.21 | 0.41 |
| 25:BC:80:LEU:HD21 | 25:BC:109:LEU:HG | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:2580:U:H5' | 26:BD:136:ASN:H | 1.86 | 0.41 |
| 28:BF:11:VAL:HG13 | 28:BF:171:ALA:HB1 | 2.03 | 0.41 |
| 30:BH:40:THR:C | 30:BH:42:LYS:H | 2.21 | 0.41 |
| 30:BH:58:LEU:HB3 | 30:BH:59:ALA:H | 1.73 | 0.41 |
| 52:BI:83:ALA:N | 52:BI:100:ILE:HD11 | 2.35 | 0.41 |
| 52:BI:35:MET:C | 52:BI:35:MET:SD | 2.99 | 0.41 |
| 52:BI:14:ALA:CB | 52:BI:50:LYS:HA | 2.50 | 0.41 |
| 32:BK:33:ALA:CB | 32:BK:39:ILE:HD11 | 2.51 | 0.41 |
| 27:BE:181:ILE:CG1 | 33:BL:2:ARG:HB3 | 2.46 | 0.41 |
| 34:BM:61:GLY:HA2 | 34:BM:107:GLY:C | 2.41 | 0.41 |
| 35:BN:79:LEU:HA | 35:BN:83:LEU:HD12 | 2.03 | 0.41 |
| 41:BT:28:ASN:C | 41:BT:29:THR:HG23 | 2.41 | 0.41 |
| 43:BW:56:HIS:O | 43:BW:57:THR:C | 2.59 | 0.41 |
| 1:CA:1073:U:OP1 | 4:CE:61:LYS:HE3 | 2.21 | 0.41 |
| 1:CA:1125:U:H5' | 9:CJ:40:ILE:HD11 | 2.03 | 0.41 |
| 1:CA:1174:G:O2' | 1:CA:1175:G:H5' | 2.20 | 0.41 |
| 1:CA:1296:C:C5' | 1:CA:1302:C:H42 | 2.34 | 0.41 |
| 1:CA:141:G:H2' | 1:CA:142:G:O4' | 2.20 | 0.41 |
| 1:CA:451:A:H1' | 1:CA:452:A:C8 | 2.56 | 0.41 |
| 1:CA:538:G:O3' | 11:CL:110:LYS:HG3 | 2.21 | 0.41 |
| 1:CA:601:G:O2' | 1:CA:602:A:H5' | 2.21 | 0.41 |
| 20:CB:26:MET:HG3 | 20:CB:188:THR:O | 2.19 | 0.41 |
| 20:CB:75:ALA:O | 20:CB:76:SER:C | 2.59 | 0.41 |
| 3:CD:141:VAL:HA | 3:CD:179:GLY:O | 2.20 | 0.41 |
| 3:CD:29:THR:CG2 | 3:CD:30:LYS:HD3 | 2.49 | 0.41 |
| 3:CD:7:LYS:HD2 | 3:CD:21:LYS:NZ | 2.35 | 0.41 |
| 4:CE:117:ALA:HB3 | 4:CE:119:VAL:HG23 | 2.03 | 0.41 |
| 5:CF:68:GLN:HA | 5:CF:71:ILE:HG12 | 2.02 | 0.41 |
| 6:CG:80:GLY:C | 6:CG:82:SER:H | 2.25 | 0.41 |
| 8:CI:28:VAL:HA | 8:CI:32:ARG:O | 2.21 | 0.41 |
| 8:CI:50:PRO:HD3 | 8:CI:79:ARG:HG3 | 2.03 | 0.41 |
| 8:CI:87:MET:SD | 8:CI:88:GLU:N | 2.93 | 0.41 |
| 9:CJ:8:ILE:O | 9:CJ:74:VAL:HB | 2.20 | 0.41 |
| 49:D2:41:ARG:O | 49:D2:42:LEU:C | 2.59 | 0.41 |
| 22:DA:17:C:O2' | 22:DA:18:G:H5' | 2.21 | 0.41 |
| 22:DA:49:C:O2' | 22:DA:50:A:H5' | 2.21 | 0.41 |
| 23:DB:1032:A:H4' | 51:D4:16:ILE:HD13 | 2.01 | 0.41 |
| 23:DB:1058:U:H1' | 52:DI:117:THR:HG22 | 2.03 | 0.41 |
| 23:DB:1080:A:O2' | 23:DB:1081:U:H5' | 2.21 | 0.41 |
| 23:DB:1159:U:O2' | 23:DB:1160:G:H5' | 2.20 | 0.41 |
| 23:DB:1210:G:H4' | 23:DB:1211:C:OP2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:1233:C:O2' | 23:DB:1234:U:H5' | 2.21 | 0.41 |
| 23:DB:1392:A:H2' | 23:DB:1393:A:C8 | 2.56 | 0.41 |
| 23:DB:1463:C:H2' | 23:DB:1464:G:H8 | 1.85 | 0.41 |
| 23:DB:1513:U:H2' | 23:DB:1514:G:O4' | 2.20 | 0.41 |
| 23:DB:1736:U:H2' | 23:DB:1737:G:O4' | 2.21 | 0.41 |
| 23:DB:1862:G:O2' | 23:DB:1863:G:H5' | 2.21 | 0.41 |
| 23:DB:2081:U:H2' | 23:DB:2082:A:C8 | 2.56 | 0.41 |
| 23:DB:2143:C:H3' | 23:DB:2144:G:O4' | 2.21 | 0.41 |
| 23:DB:2212:A:C8 | 23:DB:2214:C:N4 | 2.88 | 0.41 |
| 23:DB:2305:U:C5 | 28:DF:151:LEU:HA | 2.56 | 0.41 |
| 23:DB:2393:U:H5'' | 33:DL:62:PRO:CG | 2.44 | 0.41 |
| 23:DB:707:G:O2' | 23:DB:708:G:H5' | 2.20 | 0.41 |
| 23:DB:942:G:O2' | 23:DB:943:A:H5' | 2.21 | 0.41 |
| 25:DC:259:ASN:OD1 | 25:DC:261:ARG:HB3 | 2.21 | 0.41 |
| 23:DB:1568:G:H4' | 25:DC:58:LYS:HB3 | 2.03 | 0.41 |
| 28:DF:81:GLY:O | 28:DF:82:TYR:C | 2.59 | 0.41 |
| 30:DH:50:ARG:HG3 | 30:DH:54:LEU:HD11 | 2.03 | 0.41 |
| 31:DJ:25:LEU:HA | 31:DJ:28:LEU:HD23 | 2.03 | 0.41 |
| 31:DJ:6:ALA:CB | 31:DJ:45:THR:HG21 | 2.46 | 0.41 |
| 31:DJ:72:LYS:HB3 | 31:DJ:73:VAL:H | 1.52 | 0.41 |
| 26:DD:21:SER:HB2 | 32:DK:73:ASP:HA | 2.02 | 0.41 |
| 33:DL:47:ARG:HG3 | 33:DL:48:ARG:N | 2.36 | 0.41 |
| 24:DV:29:ILE:O | 24:DV:29:ILE:HD12 | 2.20 | 0.41 |
| 1:AA:1095:U:H5'' | 1:AA:1109:C:O2 | 2.19 | 0.41 |
| 1:AA:1254:A:H2' | 1:AA:1255:G:O4' | 2.21 | 0.41 |
| 1:AA:1307:U:H2' | 1:AA:1308:U:H6 | 1.82 | 0.41 |
| 1:AA:488:C:H2' | 1:AA:489:C:H6 | 1.86 | 0.41 |
| 2:AC:126:ARG:HA | 2:AC:126:ARG:NE | 2.36 | 0.41 |
| 3:AD:72:ARG:O | 3:AD:75:TYR:HB3 | 2.21 | 0.41 |
| 5:AF:18:VAL:O | 5:AF:22:ILE:HG13 | 2.20 | 0.41 |
| 6:AG:149:ALA:H | 10:AK:55:ARG:HH21 | 1.63 | 0.41 |
| 7:AH:68:LYS:HZ3 | 7:AH:69:ALA:HB3 | 1.86 | 0.41 |
| 8:AI:48:ARG:HA | 8:AI:51:LEU:HD12 | 2.02 | 0.41 |
| 8:AI:14:SER:HB2 | 8:AI:69:GLY:HA3 | 2.01 | 0.41 |
| 9:AJ:53:ILE:HG23 | 9:AJ:54:SER:N | 2.36 | 0.41 |
| 12:AM:15:VAL:HG22 | 12:AM:33:LEU:HD12 | 2.02 | 0.41 |
| 13:AN:68:ARG:HH11 | 13:AN:68:ARG:HG2 | 1.86 | 0.41 |
| 14:AO:80:LEU:HD23 | 14:AO:80:LEU:C | 2.41 | 0.41 |
| 16:AQ:75:VAL:CG2 | 16:AQ:76:ARG:N | 2.83 | 0.41 |
| 1:AA:664:G:P | 17:AR:52:ARG:HH21 | 2.44 | 0.41 |
| 48:B1:35:LEU:N | 48:B1:35:LEU:CD2 | 2.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:B1:39:ASP:O | 48:B1:43:ARG:N | 2.53 | 0.41 |
| 48:B1:46:VAL:HG22 | 48:B1:47:ILE:N | 2.28 | 0.41 |
| 23:BB:1076:C:H4' | 52:BI:94:LYS:CE | 2.50 | 0.41 |
| 23:BB:1188:U:O2' | 23:BB:1189:A:H5' | 2.21 | 0.41 |
| 23:BB:1341:G:C2 | 23:BB:1398:C:H4' | 2.56 | 0.41 |
| 23:BB:141:G:H5'' | 23:BB:142:A:C6 | 2.56 | 0.41 |
| 23:BB:1537:G:N3 | 23:BB:1537:G:H5'' | 2.36 | 0.41 |
| 23:BB:1773:A:H2' | 23:BB:1774:C:O4' | 2.20 | 0.41 |
| 23:BB:1948:G:C6 | 23:BB:1959:G:C6 | 3.09 | 0.41 |
| 23:BB:268:C:H2' | 23:BB:268:C:O2 | 2.21 | 0.41 |
| 23:BB:2800:A:H2' | 23:BB:2801:G:C4' | 2.51 | 0.41 |
| 23:BB:2800:A:C2 | 23:BB:2801:G:H1' | 2.56 | 0.41 |
| 23:BB:325:G:O2' | 23:BB:326:G:H5' | 2.20 | 0.41 |
| 23:BB:699:A:H2' | 23:BB:700:G:O4' | 2.21 | 0.41 |
| 23:BB:769:U:H2' | 23:BB:770:G:C8 | 2.55 | 0.41 |
| 23:BB:949:G:O2' | 23:BB:950:G:H5' | 2.21 | 0.41 |
| 25:BC:128:THR:HG22 | 25:BC:188:ARG:HB3 | 2.03 | 0.41 |
| 25:BC:83:ASP:HA | 25:BC:84:PRO:HD3 | 1.89 | 0.41 |
| 23:BB:2635:A:C5' | 26:BD:79:LEU:HB2 | 2.51 | 0.41 |
| 27:BE:166:LYS:O | 27:BE:167:VAL:CB | 2.69 | 0.41 |
| 27:BE:46:GLN:HB3 | 27:BE:86:ALA:CA | 2.51 | 0.41 |
| 28:BF:107:VAL:O | 28:BF:110:ILE:HG22 | 2.20 | 0.41 |
| 28:BF:133:GLU:HA | 28:BF:150:GLY:CA | 2.50 | 0.41 |
| 29:BG:84:LYS:HB2 | 29:BG:132:LEU:H | 1.86 | 0.41 |
| 30:BH:141:LYS:N | 30:BH:141:LYS:CD | 2.83 | 0.41 |
| 31:BJ:43:GLU:O | 31:BJ:44:TYR:C | 2.58 | 0.41 |
| 23:BB:670:A:H3' | 33:BL:43:GLY:H | 1.86 | 0.41 |
| 33:BL:56:PRO:O | 33:BL:59:ARG:HB2 | 2.21 | 0.41 |
| 35:BN:80:PHE:N | 35:BN:84:GLY:HA3 | 2.36 | 0.41 |
| 40:BS:20:VAL:HG13 | 40:BS:21:ALA:N | 2.36 | 0.41 |
| 41:BT:63:VAL:HG12 | 41:BT:65:GLY:H | 1.86 | 0.41 |
| 24:BV:14:LYS:HE3 | 24:BV:18:ARG:HH21 | 1.85 | 0.41 |
| 24:BV:4:ILE:HB | 24:BV:63:ILE:HA | 2.02 | 0.41 |
| 44:BX:25:GLN:HB3 | 44:BX:25:GLN:HE21 | 1.53 | 0.41 |
| 1:CA:1115:U:H2' | 1:CA:1116:U:C6 | 2.56 | 0.41 |
| 1:CA:1194:U:H2' | 1:CA:1195:C:C6 | 2.56 | 0.41 |
| 1:CA:1258:G:C2 | 1:CA:1278:G:N2 | 2.89 | 0.41 |
| 1:CA:1319:A:H4' | 1:CA:1320:C:OP1 | 2.20 | 0.41 |
| 1:CA:170:U:O2' | 1:CA:171:A:H5' | 2.20 | 0.41 |
| 1:CA:264:C:H2' | 1:CA:265:G:O4' | 2.21 | 0.41 |
| 1:CA:284:C:O2' | 1:CA:285:C:H5' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:653:U:C6 | 7:CH:55:LYS:HE2 | 2.56 | 0.41 |
| 1:CA:736:C:H2' | 1:CA:737:C:H6 | 1.85 | 0.41 |
| 1:CA:986:U:H2' | 1:CA:987:G:O4' | 2.21 | 0.41 |
| 20:CB:165:ALA:H | 20:CB:186:VAL:CG1 | 2.34 | 0.41 |
| 20:CB:67:LEU:HG | 20:CB:153:MET:HE2 | 2.03 | 0.41 |
| 2:CC:102:ILE:HD12 | 2:CC:102:ILE:N | 2.36 | 0.41 |
| 2:CC:112:ALA:CB | 2:CC:184:ASN:HB2 | 2.47 | 0.41 |
| 2:CC:85:LYS:O | 2:CC:89:VAL:HG23 | 2.21 | 0.41 |
| 3:CD:148:ALA:O | 3:CD:154:VAL:HG11 | 2.21 | 0.41 |
| 4:CE:77:ASN:CG | 4:CE:78:GLY:H | 2.19 | 0.41 |
| 5:CF:36:ILE:HA | 5:CF:64:VAL:HG13 | 2.02 | 0.41 |
| 8:CI:44:ARG:NE | 8:CI:48:ARG:HH22 | 2.19 | 0.41 |
| 12:CM:29:SER:HA | 12:CM:32:ILE:HG22 | 2.03 | 0.41 |
| 18:CS:35:ARG:HB3 | 18:CS:50:VAL:CG1 | 2.51 | 0.41 |
| 48:D1:28:THR:C | 48:D1:30:PRO:HD3 | 2.41 | 0.41 |
| 50:D3:7:ARG:NH1 | 50:D3:7:ARG:HG3 | 2.36 | 0.41 |
| 23:DB:1068:G:C6 | 23:DB:1069:A:N6 | 2.89 | 0.41 |
| 23:DB:1409:U:O2' | 23:DB:1410:G:H5' | 2.21 | 0.41 |
| 23:DB:1573:G:H2' | 23:DB:1574:C:H5' | 2.02 | 0.41 |
| 23:DB:1689:A:O2' | 23:DB:1690:A:H5' | 2.20 | 0.41 |
| 23:DB:1824:G:O2' | 23:DB:1825:U:H5' | 2.21 | 0.41 |
| 23:DB:1902:C:H2' | 23:DB:1903:G:O4' | 2.19 | 0.41 |
| 23:DB:1914:C:O2' | 23:DB:1915:U:H5' | 2.21 | 0.41 |
| 23:DB:2455:G:H2' | 23:DB:2456:C:H6 | 1.85 | 0.41 |
| 23:DB:2480:C:O2' | 23:DB:2481:G:H5' | 2.21 | 0.41 |
| 23:DB:2818:U:O5' | 23:DB:2837:A:H1' | 2.21 | 0.41 |
| 23:DB:524:G:O2' | 23:DB:525:U:H5' | 2.20 | 0.41 |
| 23:DB:597:G:H2' | 23:DB:598:U:C6 | 2.55 | 0.41 |
| 23:DB:783:A:C2' | 23:DB:784:G:O5' | 2.68 | 0.41 |
| 23:DB:858:G:C2 | 23:DB:2268:A:C4 | 3.09 | 0.41 |
| 25:DC:109:LEU:O | 25:DC:110:LYS:C | 2.59 | 0.41 |
| 25:DC:115:ILE:HG13 | 25:DC:115:ILE:O | 2.20 | 0.41 |
| 25:DC:146:LYS:CB | 25:DC:147:PRO:HD2 | 2.32 | 0.41 |
| 25:DC:72:GLY:O | 25:DC:73:ILE:HD13 | 2.20 | 0.41 |
| 26:DD:151:THR:CB | 26:DD:152:PRO:HD3 | 2.51 | 0.41 |
| 26:DD:68:PHE:CB | 26:DD:73:VAL:HG23 | 2.51 | 0.41 |
| 27:DE:112:LEU:C | 27:DE:114:ARG:N | 2.75 | 0.41 |
| 29:DG:49:LEU:HG | 29:DG:50:THR:H | 1.86 | 0.41 |
| 52:DI:10:LEU:C | 52:DI:10:LEU:HD12 | 2.40 | 0.41 |
| 33:DL:124:GLY:CA | 33:DL:143:GLU:HG3 | 2.50 | 0.41 |
| 33:DL:81:ASP:HA | 33:DL:84:LYS:CD | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DN:24:MET:HE1 | 35:DN:40:LYS:HB3 | 2.03 | 0.41 |
| 35:DN:87:PHE:C | 35:DN:89:SER:H | 2.25 | 0.41 |
| 41:DT:27:SER:O | 41:DT:28:ASN:CB | 2.69 | 0.41 |
| 42:DU:21:ARG:HD3 | 42:DU:72:PHE:CG | 2.56 | 0.41 |
| 24:DV:42:LEU:HB2 | 24:DV:47:VAL:HG21 | 2.02 | 0.41 |
| 43:DW:65:LYS:H | 43:DW:84:GLU:HB3 | 1.86 | 0.41 |
| 46:DZ:36:HIS:HB3 | 46:DZ:38:PHE:CE2 | 2.56 | 0.41 |
| 1:AA:1072:G:H2' | 1:AA:1073:U:H6 | 1.85 | 0.41 |
| 1:AA:1176:A:H2' | 1:AA:1177:G:O4' | 2.21 | 0.41 |
| 1:AA:176:C:H3' | 1:AA:177:G:N2 | 2.35 | 0.41 |
| 1:AA:20:U:H2' | 1:AA:21:G:O4' | 2.21 | 0.41 |
| 1:AA:270:A:H2' | 1:AA:271:C:H6 | 1.82 | 0.41 |
| 1:AA:334:C:H2' | 1:AA:335:C:C6 | 2.56 | 0.41 |
| 1:AA:451:A:N6 | 1:AA:480:U:H2' | 2.36 | 0.41 |
| 1:AA:402:G:H5' | 1:AA:621:A:H1' | 2.02 | 0.41 |
| 3:AD:124:VAL:HA | 3:AD:141:VAL:O | 2.21 | 0.41 |
| 3:AD:159:GLU:C | 3:AD:161:ALA:H | 2.24 | 0.41 |
| 5:AF:97:THR:O | 5:AF:98:GLU:O | 2.38 | 0.41 |
| 8:AI:32:ARG:HH11 | 8:AI:37:TYR:HD1 | 1.69 | 0.41 |
| 9:AJ:14:ASP:OD1 | 9:AJ:17:LEU:HB2 | 2.20 | 0.41 |
| 10:AK:42:GLY:HA3 | 10:AK:73:VAL:HG13 | 2.02 | 0.41 |
| 12:AM:82:LEU:HD21 | 18:AS:64:GLU:OE1 | 2.20 | 0.41 |
| 15:AP:3:THR:CG2 | 15:AP:66:THR:HB | 2.44 | 0.41 |
| 16:AQ:58:VAL:HB | 16:AQ:74:LEU:CD2 | 2.51 | 0.41 |
| 21:AU:48:LYS:HG3 | 21:AU:49:ALA:N | 2.34 | 0.41 |
| 49:B2:10:LEU:HD11 | 49:B2:14:ARG:CZ | 2.51 | 0.41 |
| 51:B4:2:LYS:CE | 51:B4:4:ARG:HE | 2.34 | 0.41 |
| 23:BB:83:A:H2 | 23:BB:103:A:N7 | 2.19 | 0.41 |
| 23:BB:1064:C:O2' | 23:BB:1065:U:H5' | 2.21 | 0.41 |
| 23:BB:1079:C:O2' | 52:BI:133:ARG:NH2 | 2.53 | 0.41 |
| 23:BB:1392:A:H2' | 23:BB:1393:A:C8 | 2.56 | 0.41 |
| 23:BB:142:A:C8 | 23:BB:142:A:O5' | 2.74 | 0.41 |
| 23:BB:1528:A:H2' | 23:BB:1529:G:O4' | 2.21 | 0.41 |
| 23:BB:1723:G:H2' | 23:BB:1724:G:H5' | 2.02 | 0.41 |
| 23:BB:1841:U:O2' | 23:BB:1842:G:H5' | 2.21 | 0.41 |
| 23:BB:1859:U:H2' | 23:BB:1860:G:C8 | 2.56 | 0.41 |
| 23:BB:1889:A:H2' | 23:BB:1890:A:C8 | 2.56 | 0.41 |
| 23:BB:2314:A:H2' | 23:BB:2315:G:C8 | 2.56 | 0.41 |
| 23:BB:2317:A:C2' | 23:BB:2318:G:H5' | 2.51 | 0.41 |
| 23:BB:345:A:N3 | 23:BB:346:A:N1 | 2.69 | 0.41 |
| 23:BB:729:G:H5'' | 23:BB:730:A:C5' | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:940:G:H2' | 23:BB:941:A:O4' | 2.21 | 0.41 |
| 25:BC:92:LEU:HD12 | 25:BC:101:ARG:O | 2.21 | 0.41 |
| 25:BC:18:VAL:O | 25:BC:18:VAL:HG22 | 2.21 | 0.41 |
| 26:BD:138:LEU:N | 26:BD:138:LEU:HD22 | 2.36 | 0.41 |
| 26:BD:161:MET:O | 26:BD:162:ALA:C | 2.58 | 0.41 |
| 26:BD:54:ALA:HA | 26:BD:76:GLY:N | 2.36 | 0.41 |
| 26:BD:90:PHE:HD2 | 26:BD:94:GLN:HG3 | 1.86 | 0.41 |
| 27:BE:137:LYS:O | 27:BE:141:MET:HG3 | 2.21 | 0.41 |
| 28:BF:46:LYS:HZ2 | 28:BF:83:PRO:HD2 | 1.85 | 0.41 |
| 30:BH:26:ALA:O | 30:BH:28:ASN:N | 2.54 | 0.41 |
| 31:BJ:20:ALA:CB | 31:BJ:23:LYS:HB2 | 2.45 | 0.41 |
| 31:BJ:45:THR:N | 31:BJ:46:PRO:CD | 2.84 | 0.41 |
| 31:BJ:6:ALA:HB3 | 31:BJ:45:THR:CG2 | 2.48 | 0.41 |
| 32:BK:24:VAL:CG1 | 32:BK:33:ALA:HB2 | 2.51 | 0.41 |
| 34:BM:42:THR:H | 34:BM:45:GLN:HB2 | 1.86 | 0.41 |
| 34:BM:63:ILE:HA | 34:BM:104:GLU:O | 2.20 | 0.41 |
| 37:BP:101:GLU:OE2 | 37:BP:101:GLU:N | 2.54 | 0.41 |
| 37:BP:109:ILE:HD12 | 37:BP:109:ILE:O | 2.21 | 0.41 |
| 38:BQ:73:ILE:HD11 | 38:BQ:77:LYS:HB3 | 2.03 | 0.41 |
| 40:BS:26:GLY:O | 40:BS:28:LYS:N | 2.53 | 0.41 |
| 45:BY:6:ILE:HA | 45:BY:56:VAL:CG2 | 2.48 | 0.41 |
| 1:CA:1042:A:H2' | 1:CA:1043:G:O4' | 2.20 | 0.41 |
| 1:CA:1260:G:H4' | 1:CA:1283:U:O2' | 2.20 | 0.41 |
| 1:CA:1531:A:C2' | 1:CA:1532:U:H5' | 2.51 | 0.41 |
| 1:CA:159:G:N1 | 1:CA:163:C:N4 | 2.69 | 0.41 |
| 1:CA:178:C:O2' | 1:CA:179:A:H5' | 2.21 | 0.41 |
| 1:CA:242:G:H2' | 1:CA:243:A:C5' | 2.51 | 0.41 |
| 1:CA:332:G:O2' | 1:CA:333:U:H5' | 2.21 | 0.41 |
| 1:CA:51:A:H4' | 1:CA:52:C:C5' | 2.50 | 0.41 |
| 1:CA:742:G:H2' | 1:CA:743:A:C8 | 2.52 | 0.41 |
| 1:CA:842:U:O2' | 1:CA:846:G:N1 | 2.54 | 0.41 |
| 2:CC:99:GLN:O | 2:CC:100:ILE:HB | 2.21 | 0.41 |
| 2:CC:171:ARG:HH11 | 2:CC:171:ARG:CB | 2.27 | 0.41 |
| 4:CE:105:ILE:HG12 | 4:CE:122:VAL:O | 2.21 | 0.41 |
| 5:CF:81:ASN:OD1 | 5:CF:83:ALA:HB3 | 2.21 | 0.41 |
| 1:CA:878:A:H5'' | 7:CH:80:PRO:HG2 | 2.03 | 0.41 |
| 1:CA:1347:G:H8 | 8:CI:108:ARG:HB3 | 1.85 | 0.41 |
| 10:CK:111:ASP:HB2 | 21:CU:19:LYS:CE | 2.51 | 0.41 |
| 14:CO:31:LEU:O | 14:CO:35:ILE:HG12 | 2.21 | 0.41 |
| 16:CQ:61:ARG:O | 16:CQ:61:ARG:HD2 | 2.21 | 0.41 |
| 16:CQ:65:PRO:HA | 16:CQ:71:SER:OG | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CQ:75:VAL:CG2 | 16:CQ:76:ARG:N | 2.83 | 0.41 |
| 21:CU:48:LYS:C | 21:CU:50:SER:N | 2.75 | 0.41 |
| 47:D0:27:LEU:H | 47:D0:27:LEU:HD12 | 1.85 | 0.41 |
| 22:DA:93:C:O2' | 22:DA:94:A:H5' | 2.21 | 0.41 |
| 23:DB:1174:U:H2' | 23:DB:1176:U:OP2 | 2.21 | 0.41 |
| 23:DB:585:G:H2' | 23:DB:1251:C:H42 | 1.86 | 0.41 |
| 23:DB:1338:G:O2' | 23:DB:1339:G:H5' | 2.21 | 0.41 |
| 23:DB:1389:G:H2' | 23:DB:1390:U:O4' | 2.21 | 0.41 |
| 23:DB:1408:G:H2' | 23:DB:1409:U:C6 | 2.56 | 0.41 |
| 23:DB:1900:A:N1 | 23:DB:1970:A:C6 | 2.89 | 0.41 |
| 23:DB:1911:U:O4 | 23:DB:1918:A:H2' | 2.21 | 0.41 |
| 23:DB:1939:U:H5' | 23:DB:1939:U:C6 | 2.49 | 0.41 |
| 23:DB:2082:A:N6 | 23:DB:2237:G:H1' | 2.36 | 0.41 |
| 23:DB:2391:G:O6 | 23:DB:2427:C:H1' | 2.21 | 0.41 |
| 23:DB:2590:A:O2' | 23:DB:2591:C:H5' | 2.21 | 0.41 |
| 23:DB:269:C:C2 | 23:DB:270:A:C8 | 3.09 | 0.41 |
| 23:DB:2776:A:H4' | 23:DB:2777:G:C5' | 2.51 | 0.41 |
| 23:DB:453:A:H1' | 23:DB:457:A:O2' | 2.21 | 0.41 |
| 23:DB:581:C:OP1 | 38:DQ:32:ARG:HG3 | 2.21 | 0.41 |
| 23:DB:678:C:H2' | 23:DB:679:C:H6 | 1.86 | 0.41 |
| 25:DC:16:VAL:N | 25:DC:203:VAL:HG12 | 2.33 | 0.41 |
| 23:DB:729:G:C5 | 25:DC:206:LYS:HB2 | 2.56 | 0.41 |
| 25:DC:226:PRO:HG3 | 25:DC:233:GLY:N | 2.24 | 0.41 |
| 25:DC:51:ARG:NH2 | 25:DC:246:PRO:HG2 | 2.36 | 0.41 |
| 25:DC:54:GLY:O | 25:DC:55:GLY:C | 2.59 | 0.41 |
| 26:DD:130:GLN:HE21 | 26:DD:130:GLN:HB3 | 1.74 | 0.41 |
| 27:DE:122:GLU:O | 27:DE:123:LYS:HB2 | 2.20 | 0.41 |
| 27:DE:12:LEU:HD11 | 27:DE:14:VAL:HG13 | 2.02 | 0.41 |
| 27:DE:176:ASP:OD1 | 27:DE:176:ASP:C | 2.59 | 0.41 |
| 29:DG:101:VAL:HG12 | 29:DG:115:GLN:HB3 | 2.02 | 0.41 |
| 29:DG:167:VAL:HG23 | 29:DG:168:VAL:N | 2.27 | 0.41 |
| 29:DG:24:THR:CG2 | 29:DG:32:LEU:HD22 | 2.51 | 0.41 |
| 35:DN:49:GLU:N | 35:DN:50:PRO:CD | 2.83 | 0.41 |
| 37:DP:85:VAL:HG21 | 37:DP:88:ARG:NH1 | 2.29 | 0.41 |
| 38:DQ:89:ILE:C | 38:DQ:91:ARG:N | 2.74 | 0.41 |
| 41:DT:53:VAL:HG12 | 41:DT:54:GLU:N | 2.36 | 0.41 |
| 42:DU:51:LEU:O | 42:DU:52:ASN:C | 2.60 | 0.41 |
| 24:DV:1:MET:HE3 | 24:DV:2:PHE:N | 2.36 | 0.41 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:C8 | 2.56 | 0.40 |
| 1:AA:1167:A:O2' | 1:AA:1168:U:H2' | 2.21 | 0.40 |
| 1:AA:1314:C:H2' | 1:AA:1315:U:H6 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1317:C:O2' | 13:AN:49:THR:HG23 | 2.21 | 0.40 |
| 1:AA:451:A:C1' | 1:AA:452:A:C8 | 3.05 | 0.40 |
| 1:AA:56:U:H2' | 1:AA:57:G:C8 | 2.54 | 0.40 |
| 1:AA:681:A:H2' | 1:AA:682:G:C8 | 2.56 | 0.40 |
| 1:AA:6:G:N3 | 1:AA:6:G:C3' | 2.81 | 0.40 |
| 1:AA:766:A:H2' | 1:AA:767:A:O4' | 2.21 | 0.40 |
| 20:AB:77:GLU:O | 20:AB:77:GLU:HG2 | 2.21 | 0.40 |
| 3:AD:56:GLU:OE1 | 3:AD:195:ASN:HB2 | 2.21 | 0.40 |
| 4:AE:25:LYS:HG3 | 4:AE:26:GLY:N | 2.36 | 0.40 |
| 6:AG:92:PRO:HG2 | 6:AG:93:VAL:H | 1.86 | 0.40 |
| 7:AH:106:SER:C | 7:AH:107:LYS:HE2 | 2.42 | 0.40 |
| 10:AK:101:ALA:C | 10:AK:103:GLY:H | 2.24 | 0.40 |
| 12:AM:7:ASN:ND2 | 12:AM:7:ASN:N | 2.69 | 0.40 |
| 18:AS:4:LEU:HD22 | 18:AS:7:GLY:O | 2.21 | 0.40 |
| 19:AT:32:LYS:O | 19:AT:33:LYS:C | 2.59 | 0.40 |
| 19:AT:81:GLN:C | 19:AT:83:ASN:H | 2.23 | 0.40 |
| 21:AU:33:ARG:NE | 21:AU:34:ARG:HG3 | 2.36 | 0.40 |
| 10:AK:111:ASP:HB3 | 21:AU:3:ILE:N | 2.36 | 0.40 |
| 48:B1:33:LEU:HD12 | 48:B1:34:GLU:H | 1.86 | 0.40 |
| 49:B2:41:ARG:O | 49:B2:42:LEU:C | 2.59 | 0.40 |
| 22:BA:17:C:O2' | 22:BA:18:G:H5' | 2.21 | 0.40 |
| 22:BA:87:U:H2' | 22:BA:88:C:O5' | 2.21 | 0.40 |
| 23:BB:116:C:O2' | 23:BB:117:G:H5' | 2.21 | 0.40 |
| 23:BB:1878:G:H2' | 23:BB:1879:C:O4' | 2.22 | 0.40 |
| 23:BB:1999:C:H2' | 23:BB:2000:C:O4' | 2.21 | 0.40 |
| 23:BB:2013:A:H2' | 23:BB:2014:A:H5' | 2.04 | 0.40 |
| 23:BB:2098:U:O2' | 23:BB:2099:U:H5' | 2.21 | 0.40 |
| 23:BB:2282:G:H5' | 23:BB:2389:G:H1' | 2.03 | 0.40 |
| 23:BB:2306:C:H6 | 23:BB:2306:C:O5' | 2.04 | 0.40 |
| 23:BB:2317:A:H2' | 23:BB:2318:G:O4' | 2.21 | 0.40 |
| 23:BB:2341:G:H2' | 23:BB:2342:C:H6 | 1.85 | 0.40 |
| 23:BB:2345:G:H4' | 23:BB:2346:A:O5' | 2.21 | 0.40 |
| 23:BB:2843:G:O2' | 23:BB:2844:G:H5' | 2.20 | 0.40 |
| 23:BB:2843:G:H2' | 23:BB:2844:G:O4' | 2.20 | 0.40 |
| 23:BB:29:U:H2' | 23:BB:30:G:C8 | 2.56 | 0.40 |
| 23:BB:317:G:H2' | 23:BB:318:C:C6 | 2.55 | 0.40 |
| 23:BB:340:A:H2' | 23:BB:341:C:O4' | 2.21 | 0.40 |
| 23:BB:516:C:O2' | 23:BB:517:C:H5' | 2.21 | 0.40 |
| 23:BB:53:A:H2' | 23:BB:54:G:O4' | 2.21 | 0.40 |
| 23:BB:575:A:C2' | 23:BB:576:U:H5' | 2.51 | 0.40 |
| 25:BC:137:GLY:N | 25:BC:163:ILE:O | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BC:246:PRO:HB2 | 25:BC:247:TRP:CZ3 | 2.57 | 0.40 |
| 26:BD:148:GLN:CB | 26:BD:152:PRO:HG2 | 2.41 | 0.40 |
| 28:BF:35:LEU:HD12 | 28:BF:88:VAL:O | 2.21 | 0.40 |
| 30:BH:103:VAL:HG21 | 30:BH:110:VAL:HG13 | 2.03 | 0.40 |
| 32:BK:71:ARG:HG3 | 32:BK:105:ARG:NH2 | 2.34 | 0.40 |
| 33:BL:111:ILE:HG22 | 33:BL:112:LEU:H | 1.86 | 0.40 |
| 33:BL:115:GLU:OE1 | 33:BL:115:GLU:N | 2.54 | 0.40 |
| 33:BL:42:SER:C | 33:BL:44:GLY:N | 2.74 | 0.40 |
| 33:BL:65:GLY:O | 33:BL:66:PHE:CB | 2.69 | 0.40 |
| 34:BM:18:ARG:HD2 | 34:BM:18:ARG:HA | 1.95 | 0.40 |
| 34:BM:2:LEU:O | 34:BM:69:PRO:HG3 | 2.21 | 0.40 |
| 23:BB:2838:G:H1' | 35:BN:45:ARG:CZ | 2.51 | 0.40 |
| 35:BN:96:ARG:CG | 35:BN:98:LEU:HD13 | 2.51 | 0.40 |
| 37:BP:12:MET:HG2 | 37:BP:76:HIS:CD2 | 2.56 | 0.40 |
| 38:BQ:68:ALA:C | 38:BQ:71:ASN:HB3 | 2.41 | 0.40 |
| 38:BQ:46:TYR:CE1 | 39:BR:76:LYS:HE3 | 2.56 | 0.40 |
| 41:BT:30:ILE:O | 41:BT:85:VAL:HG23 | 2.21 | 0.40 |
| 41:BT:45:ALA:HA | 41:BT:48:GLN:CB | 2.51 | 0.40 |
| 41:BT:61:LEU:C | 41:BT:61:LEU:HD12 | 2.40 | 0.40 |
| 1:CA:1058:G:H2' | 1:CA:1059:C:H6 | 1.86 | 0.40 |
| 1:CA:1071:C:H2' | 1:CA:1072:G:C8 | 2.51 | 0.40 |
| 1:CA:107:G:O6 | 19:CT:9:ARG:HD3 | 2.21 | 0.40 |
| 1:CA:1225:A:H5'' | 1:CA:1226:C:C5 | 2.55 | 0.40 |
| 1:CA:122:G:C2' | 1:CA:123:U:H5' | 2.52 | 0.40 |
| 1:CA:160:A:H2' | 1:CA:161:A:C8 | 2.56 | 0.40 |
| 1:CA:33:A:O2' | 1:CA:34:C:H5' | 2.21 | 0.40 |
| 1:CA:340:U:O2' | 1:CA:341:C:H5' | 2.21 | 0.40 |
| 1:CA:450:G:H4' | 15:CP:41:PRO:HB2 | 2.03 | 0.40 |
| 1:CA:451:A:C1' | 1:CA:452:A:C8 | 3.04 | 0.40 |
| 1:CA:488:C:H2' | 1:CA:489:C:H6 | 1.86 | 0.40 |
| 1:CA:584:G:H2' | 1:CA:585:G:H8 | 1.85 | 0.40 |
| 1:CA:633:G:H2' | 1:CA:634:C:C6 | 2.56 | 0.40 |
| 1:CA:648:A:O2' | 1:CA:649:A:H5' | 2.21 | 0.40 |
| 1:CA:660:C:H2' | 1:CA:661:G:C8 | 2.57 | 0.40 |
| 1:CA:78:A:O2' | 1:CA:79:G:H5' | 2.22 | 0.40 |
| 1:CA:999:C:H2' | 1:CA:1000:A:C8 | 2.57 | 0.40 |
| 20:CB:114:LYS:O | 20:CB:117:GLU:HB3 | 2.22 | 0.40 |
| 2:CC:106:ARG:HG2 | 2:CC:106:ARG:NH1 | 2.35 | 0.40 |
| 3:CD:97:LEU:HD13 | 3:CD:136:VAL:CG1 | 2.51 | 0.40 |
| 6:CG:100:MET:O | 6:CG:104:VAL:HG23 | 2.21 | 0.40 |
| 6:CG:16:LYS:HB3 | 6:CG:43:TYR:CE1 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CI:44:ARG:O | 8:CI:48:ARG:HG3 | 2.21 | 0.40 |
| 8:CI:58:GLU:O | 8:CI:59:LYS:HD2 | 2.20 | 0.40 |
| 8:CI:93:LEU:HD13 | 8:CI:97:LEU:CD1 | 2.46 | 0.40 |
| 1:CA:975:A:N1 | 9:CJ:50:THR:HB | 2.36 | 0.40 |
| 10:CK:14:GLN:HA | 10:CK:76:TYR:O | 2.21 | 0.40 |
| 11:CL:23:LEU:O | 11:CL:25:ALA:N | 2.54 | 0.40 |
| 16:CQ:13:SER:HB3 | 16:CQ:21:VAL:CB | 2.50 | 0.40 |
| 47:D0:25:THR:O | 47:D0:26:SER:HB3 | 2.21 | 0.40 |
| 23:DB:1029:A:H2' | 23:DB:1030:C:O4' | 2.21 | 0.40 |
| 23:DB:1159:U:H2' | 23:DB:1160:G:H8 | 1.85 | 0.40 |
| 23:DB:1346:G:C6 | 23:DB:1601:G:C6 | 3.08 | 0.40 |
| 23:DB:1635:A:H2' | 23:DB:1636:U:C5' | 2.52 | 0.40 |
| 23:DB:1703:G:H2' | 23:DB:1704:C:C6 | 2.56 | 0.40 |
| 23:DB:1742:U:O2' | 23:DB:1743:G:H5' | 2.21 | 0.40 |
| 23:DB:1777:U:O2' | 23:DB:1778:U:H5' | 2.21 | 0.40 |
| 23:DB:1798:U:OP1 | 25:DC:257:ARG:HB2 | 2.21 | 0.40 |
| 23:DB:1810:A:H2' | 23:DB:1811:G:O4' | 2.21 | 0.40 |
| 23:DB:2016:U:C4 | 23:DB:2017:U:C4 | 3.09 | 0.40 |
| 23:DB:2353:G:N3 | 43:DW:30:VAL:CG1 | 2.81 | 0.40 |
| 23:DB:2331:G:N2 | 23:DB:2385:C:C4 | 2.90 | 0.40 |
| 23:DB:2282:G:H5' | 23:DB:2389:G:H1' | 2.03 | 0.40 |
| 23:DB:2518:A:N3 | 23:DB:2518:A:H5' | 2.36 | 0.40 |
| 23:DB:2846:G:OP1 | 37:DP:52:ARG:NH1 | 2.48 | 0.40 |
| 23:DB:689:A:H2' | 23:DB:690:G:C8 | 2.57 | 0.40 |
| 23:DB:957:C:N4 | 23:DB:2459:A:C8 | 2.88 | 0.40 |
| 25:DC:189:ALA:C | 25:DC:190:THR:HG23 | 2.41 | 0.40 |
| 26:DD:54:ALA:HA | 26:DD:76:GLY:N | 2.35 | 0.40 |
| 28:DF:94:ARG:HD3 | 28:DF:97:GLU:OE2 | 2.21 | 0.40 |
| 23:DB:2745:C:O3' | 29:DG:141:GLY:HA3 | 2.21 | 0.40 |
| 29:DG:152:ARG:HG3 | 29:DG:153:PRO:CD | 2.50 | 0.40 |
| 52:DI:112:LYS:HB2 | 52:DI:116:MET:SD | 2.61 | 0.40 |
| 52:DI:5:GLN:O | 52:DI:6:ALA:CB | 2.68 | 0.40 |
| 31:DJ:20:ALA:HB2 | 31:DJ:28:LEU:HD22 | 2.02 | 0.40 |
| 31:DJ:43:GLU:O | 31:DJ:44:TYR:C | 2.58 | 0.40 |
| 31:DJ:58:ASN:O | 31:DJ:59:ALA:HB3 | 2.21 | 0.40 |
| 32:DK:111:LYS:HD3 | 32:DK:111:LYS:N | 2.36 | 0.40 |
| 23:DB:2684:U:O4' | 32:DK:70:ARG:NH2 | 2.55 | 0.40 |
| 34:DM:2:LEU:O | 34:DM:69:PRO:HG3 | 2.21 | 0.40 |
| 36:DO:105:ALA:C | 36:DO:107:ALA:H | 2.24 | 0.40 |
| 37:DP:6:GLN:CA | 37:DP:9:GLN:HG2 | 2.48 | 0.40 |
| 23:DB:1249:U:O4' | 38:DQ:3:VAL:HG21 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DQ:47:ARG:O | 38:DQ:51:GLN:HG3 | 2.21 | 0.40 |
| 24:DV:65:VAL:C | 24:DV:67:GLY:N | 2.73 | 0.40 |
| 1:AA:1096:C:O2' | 1:AA:1097:C:H5' | 2.20 | 0.40 |
| 1:AA:126:G:H4' | 1:AA:634:C:O2 | 2.22 | 0.40 |
| 1:AA:1288:A:H2' | 1:AA:1289:A:O4' | 2.21 | 0.40 |
| 1:AA:1308:U:H3' | 12:AM:97:ARG:NH1 | 2.36 | 0.40 |
| 1:AA:1313:U:O5' | 1:AA:1313:U:H6 | 2.04 | 0.40 |
| 1:AA:264:C:H2' | 1:AA:265:G:O4' | 2.22 | 0.40 |
| 1:AA:327:A:O2' | 1:AA:329:A:H5'' | 2.21 | 0.40 |
| 1:AA:665:A:H2' | 1:AA:725:G:N2 | 2.36 | 0.40 |
| 1:AA:883:C:O2' | 1:AA:884:U:H5' | 2.20 | 0.40 |
| 20:AB:18:GLN:C | 20:AB:37:VAL:HG23 | 2.42 | 0.40 |
| 20:AB:71:THR:HG21 | 20:AB:94:ARG:H | 1.85 | 0.40 |
| 2:AC:174:LEU:HD23 | 2:AC:174:LEU:O | 2.21 | 0.40 |
| 2:AC:31:ASN:ND2 | 2:AC:58:ARG:NE | 2.69 | 0.40 |
| 3:AD:196:GLU:HG3 | 3:AD:197:HIS:N | 2.36 | 0.40 |
| 6:AG:107:ALA:O | 6:AG:118:ARG:HB3 | 2.22 | 0.40 |
| 6:AG:147:ASN:C | 10:AK:55:ARG:HH21 | 2.24 | 0.40 |
| 7:AH:57:GLU:HG3 | 7:AH:58:LEU:H | 1.86 | 0.40 |
| 9:AJ:59:LYS:C | 9:AJ:61:ALA:H | 2.25 | 0.40 |
| 13:AN:63:CYS:HB3 | 13:AN:68:ARG:H | 1.86 | 0.40 |
| 14:AO:77:TYR:O | 14:AO:81:ILE:HG13 | 2.21 | 0.40 |
| 15:AP:75:ILE:HG13 | 15:AP:75:ILE:H | 1.73 | 0.40 |
| 16:AQ:66:LEU:HB2 | 16:AQ:70:LYS:HG2 | 2.04 | 0.40 |
| 18:AS:12:LEU:O | 18:AS:16:LYS:HE2 | 2.21 | 0.40 |
| 21:AU:16:ARG:CZ | 21:AU:19:LYS:HD3 | 2.51 | 0.40 |
| 51:B4:1:MET:SD | 51:B4:36:ARG:HG3 | 2.61 | 0.40 |
| 51:B4:18:LYS:HE3 | 51:B4:21:GLY:HA2 | 2.02 | 0.40 |
| 51:B4:22:VAL:O | 51:B4:24:ARG:HG3 | 2.21 | 0.40 |
| 22:BA:2:G:N3 | 22:BA:2:G:H2' | 2.37 | 0.40 |
| 23:BB:999:U:O2' | 23:BB:1000:A:H5' | 2.21 | 0.40 |
| 23:BB:1165:A:O2' | 23:BB:1166:G:H5' | 2.22 | 0.40 |
| 23:BB:1190:G:O2' | 23:BB:1191:G:H5' | 2.21 | 0.40 |
| 23:BB:1280:G:C2' | 23:BB:1281:G:H5' | 2.51 | 0.40 |
| 23:BB:139:U:H2' | 23:BB:139:U:OP1 | 2.21 | 0.40 |
| 23:BB:1513:U:H2' | 23:BB:1514:G:O4' | 2.22 | 0.40 |
| 23:BB:169:G:O2' | 23:BB:170:U:H5' | 2.21 | 0.40 |
| 23:BB:2143:C:O5' | 23:BB:2143:C:H6 | 2.04 | 0.40 |
| 23:BB:2199:A:O2' | 46:BZ:36:HIS:CE1 | 2.74 | 0.40 |
| 23:BB:2248:C:C2' | 23:BB:2249:U:H5' | 2.52 | 0.40 |
| 23:BB:2580:U:H3' | 23:BB:2581:G:C2 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 23:BB:2591:C:O2' | 23:BB:2592:G:H5' | 2.20 | 0.40 |
| 23:BB:2667:C:H1' | 29:BG:108:PHE:HD2 | 1.87 | 0.40 |
| 23:BB:2758:A:H2' | 23:BB:2759:G:H5' | 2.03 | 0.40 |
| 23:BB:65:U:C2 | 23:BB:66:C:C5 | 3.09 | 0.40 |
| 23:BB:858:G:C2 | 23:BB:2268:A:C4 | 3.08 | 0.40 |
| 23:BB:864:G:O2' | 23:BB:865:C:H5' | 2.21 | 0.40 |
| 25:BC:245:THR:C | 25:BC:247:TRP:N | 2.75 | 0.40 |
| 25:BC:63:ILE:HD13 | 25:BC:63:ILE:HA | 1.79 | 0.40 |
| 27:BE:129:PRO:HG3 | 27:BE:156:ASN:OD1 | 2.21 | 0.40 |
| 27:BE:21:ARG:HG3 | 27:BE:22:ASP:O | 2.22 | 0.40 |
| 28:BF:108:PRO:O | 28:BF:110:ILE:HG23 | 2.22 | 0.40 |
| 28:BF:3:LEU:HB2 | 28:BF:100:GLU:OE1 | 2.21 | 0.40 |
| 30:BH:70:GLU:O | 30:BH:71:LYS:C | 2.59 | 0.40 |
| 52:BI:116:MET:HE1 | 52:BI:124:MET:O | 2.20 | 0.40 |
| 52:BI:73:PRO:HA | 52:BI:74:PRO:HD3 | 1.99 | 0.40 |
| 52:BI:79:LEU:HD11 | 52:BI:131:THR:OG1 | 2.20 | 0.40 |
| 31:BJ:29:ALA:O | 31:BJ:32:LEU:HB2 | 2.21 | 0.40 |
| 32:BK:10:VAL:CG2 | 32:BK:16:ALA:HA | 2.52 | 0.40 |
| 32:BK:31:ARG:HG3 | 32:BK:31:ARG:HH11 | 1.85 | 0.40 |
| 32:BK:93:GLN:CD | 32:BK:94:PRO:HD2 | 2.41 | 0.40 |
| 23:BB:2415:G:H4' | 33:BL:66:PHE:HB2 | 2.03 | 0.40 |
| 34:BM:56:ALA:C | 34:BM:58:LYS:N | 2.74 | 0.40 |
| 39:BR:6:GLN:HE22 | 39:BR:9:GLY:C | 2.25 | 0.40 |
| 23:BB:137:U:H2' | 41:BT:1:MET:H2 | 1.86 | 0.40 |
| 41:BT:36:LYS:C | 41:BT:36:LYS:HD3 | 2.42 | 0.40 |
| 42:BU:54:PRO:HG2 | 42:BU:55:GLY:H | 1.87 | 0.40 |
| 43:BW:17:ALA:CA | 43:BW:35:ILE:HG23 | 2.46 | 0.40 |
| 1:CA:1080:A:H5'' | 4:CE:20:VAL:HG11 | 2.03 | 0.40 |
| 1:CA:1211:U:H5' | 1:CA:1212:U:H5' | 2.03 | 0.40 |
| 1:CA:1296:C:H5'' | 1:CA:1302:C:H42 | 1.86 | 0.40 |
| 1:CA:1493:A:H1' | 54:CA:2062:HYG:H362 | 1.86 | 0.40 |
| 1:CA:1520:C:H2' | 1:CA:1521:C:C6 | 2.57 | 0.40 |
| 1:CA:360:G:O2' | 1:CA:361:G:H5' | 2.22 | 0.40 |
| 1:CA:537:G:H2' | 1:CA:538:G:C8 | 2.55 | 0.40 |
| 1:CA:789:U:H2' | 1:CA:791:G:OP2 | 2.20 | 0.40 |
| 20:CB:48:MET:SD | 20:CB:200:PRO:HD2 | 2.61 | 0.40 |
| 2:CC:46:LEU:HB3 | 2:CC:49:ALA:HB3 | 2.03 | 0.40 |
| 3:CD:97:LEU:HA | 3:CD:100:VAL:CG2 | 2.51 | 0.40 |
| 3:CD:117:VAL:HA | 3:CD:122:ILE:HG12 | 2.03 | 0.40 |
| 4:CE:104:ILE:HG13 | 4:CE:122:VAL:HG23 | 2.02 | 0.40 |
| 4:CE:25:LYS:HG3 | 4:CE:26:GLY:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CF:55:HIS:CD2 | 5:CF:56:LYS:HE3 | 2.57 | 0.40 |
| 6:CG:3:ARG:NH1 | 6:CG:3:ARG:HG3 | 2.36 | 0.40 |
| 8:CI:48:ARG:HA | 8:CI:51:LEU:HD12 | 2.03 | 0.40 |
| 11:CL:73:LEU:HD21 | 11:CL:103:CYS:CB | 2.50 | 0.40 |
| 11:CL:56:LEU:HD12 | 11:CL:60:PHE:HB2 | 2.04 | 0.40 |
| 12:CM:102:LYS:HB2 | 12:CM:102:LYS:NZ | 2.37 | 0.40 |
| 12:CM:22:TYR:N | 12:CM:22:TYR:CD2 | 2.88 | 0.40 |
| 14:CO:69:LEU:HD12 | 14:CO:77:TYR:HB2 | 2.01 | 0.40 |
| 15:CP:22:ALA:HA | 15:CP:33:ILE:HG13 | 2.03 | 0.40 |
| 17:CR:61:ALA:HB3 | 17:CR:67:LEU:HD12 | 2.04 | 0.40 |
| 18:CS:52:ASN:CG | 18:CS:53:GLY:N | 2.72 | 0.40 |
| 21:CU:42:THR:O | 21:CU:45:LYS:N | 2.54 | 0.40 |
| 49:D2:21:ARG:HD3 | 49:D2:43:THR:HG21 | 2.04 | 0.40 |
| 51:D4:7:VAL:HG23 | 51:D4:35:GLN:CB | 2.51 | 0.40 |
| 22:DA:47:C:H5' | 22:DA:48:U:OP2 | 2.21 | 0.40 |
| 22:DA:63:C:H2' | 22:DA:64:G:H8 | 1.86 | 0.40 |
| 23:DB:1076:C:H2' | 23:DB:1077:A:C8 | 2.57 | 0.40 |
| 23:DB:1076:C:H2' | 23:DB:1077:A:H8 | 1.86 | 0.40 |
| 23:DB:126:A:H5' | 49:D2:19:ARG:HB2 | 2.03 | 0.40 |
| 23:DB:1870:C:H2' | 23:DB:1871:A:C8 | 2.56 | 0.40 |
| 23:DB:2026:U:C2 | 23:DB:2027:G:C8 | 3.08 | 0.40 |
| 23:DB:2027:G:C6 | 23:DB:2028:U:C4 | 3.09 | 0.40 |
| 23:DB:2252:G:H2' | 23:DB:2253:G:C8 | 2.56 | 0.40 |
| 23:DB:2376:A:O2' | 36:DO:111:ARG:NH2 | 2.54 | 0.40 |
| 23:DB:2515:C:O2' | 23:DB:2516:A:H5' | 2.20 | 0.40 |
| 23:DB:2536:G:H2' | 23:DB:2537:U:O4' | 2.22 | 0.40 |
| 23:DB:2579:C:H6 | 23:DB:2579:C:O5' | 2.04 | 0.40 |
| 23:DB:2699:C:H2' | 23:DB:2700:A:C8 | 2.56 | 0.40 |
| 23:DB:2772:C:H4' | 26:DD:171:THR:CG2 | 2.51 | 0.40 |
| 23:DB:2848:G:N2 | 23:DB:2867:G:C2 | 2.89 | 0.40 |
| 23:DB:613:A:H4' | 23:DB:614:A:OP2 | 2.21 | 0.40 |
| 23:DB:666:A:O2' | 23:DB:667:U:H5' | 2.21 | 0.40 |
| 23:DB:818:G:H4' | 23:DB:838:C:O3' | 2.22 | 0.40 |
| 25:DC:145:MET:HE1 | 25:DC:153:LEU:HD21 | 2.03 | 0.40 |
| 25:DC:254:LYS:HB3 | 25:DC:255:LYS:H | 1.72 | 0.40 |
| 26:DD:117:GLY:O | 26:DD:118:PHE:C | 2.59 | 0.40 |
| 26:DD:2:ILE:H | 26:DD:2:ILE:HG13 | 1.69 | 0.40 |
| 27:DE:38:GLY:C | 27:DE:40:ARG:N | 2.75 | 0.40 |
| 28:DF:137:PHE:O | 28:DF:139:GLU:N | 2.55 | 0.40 |
| 28:DF:45:ASP:C | 28:DF:47:LYS:H | 2.25 | 0.40 |
| 30:DH:108:VAL:HG12 | 30:DH:110:VAL:HG12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DH:57:LYS:O | 30:DH:61:VAL:N | 2.50 | 0.40 |
| 31:DJ:64:VAL:HG22 | 31:DJ:68:LYS:CD | 2.50 | 0.40 |
| 33:DL:74:THR:HA | 33:DL:107:PHE:O | 2.21 | 0.40 |
| 34:DM:71:LYS:HB3 | 34:DM:93:VAL:O | 2.21 | 0.40 |
| 37:DP:101:GLU:OE2 | 37:DP:101:GLU:N | 2.53 | 0.40 |
| 39:DR:49:ILE:HG22 | 39:DR:54:VAL:HB | 2.02 | 0.40 |
| 40:DS:36:LEU:HD22 | 40:DS:36:LEU:N | 2.33 | 0.40 |
| 41:DT:45:ALA:HA | 41:DT:48:GLN:CB | 2.50 | 0.40 |
| 42:DU:65:GLN:HG2 | 42:DU:65:GLN:H | 1.54 | 0.40 |
| 46:DZ:76:GLU:HG3 | 46:DZ:77:LYS:N | 2.36 | 0.40 |
| 1:AA:1033:G:H2' | 1:AA:1034:G:H5'' | 2.03 | 0.40 |
| 1:AA:105:G:H2' | 1:AA:106:C:C6 | 2.57 | 0.40 |
| 1:AA:1067:A:H4' | 1:AA:1068:G:O5' | 2.21 | 0.40 |
| 1:AA:116:A:H8 | 1:AA:116:A:O5' | 2.04 | 0.40 |
| 1:AA:123:U:H2' | 1:AA:124:C:C6 | 2.57 | 0.40 |
| 1:AA:191:G:H2' | 1:AA:192:A:C8 | 2.57 | 0.40 |
| 1:AA:201:G:H2' | 1:AA:202:G:C8 | 2.56 | 0.40 |
| 1:AA:201:G:O2' | 1:AA:202:G:H5' | 2.22 | 0.40 |
| 1:AA:818:G:H3' | 1:AA:819:A:H5'' | 2.04 | 0.40 |
| 1:AA:81:A:O4' | 1:AA:81:A:OP2 | 2.39 | 0.40 |
| 1:AA:880:C:H2' | 1:AA:881:G:H8 | 1.85 | 0.40 |
| 20:AB:26:MET:HG3 | 20:AB:188:THR:O | 2.21 | 0.40 |
| 20:AB:68:PHE:HD1 | 20:AB:89:PHE:O | 2.05 | 0.40 |
| 3:AD:195:ASN:HD22 | 3:AD:195:ASN:HA | 1.57 | 0.40 |
| 4:AE:105:ILE:HG12 | 4:AE:122:VAL:O | 2.21 | 0.40 |
| 5:AF:54:LEU:C | 5:AF:56:LYS:H | 2.24 | 0.40 |
| 8:AI:29:ILE:HG12 | 8:AI:64:ILE:HD13 | 2.03 | 0.40 |
| 12:AM:80:MET:C | 12:AM:82:LEU:H | 2.24 | 0.40 |
| 13:AN:30:ILE:CG2 | 13:AN:44:VAL:HG21 | 2.49 | 0.40 |
| 14:AO:57:ARG:CZ | 14:AO:61:GLN:HE22 | 2.34 | 0.40 |
| 14:AO:69:LEU:HD12 | 14:AO:77:TYR:HB2 | 2.03 | 0.40 |
| 16:AQ:13:SER:HB3 | 16:AQ:21:VAL:CB | 2.49 | 0.40 |
| 16:AQ:22:VAL:O | 16:AQ:42:LYS:HA | 2.22 | 0.40 |
| 18:AS:77:ARG:HB3 | 18:AS:77:ARG:HE | 1.64 | 0.40 |
| 21:AU:42:THR:O | 21:AU:45:LYS:N | 2.55 | 0.40 |
| 47:B0:18:HIS:ND1 | 47:B0:18:HIS:N | 2.70 | 0.40 |
| 48:B1:10:LEU:HD23 | 48:B1:35:LEU:HD21 | 2.03 | 0.40 |
| 49:B2:32:ALA:HA | 49:B2:35:ARG:HB2 | 2.03 | 0.40 |
| 50:B3:26:ALA:O | 50:B3:27:ASN:C | 2.59 | 0.40 |
| 23:BB:1179:G:C2' | 23:BB:1180:U:H5' | 2.51 | 0.40 |
| 23:BB:1390:U:O2' | 23:BB:1391:U:H5' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:1446:C:H2' | 23:BB:1447:C:C6 | 2.56 | 0.40 |
| 23:BB:1616:A:H4' | 23:BB:1617:C:OP2 | 2.22 | 0.40 |
| 23:BB:1688:U:O2 | 23:BB:1700:A:H8 | 2.05 | 0.40 |
| 23:BB:783:A:H4' | 23:BB:1779:U:O2 | 2.22 | 0.40 |
| 23:BB:1992:G:N2 | 23:BB:1996:C:O2' | 2.54 | 0.40 |
| 23:BB:1997:C:OP2 | 26:BD:129:THR:HB | 2.21 | 0.40 |
| 23:BB:2437:G:H2' | 23:BB:2438:U:C6 | 2.57 | 0.40 |
| 23:BB:2769:U:O2' | 23:BB:2770:G:H5' | 2.21 | 0.40 |
| 23:BB:2622:U:O2' | 23:BB:2825:G:N7 | 2.54 | 0.40 |
| 23:BB:2840:C:OP1 | 35:BN:50:PRO:HA | 2.21 | 0.40 |
| 23:BB:548:G:C8 | 23:BB:548:G:OP2 | 2.74 | 0.40 |
| 23:BB:711:G:O2' | 23:BB:712:G:H5' | 2.22 | 0.40 |
| 23:BB:755:U:H2' | 23:BB:756:A:H8 | 1.86 | 0.40 |
| 23:BB:858:G:H21 | 23:BB:2268:A:C3' | 2.29 | 0.40 |
| 25:BC:110:LYS:O | 25:BC:111:ALA:C | 2.59 | 0.40 |
| 25:BC:34:GLU:O | 25:BC:34:GLU:HG3 | 2.22 | 0.40 |
| 28:BF:139:GLU:OE2 | 28:BF:142:TYR:HA | 2.20 | 0.40 |
| 28:BF:8:LYS:HA | 28:BF:12:VAL:CG2 | 2.46 | 0.40 |
| 29:BG:106:LEU:N | 29:BG:106:LEU:HD23 | 2.37 | 0.40 |
| 52:BI:49:GLU:OE1 | 52:BI:52:LEU:HD22 | 2.21 | 0.40 |
| 32:BK:105:ARG:N | 32:BK:105:ARG:CD | 2.84 | 0.40 |
| 34:BM:61:GLY:HA2 | 34:BM:107:GLY:HA3 | 2.04 | 0.40 |
| 34:BM:38:ARG:HG3 | 34:BM:98:PRO:HD3 | 2.02 | 0.40 |
| 35:BN:21:PHE:HA | 35:BN:24:MET:HB2 | 2.04 | 0.40 |
| 35:BN:49:GLU:HA | 35:BN:94:TYR:CD2 | 2.55 | 0.40 |
| 36:BO:36:TYR:HA | 36:BO:52:SER:CB | 2.51 | 0.40 |
| 23:BB:580:U:O3' | 38:BQ:30:VAL:HG13 | 2.21 | 0.40 |
| 40:BS:2:GLU:O | 40:BS:3:THR:C | 2.60 | 0.40 |
| 40:BS:49:LYS:HA | 40:BS:52:GLU:HG2 | 2.04 | 0.40 |
| 42:BU:21:ARG:HD3 | 42:BU:72:PHE:CB | 2.51 | 0.40 |
| 43:BW:18:LYS:CA | 43:BW:36:ILE:HG12 | 2.38 | 0.40 |
| 23:BB:2387:U:H1' | 43:BW:38:ARG:CZ | 2.52 | 0.40 |
| 41:BT:12:ARG:CG | 44:BX:29:ARG:HH12 | 2.33 | 0.40 |
| 1:CA:1176:A:H2' | 1:CA:1177:G:O4' | 2.22 | 0.40 |
| 1:CA:1238:A:C2 | 1:CA:1241:G:N3 | 2.88 | 0.40 |
| 1:CA:1271:A:H5' | 1:CA:1314:C:C5' | 2.49 | 0.40 |
| 1:CA:1324:A:H4' | 1:CA:1363:A:OP1 | 2.22 | 0.40 |
| 1:CA:1329:A:H5'' | 12:CM:24:VAL:HA | 2.03 | 0.40 |
| 1:CA:1489:G:H2' | 1:CA:1490:U:C6 | 2.55 | 0.40 |
| 1:CA:176:C:H3' | 1:CA:177:G:N2 | 2.35 | 0.40 |
| 1:CA:549:C:H2' | 1:CA:550:G:H8 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:625:U:H4' | 15:CP:16:PHE:CE1 | 2.56 | 0.40 |
| 1:CA:668:G:O2' | 1:CA:669:G:H5' | 2.22 | 0.40 |
| 1:CA:812:G:O2' | 1:CA:813:U:C6 | 2.56 | 0.40 |
| 1:CA:930:C:H2' | 1:CA:931:C:C6 | 2.56 | 0.40 |
| 1:CA:994:A:C5 | 1:CA:1216:A:H4' | 2.56 | 0.40 |
| 3:CD:196:GLU:HG3 | 3:CD:197:HIS:N | 2.35 | 0.40 |
| 4:CE:107:GLY:C | 4:CE:109:ALA:H | 2.25 | 0.40 |
| 4:CE:84:VAL:CG1 | 4:CE:146:MET:HB3 | 2.49 | 0.40 |
| 6:CG:92:PRO:HG2 | 6:CG:93:VAL:H | 1.86 | 0.40 |
| 7:CH:74:ILE:CG1 | 7:CH:128:VAL:HG22 | 2.47 | 0.40 |
| 8:CI:44:ARG:HB3 | 8:CI:48:ARG:NH2 | 2.36 | 0.40 |
| 9:CJ:26:VAL:HG12 | 9:CJ:30:LYS:HG3 | 2.04 | 0.40 |
| 9:CJ:8:ILE:HB | 9:CJ:74:VAL:HB | 2.02 | 0.40 |
| 10:CK:107:THR:HB | 10:CK:108:ASN:OD1 | 2.20 | 0.40 |
| 10:CK:51:PHE:O | 10:CK:51:PHE:HD1 | 2.04 | 0.40 |
| 11:CL:33:CYS:H | 11:CL:54:VAL:CG1 | 2.33 | 0.40 |
| 11:CL:73:LEU:HD21 | 11:CL:103:CYS:HB2 | 2.04 | 0.40 |
| 12:CM:18:LEU:C | 12:CM:20:SER:N | 2.75 | 0.40 |
| 12:CM:85:TYR:HA | 12:CM:88:LEU:CD1 | 2.52 | 0.40 |
| 13:CN:56:PRO:C | 13:CN:58:ARG:H | 2.25 | 0.40 |
| 16:CQ:58:VAL:HB | 16:CQ:74:LEU:CD2 | 2.51 | 0.40 |
| 16:CQ:59:GLU:HG3 | 16:CQ:78:VAL:HG21 | 2.02 | 0.40 |
| 1:CA:1220:G:O3' | 18:CS:35:ARG:HD2 | 2.20 | 0.40 |
| 47:D0:27:LEU:HB2 | 47:D0:28:SER:H | 1.65 | 0.40 |
| 48:D1:22:THR:OG1 | 48:D1:23:THR:N | 2.53 | 0.40 |
| 50:D3:31:ILE:CG1 | 50:D3:35:LYS:HE3 | 2.51 | 0.40 |
| 22:DA:3:C:H2' | 22:DA:4:C:H6 | 1.85 | 0.40 |
| 22:DA:42:C:O2' | 28:DF:91:ARG:NH1 | 2.54 | 0.40 |
| 22:DA:49:C:OP1 | 36:DO:101:GLY:HA3 | 2.22 | 0.40 |
| 22:DA:98:G:HO2' | 22:DA:99:A:H5'' | 1.86 | 0.40 |
| 23:DB:1126:A:H4' | 23:DB:1127:A:H5'' | 2.03 | 0.40 |
| 23:DB:1204:A:N1 | 23:DB:1241:A:C2 | 2.89 | 0.40 |
| 23:DB:1933:G:H2' | 23:DB:1934:C:H6 | 1.86 | 0.40 |
| 23:DB:2142:A:H2' | 23:DB:2143:C:O4' | 2.22 | 0.40 |
| 23:DB:1420:A:C2' | 23:DB:2211:A:H62 | 2.15 | 0.40 |
| 23:DB:2484:G:O2' | 23:DB:2485:G:H5' | 2.21 | 0.40 |
| 23:DB:2846:G:H2' | 23:DB:2847:U:O4' | 2.21 | 0.40 |
| 23:DB:689:A:H2' | 23:DB:690:G:H8 | 1.86 | 0.40 |
| 23:DB:760:G:H2' | 23:DB:761:A:O4' | 2.21 | 0.40 |
| 25:DC:20:ASN:O | 25:DC:23:LEU:HB2 | 2.22 | 0.40 |
| 23:DB:1805:A:H5'' | 25:DC:247:TRP:CE2 | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DC:4:LYS:HE3 | 25:DC:13:ARG:O | 2.22 | 0.40 |
| 25:DC:86:ARG:NH1 | 25:DC:86:ARG:HB3 | 2.36 | 0.40 |
| 27:DE:29:HIS:O | 27:DE:32:VAL:HG22 | 2.21 | 0.40 |
| 29:DG:39:ALA:HB2 | 29:DG:57:TYR:CD2 | 2.57 | 0.40 |
| 30:DH:38:PRO:O | 30:DH:40:THR:HG23 | 2.22 | 0.40 |
| 31:DJ:25:LEU:HB2 | 31:DJ:62:VAL:HG21 | 2.02 | 0.40 |
| 31:DJ:83:GLY:O | 31:DJ:84:ILE:C | 2.60 | 0.40 |
| 32:DK:60:ALA:CB | 32:DK:86:LEU:HA | 2.51 | 0.40 |
| 32:DK:86:LEU:CD2 | 32:DK:86:LEU:H | 2.23 | 0.40 |
| 34:DM:42:THR:H | 34:DM:45:GLN:HB2 | 1.87 | 0.40 |
| 37:DP:109:ILE:HG13 | 37:DP:109:ILE:H | 1.67 | 0.40 |
| 37:DP:61:ARG:HE | 37:DP:100:ARG:HD2 | 1.87 | 0.40 |
| 38:DQ:16:ILE:C | 38:DQ:18:LYS:H | 2.24 | 0.40 |
| 39:DR:101:ILE:HG22 | 39:DR:101:ILE:O | 2.22 | 0.40 |
| 39:DR:7:SER:HA | 39:DR:22:LEU:HD13 | 2.02 | 0.40 |
| 46:DZ:40:VAL:HG22 | 46:DZ:45:ARG:N | 2.36 | 0.40 |
| 1:AA:1107:C:C4 | 1:AA:1108:G:N7 | 2.89 | 0.40 |
| 1:AA:1336:C:O4' | 1:AA:1337:G:C2 | 2.74 | 0.40 |
| 1:AA:140:U:H2' | 1:AA:141:G:H8 | 1.86 | 0.40 |
| 1:AA:177:G:N3 | 1:AA:177:G:O4' | 2.54 | 0.40 |
| 1:AA:430:A:P | 3:AD:6:PRO:HA | 2.61 | 0.40 |
| 1:AA:761:G:O2' | 1:AA:762:U:H5' | 2.21 | 0.40 |
| 1:AA:78:A:O5' | 1:AA:78:A:H8 | 2.03 | 0.40 |
| 1:AA:832:G:H2' | 1:AA:833:G:H8 | 1.86 | 0.40 |
| 2:AC:18:ASN:HB2 | 13:AN:90:GLY:HA3 | 2.04 | 0.40 |
| 4:AE:94:PHE:O | 4:AE:124:ALA:HB1 | 2.22 | 0.40 |
| 6:AG:10:LYS:NZ | 6:AG:10:LYS:HB2 | 2.35 | 0.40 |
| 6:AG:147:ASN:CA | 10:AK:55:ARG:HH21 | 2.35 | 0.40 |
| 9:AJ:71:LEU:H | 9:AJ:71:LEU:HD23 | 1.87 | 0.40 |
| 12:AM:22:TYR:CD2 | 12:AM:22:TYR:N | 2.88 | 0.40 |
| 16:AQ:32:ILE:HG23 | 16:AQ:33:TYR:CD2 | 2.56 | 0.40 |
| 17:AR:61:ALA:HB3 | 17:AR:67:LEU:HD12 | 2.02 | 0.40 |
| 18:AS:20:LYS:HD2 | 18:AS:20:LYS:O | 2.20 | 0.40 |
| 18:AS:33:TRP:CE3 | 18:AS:33:TRP:N | 2.90 | 0.40 |
| 23:BB:1295:C:H2' | 23:BB:1296:G:C8 | 2.56 | 0.40 |
| 23:BB:1316:U:H2' | 23:BB:1317:G:C8 | 2.57 | 0.40 |
| 23:BB:1495:A:H2' | 23:BB:1496:A:H8 | 1.85 | 0.40 |
| 23:BB:2027:G:C2 | 23:BB:2028:U:C2 | 3.09 | 0.40 |
| 23:BB:981:A:H4' | 23:BB:2037:A:H5' | 2.03 | 0.40 |
| 23:BB:2104:C:H6 | 23:BB:2104:C:H3' | 1.87 | 0.40 |
| 23:BB:2208:C:O2' | 23:BB:2209:G:H5' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BB:2525:G:C2 | 23:BB:2539:C:C2 | 3.10 | 0.40 |
| 23:BB:2818:U:O5' | 23:BB:2837:A:H1' | 2.21 | 0.40 |
| 23:BB:28:A:O2' | 23:BB:29:U:H5' | 2.20 | 0.40 |
| 23:BB:459:U:O2' | 23:BB:460:A:H5' | 2.21 | 0.40 |
| 23:BB:719:C:O2' | 23:BB:720:U:H5' | 2.20 | 0.40 |
| 23:BB:996:A:H4' | 38:BQ:91:ARG:CD | 2.43 | 0.40 |
| 26:BD:118:PHE:HE2 | 35:BN:1:MET:SD | 2.44 | 0.40 |
| 27:BE:102:ARG:NH2 | 27:BE:102:ARG:HG3 | 2.36 | 0.40 |
| 27:BE:176:ASP:C | 27:BE:176:ASP:OD1 | 2.59 | 0.40 |
| 28:BF:42:ALA:O | 28:BF:45:ASP:N | 2.48 | 0.40 |
| 28:BF:81:GLY:O | 28:BF:82:TYR:C | 2.60 | 0.40 |
| 30:BH:48:GLU:CG | 30:BH:49:ALA:N | 2.84 | 0.40 |
| 52:BI:27:LEU:HB2 | 52:BI:32:VAL:HG21 | 2.02 | 0.40 |
| 52:BI:14:ALA:HA | 52:BI:45:THR:HG21 | 2.02 | 0.40 |
| 31:BJ:36:LEU:CD1 | 31:BJ:121:LYS:HE3 | 2.50 | 0.40 |
| 31:BJ:20:ALA:CB | 31:BJ:28:LEU:HD22 | 2.51 | 0.40 |
| 33:BL:50:PHE:O | 33:BL:52:GLY:N | 2.54 | 0.40 |
| 34:BM:17:ASN:HB3 | 34:BM:38:ARG:NH1 | 2.36 | 0.40 |
| 36:BO:100:HIS:ND1 | 36:BO:101:GLY:N | 2.69 | 0.40 |
| 36:BO:6:ALA:HB3 | 36:BO:10:ARG:HH11 | 1.86 | 0.40 |
| 40:BS:14:ALA:C | 40:BS:16:LYS:N | 2.75 | 0.40 |
| 41:BT:68:LYS:HB2 | 41:BT:68:LYS:HE3 | 1.79 | 0.40 |
| 42:BU:19:GLY:O | 42:BU:20:LYS:HD3 | 2.22 | 0.40 |
| 42:BU:32:LYS:H | 42:BU:32:LYS:HD3 | 1.87 | 0.40 |
| 42:BU:90:LYS:O | 42:BU:91:LYS:C | 2.59 | 0.40 |
| 45:BY:55:LYS:O | 45:BY:56:VAL:C | 2.59 | 0.40 |
| 46:BZ:51:VAL:HG12 | 46:BZ:52:SER:N | 2.36 | 0.40 |
| 46:BZ:5:CYS:HB3 | 46:BZ:10:LYS:N | 2.36 | 0.40 |
| 1:CA:120:A:C2' | 1:CA:121:U:H5'' | 2.40 | 0.40 |
| 1:CA:1256:A:O4' | 1:CA:1278:G:N2 | 2.54 | 0.40 |
| 1:CA:1320:C:H41 | 18:CS:36:ARG:CG | 2.30 | 0.40 |
| 1:CA:144:G:H2' | 1:CA:145:G:O4' | 2.22 | 0.40 |
| 1:CA:1514:G:H2' | 1:CA:1515:G:C8 | 2.55 | 0.40 |
| 1:CA:618:C:N3 | 1:CA:622:A:N6 | 2.64 | 0.40 |
| 1:CA:926:G:H5' | 1:CA:927:G:C5' | 2.51 | 0.40 |
| 1:CA:95:C:C2' | 1:CA:95:C:O2 | 2.69 | 0.40 |
| 2:CC:45:GLU:C | 2:CC:46:LEU:HD22 | 2.42 | 0.40 |
| 4:CE:33:THR:HB | 4:CE:49:TYR:CE1 | 2.57 | 0.40 |
| 5:CF:34:GLY:C | 5:CF:35:LYS:HD2 | 2.42 | 0.40 |
| 1:CA:1148:U:O4' | 8:CI:17:ARG:HD3 | 2.21 | 0.40 |
| 8:CI:40:ARG:C | 8:CI:41:GLU:HG3 | 2.41 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CI:54:VAL:HG21 | 8:CI:86:LEU:HD21 | 2.03 | 0.40 |
| 10:CK:18:GLY:HA2 | 10:CK:36:ARG:NH1 | 2.37 | 0.40 |
| 11:CL:56:LEU:HG | 11:CL:60:PHE:O | 2.21 | 0.40 |
| 12:CM:88:LEU:O | 12:CM:92:ARG:HG3 | 2.22 | 0.40 |
| 16:CQ:11:VAL:HG13 | 16:CQ:20:ILE:CG2 | 2.52 | 0.40 |
| 18:CS:4:LEU:HD22 | 18:CS:7:GLY:O | 2.21 | 0.40 |
| 23:DB:1022:G:N2 | 23:DB:1142:A:N1 | 2.69 | 0.40 |
| 23:DB:122:G:O2' | 23:DB:123:G:H5' | 2.21 | 0.40 |
| 23:DB:130:C:O2' | 23:DB:131:A:H5' | 2.21 | 0.40 |
| 23:DB:1459:G:O5' | 23:DB:1459:G:N3 | 2.54 | 0.40 |
| 23:DB:1702:G:H2' | 23:DB:1703:G:O4' | 2.21 | 0.40 |
| 23:DB:1829:A:H3' | 23:DB:1830:C:H6 | 1.87 | 0.40 |
| 23:DB:960:A:C4' | 23:DB:2457:U:H4' | 2.51 | 0.40 |
| 23:DB:2582:G:O2' | 23:DB:2583:G:H5' | 2.22 | 0.40 |
| 23:DB:483:A:N7 | 23:DB:497:A:H2 | 2.19 | 0.40 |
| 23:DB:63:A:C8 | 23:DB:63:A:OP2 | 2.69 | 0.40 |
| 23:DB:673:C:C2' | 23:DB:674:G:H5' | 2.52 | 0.40 |
| 23:DB:726:G:H5'' | 23:DB:1432:G:O2' | 2.22 | 0.40 |
| 25:DC:184:GLU:O | 25:DC:185:ALA:HB3 | 2.21 | 0.40 |
| 25:DC:249:VAL:O | 25:DC:250:GLN:C | 2.59 | 0.40 |
| 27:DE:198:GLU:O | 27:DE:199:MET:C | 2.60 | 0.40 |
| 27:DE:34:ALA:CB | 27:DE:96:VAL:HG21 | 2.51 | 0.40 |
| 28:DF:120:SER:OG | 28:DF:129:MET:HB3 | 2.22 | 0.40 |
| 23:DB:2305:U:H1' | 28:DF:132:ARG:HA | 2.03 | 0.40 |
| 28:DF:74:ALA:CB | 28:DF:78:ILE:HD13 | 2.51 | 0.40 |
| 22:DA:43:C:C1' | 28:DF:91:ARG:HD2 | 2.51 | 0.40 |
| 30:DH:14:SER:O | 30:DH:16:GLY:N | 2.54 | 0.40 |
| 52:DI:14:ALA:HB3 | 52:DI:51:GLY:H | 1.87 | 0.40 |
| 31:DJ:45:THR:N | 31:DJ:46:PRO:CD | 2.83 | 0.40 |
| 31:DJ:77:HIS:HD2 | 31:DJ:83:GLY:HA3 | 1.87 | 0.40 |
| 33:DL:123:ARG:C | 33:DL:123:ARG:HD2 | 2.41 | 0.40 |
| 34:DM:19:GLY:C | 34:DM:97:GLN:HG3 | 2.41 | 0.40 |
| 35:DN:99:LYS:O | 47:D0:41:HIS:HB2 | 2.21 | 0.40 |
| 37:DP:50:ARG:O | 37:DP:51:ASN:HB2 | 2.22 | 0.40 |
| 38:DQ:3:VAL:CG1 | 38:DQ:4:LYS:N | 2.84 | 0.40 |
| 40:DS:26:GLY:O | 40:DS:28:LYS:N | 2.54 | 0.40 |
| 41:DT:62:VAL:HG12 | 41:DT:63:VAL:N | 2.37 | 0.40 |
| 41:DT:87:LEU:HB2 | 41:DT:91:GLN:HG2 | 2.02 | 0.40 |
| 23:DB:329:G:N2 | 42:DU:16:LYS:HE3 | 2.29 | 0.40 |
| 24:DV:5:ASN:O | 24:DV:6:ALA:HB2 | 2.22 | 0.40 |
| 24:DV:80:HIS:HA | 24:DV:81:PRO:HD3 | 1.96 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:DX:22:LEU:O | 44:DX:24:GLU:N | 2.52 | 0.40 |
| 44:DX:7:ARG:HD2 | 44:DX:7:ARG:HA | 1.84 | 0.40 |
| 1:AA:1058:G:H2' | 1:AA:1059:C:H6 | 1.87 | 0.40 |
| 1:AA:1053:G:C6 | 1:AA:1199:U:H2' | 2.57 | 0.40 |
| 1:AA:1386:G:O2' | 1:AA:1387:G:H5' | 2.21 | 0.40 |
| 1:AA:242:G:H2' | 1:AA:243:A:C5' | 2.52 | 0.40 |
| 1:AA:375:U:O2' | 1:AA:376:G:H5' | 2.22 | 0.40 |
| 1:AA:58:C:O2' | 1:AA:388:G:N7 | 2.49 | 0.40 |
| 1:AA:448:A:H2' | 1:AA:449:G:H8 | 1.85 | 0.40 |
| 1:AA:7:A:H2' | 4:AE:123:LEU:HB2 | 2.03 | 0.40 |
| 1:AA:80:A:OP2 | 1:AA:81:A:N7 | 2.54 | 0.40 |
| 1:AA:977:A:H1' | 1:AA:982:U:O4 | 2.21 | 0.40 |
| 3:AD:89:LEU:HD22 | 3:AD:199:ILE:HD11 | 2.04 | 0.40 |
| 4:AE:25:LYS:HG3 | 4:AE:26:GLY:H | 1.87 | 0.40 |
| 4:AE:71:ILE:HD12 | 4:AE:73:VAL:CG2 | 2.52 | 0.40 |
| 6:AG:14:ASP:OD2 | 6:AG:22:LEU:HD22 | 2.22 | 0.40 |
| 7:AH:24:VAL:CG1 | 7:AH:60:LEU:HB3 | 2.52 | 0.40 |
| 8:AI:42:THR:O | 8:AI:45:MET:HG2 | 2.22 | 0.40 |
| 8:AI:24:ASN:O | 8:AI:60:LEU:N | 2.55 | 0.40 |
| 1:AA:1147:C:H4' | 8:AI:6:TYR:CE1 | 2.56 | 0.40 |
| 9:AJ:71:LEU:O | 9:AJ:72:ARG:HD3 | 2.22 | 0.40 |
| 12:AM:29:SER:HA | 12:AM:32:ILE:HG22 | 2.04 | 0.40 |
| 13:AN:46:LYS:HD3 | 13:AN:46:LYS:HA | 1.87 | 0.40 |
| 14:AO:31:LEU:O | 14:AO:35:ILE:HG12 | 2.21 | 0.40 |
| 14:AO:81:ILE:HG23 | 14:AO:86:LEU:HB2 | 2.04 | 0.40 |
| 15:AP:12:LYS:C | 15:AP:14:ARG:H | 2.23 | 0.40 |
| 16:AQ:11:VAL:HG13 | 16:AQ:20:ILE:CG2 | 2.52 | 0.40 |
| 16:AQ:30:HIS:HE1 | 16:AQ:32:ILE:HG22 | 1.78 | 0.40 |
| 16:AQ:40:THR:HG22 | 16:AQ:41:THR:N | 2.36 | 0.40 |
| 16:AQ:43:LEU:N | 16:AQ:43:LEU:HD12 | 2.37 | 0.40 |
| 19:AT:50:PHE:C | 19:AT:52:GLU:H | 2.24 | 0.40 |
| 48:B1:10:LEU:HB3 | 48:B1:48:TYR:HB3 | 2.04 | 0.40 |
| 48:B1:33:LEU:CB | 48:B1:51:ALA:HB3 | 2.44 | 0.40 |
| 50:B3:51:LYS:HD2 | 50:B3:54:LEU:HD22 | 2.04 | 0.40 |
| 22:BA:7:G:H5'' | 36:BO:29:HIS:CD2 | 2.57 | 0.40 |
| 23:BB:1063:G:O2' | 23:BB:1064:C:H5' | 2.22 | 0.40 |
| 23:BB:1068:G:C6 | 23:BB:1069:A:N6 | 2.89 | 0.40 |
| 23:BB:1180:U:H2' | 23:BB:1181:U:C6 | 2.56 | 0.40 |
| 23:BB:1210:G:H5' | 23:BB:1212:G:C5' | 2.50 | 0.40 |
| 23:BB:1539:U:O2 | 23:BB:1539:U:H2' | 2.19 | 0.40 |
| 23:BB:1654:A:O2' | 23:BB:1655:A:H5' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:1923:U:H2' | 23:BB:1924:C:C5 | 2.56 | 0.40 |
| 23:BB:2033:A:H1' | 23:BB:2035:G:OP2 | 2.22 | 0.40 |
| 23:BB:2438:U:O3' | 23:BB:2439:A:H3' | 2.22 | 0.40 |
| 23:BB:2737:G:H2' | 23:BB:2738:A:H8 | 1.85 | 0.40 |
| 23:BB:275:C:H2' | 23:BB:276:U:O4' | 2.21 | 0.40 |
| 23:BB:2824:C:C4 | 23:BB:2825:G:C5 | 3.10 | 0.40 |
| 23:BB:2719:G:O2' | 23:BB:2846:G:H4' | 2.21 | 0.40 |
| 23:BB:324:A:H61 | 23:BB:338:G:C2' | 2.35 | 0.40 |
| 23:BB:374:A:N6 | 23:BB:400:G:H1' | 2.36 | 0.40 |
| 23:BB:667:U:H2' | 23:BB:668:A:O4' | 2.22 | 0.40 |
| 23:BB:78:U:H2' | 23:BB:79:C:H6 | 1.83 | 0.40 |
| 23:BB:821:A:H2' | 23:BB:946:C:O4' | 2.21 | 0.40 |
| 25:BC:115:ILE:O | 25:BC:115:ILE:HG13 | 2.21 | 0.40 |
| 26:BD:109:VAL:HG11 | 26:BD:193:VAL:CG1 | 2.51 | 0.40 |
| 26:BD:2:ILE:H | 26:BD:2:ILE:HG13 | 1.69 | 0.40 |
| 27:BE:29:HIS:CA | 27:BE:32:VAL:HG22 | 2.52 | 0.40 |
| 28:BF:139:GLU:O | 28:BF:140:ILE:C | 2.60 | 0.40 |
| 28:BF:55:ASP:O | 28:BF:58:ALA:HB3 | 2.21 | 0.40 |
| 30:BH:103:VAL:CG2 | 30:BH:109:GLU:HA | 2.52 | 0.40 |
| 33:BL:111:ILE:CG2 | 33:BL:112:LEU:N | 2.85 | 0.40 |
| 35:BN:24:MET:HE3 | 35:BN:40:LYS:HB3 | 2.02 | 0.40 |
| 35:BN:44:LEU:O | 35:BN:48:VAL:HG23 | 2.22 | 0.40 |
| 35:BN:96:ARG:HG3 | 35:BN:98:LEU:HD13 | 2.04 | 0.40 |
| 36:BO:35:ILE:HD11 | 36:BO:102:ARG:NE | 2.36 | 0.40 |
| 36:BO:29:HIS:HB3 | 36:BO:36:TYR:HB2 | 2.03 | 0.40 |
| 41:BT:45:ALA:HA | 41:BT:48:GLN:CG | 2.51 | 0.40 |
| 24:BV:83:LYS:HA | 24:BV:84:PRO:HD3 | 1.93 | 0.40 |
| 43:BW:37:VAL:C | 43:BW:38:ARG:HG2 | 2.42 | 0.40 |
| 45:BY:2:LYS:H | 45:BY:2:LYS:CD | 2.30 | 0.40 |
| 45:BY:51:SER:HA | 45:BY:54:VAL:CG2 | 2.52 | 0.40 |
| 1:CA:105:G:H2' | 1:CA:106:C:C6 | 2.56 | 0.40 |
| 1:CA:1388:C:O2' | 1:CA:1389:C:H5' | 2.21 | 0.40 |
| 1:CA:423:G:N3 | 1:CA:423:G:H3' | 2.37 | 0.40 |
| 1:CA:469:C:O2' | 1:CA:470:C:H5' | 2.22 | 0.40 |
| 20:CB:184:ALA:HB3 | 20:CB:195:VAL:HG21 | 2.03 | 0.40 |
| 20:CB:185:ILE:HA | 20:CB:199:ILE:O | 2.20 | 0.40 |
| 20:CB:218:ALA:O | 20:CB:222:GLU:N | 2.53 | 0.40 |
| 2:CC:134:LYS:HA | 2:CC:167:TYR:CE2 | 2.56 | 0.40 |
| 4:CE:110:MET:O | 4:CE:113:VAL:HG22 | 2.22 | 0.40 |
| 8:CI:119:LYS:C | 8:CI:121:ARG:H | 2.25 | 0.40 |
| 9:CJ:71:LEU:H | 9:CJ:71:LEU:HD23 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:CK:34:THR:HA | 10:CK:41:LEU:CG | 2.50 | 0.40 |
| 12:CM:43:LYS:C | 12:CM:45:SER:H | 2.24 | 0.40 |
| 13:CN:78:LEU:HD23 | 13:CN:82:LYS:HB3 | 2.02 | 0.40 |
| 14:CO:77:TYR:CZ | 14:CO:81:ILE:HD11 | 2.56 | 0.40 |
| 15:CP:43:ALA:HB1 | 15:CP:46:LYS:HE3 | 2.03 | 0.40 |
| 15:CP:71:VAL:HG13 | 15:CP:72:ALA:N | 2.37 | 0.40 |
| 18:CS:2:ARG:CA | 18:CS:2:ARG:NE | 2.85 | 0.40 |
| 19:CT:20:ASN:O | 19:CT:24:ARG:HB2 | 2.22 | 0.40 |
| 1:CA:261:U:OP2 | 19:CT:70:LYS:HE2 | 2.21 | 0.40 |
| 22:DA:87:U:H2' | 22:DA:88:C:O5' | 2.21 | 0.40 |
| 23:DB:1328:A:H2' | 23:DB:1330:C:C4 | 2.56 | 0.40 |
| 23:DB:1481:U:H2' | 23:DB:1482:G:H4' | 2.03 | 0.40 |
| 23:DB:1437:C:O2' | 23:DB:1516:G:H4' | 2.21 | 0.40 |
| 23:DB:1710:G:H2' | 23:DB:1711:A:C8 | 2.57 | 0.40 |
| 23:DB:1797:G:C6 | 23:DB:1823:G:C6 | 3.09 | 0.40 |
| 23:DB:182:A:H1' | 23:DB:434:U:H5' | 2.02 | 0.40 |
| 23:DB:1843:C:O2' | 23:DB:1844:C:H5' | 2.21 | 0.40 |
| 23:DB:1859:U:H2' | 23:DB:1860:G:C8 | 2.57 | 0.40 |
| 23:DB:1998:A:H2' | 23:DB:1999:C:C6 | 2.56 | 0.40 |
| 23:DB:2255:G:H2' | 23:DB:2256:G:O4' | 2.22 | 0.40 |
| 23:DB:2314:A:H2' | 23:DB:2315:G:C8 | 2.56 | 0.40 |
| 23:DB:2379:G:H5' | 36:DO:21:LEU:HD21 | 2.03 | 0.40 |
| 23:DB:584:C:OP1 | 38:DQ:5:ARG:CB | 2.70 | 0.40 |
| 23:DB:656:G:H2' | 23:DB:657:U:O4' | 2.22 | 0.40 |
| 23:DB:78:U:H2' | 23:DB:79:C:H6 | 1.84 | 0.40 |
| 23:DB:821:A:H2' | 23:DB:946:C:O4' | 2.22 | 0.40 |
| 23:DB:901:C:H3' | 23:DB:902:C:H6 | 1.87 | 0.40 |
| 27:DE:102:ARG:O | 27:DE:106:LYS:HG3 | 2.21 | 0.40 |
| 29:DG:145:ALA:O | 29:DG:148:ARG:HG3 | 2.20 | 0.40 |
| 30:DH:121:VAL:C | 30:DH:122:LEU:HD22 | 2.41 | 0.40 |
| 30:DH:90:LEU:HD13 | 30:DH:123:ARG:C | 2.42 | 0.40 |
| 30:DH:117:LEU:HD13 | 30:DH:130:VAL:HG22 | 2.03 | 0.40 |
| 52:DI:45:THR:O | 52:DI:48:ILE:HG22 | 2.21 | 0.40 |
| 34:DM:59:ARG:CZ | 34:DM:60:GLN:HB3 | 2.52 | 0.40 |
| 35:DN:52:ILE:HB | 35:DN:94:TYR:CD2 | 2.57 | 0.40 |
| 35:DN:96:ARG:CG | 35:DN:98:LEU:HD13 | 2.52 | 0.40 |
| 37:DP:20:ARG:C | 37:DP:22:GLY:H | 2.25 | 0.40 |
| 37:DP:62:LYS:HB3 | 37:DP:69:VAL:CG2 | 2.51 | 0.40 |
| 46:DZ:30:LEU:HA | 46:DZ:31:PRO:HD3 | 1.95 | 0.40 |
| 46:DZ:54:LYS:C | 46:DZ:56:MET:N | 2.75 | 0.40 |
| 46:DZ:53:ALA:C | 46:DZ:55:GLY:N | 2.75 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%) | 147 (72%) | 40 (20%) | 17 (8%) | 1 | 9 |
| 2 | CC | 204/232 (88%) | 148 (72%) | 40 (20%) | 16 (8%) | 1 | 10 |
| 3 | AD | 203/205 (99%) | 136 (67%) | 52 (26%) | 15 (7%) | 1 | 11 |
| 3 | CD | 203/205 (99%) | 134 (66%) | 54 (27%) | 15 (7%) | 1 | 11 |
| 4 | AE | 148/166 (89%) | 117 (79%) | 27 (18%) | 4 (3%) | 5 | 33 |
| 4 | CE | 148/166 (89%) | 117 (79%) | 25 (17%) | 6 (4%) | 3 | 23 |
| 5 | AF | 98/135 (73%) | 66 (67%) | 21 (21%) | 11 (11%) | 0 | 6 |
| 5 | CF | 98/135 (73%) | 67 (68%) | 21 (21%) | 10 (10%) | 0 | 7 |
| 6 | AG | 148/178 (83%) | 122 (82%) | 18 (12%) | 8 (5%) | 2 | 17 |
| 6 | CG | 150/178 (84%) | 124 (83%) | 20 (13%) | 6 (4%) | 3 | 24 |
| 7 | AH | 127/129 (98%) | 92 (72%) | 26 (20%) | 9 (7%) | 1 | 12 |
| 7 | CH | 127/129 (98%) | 90 (71%) | 28 (22%) | 9 (7%) | 1 | 12 |
| 8 | AI | 125/129 (97%) | 88 (70%) | 29 (23%) | 8 (6%) | 1 | 14 |
| 8 | CI | 125/129 (97%) | 88 (70%) | 29 (23%) | 8 (6%) | 1 | 14 |
| 9 | AJ | 96/103 (93%) | 69 (72%) | 17 (18%) | 10 (10%) | 0 | 7 |
| 9 | CJ | 96/103 (93%) | 68 (71%) | 18 (19%) | 10 (10%) | 0 | 7 |
| 10 | AK | 115/128 (90%) | 81 (70%) | 26 (23%) | 8 (7%) | 1 | 12 |
| 10 | CK | 115/128 (90%) | 80 (70%) | 27 (24%) | 8 (7%) | 1 | 12 |
| 11 | AL | 121/123 (98%) | 78 (64%) | 29 (24%) | 14 (12%) | 0 | 5 |
| 11 | CL | 121/123 (98%) | 79 (65%) | 28 (23%) | 14 (12%) | 0 | 5 |
| 12 | AM | 112/117 (96%) | 72 (64%) | 36 (32%) | 4 (4%) | 3 | 26 |
| 12 | CM | 111/117 (95%) | 69 (62%) | 38 (34%) | 4 (4%) | 3 | 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 13 | AN | 92/100 (92%) | 57 (62%) | 25 (27%) | 10 (11%) | 0 | 6 |
| 13 | CN | 92/100 (92%) | 56 (61%) | 26 (28%) | 10 (11%) | 0 | 6 |
| 14 | AO | 86/89 (97%) | 65 (76%) | 16 (19%) | 5 (6%) | 1 | 16 |
| 14 | CO | 86/89 (97%) | 65 (76%) | 16 (19%) | 5 (6%) | 1 | 16 |
| 15 | AP | 80/82 (98%) | 56 (70%) | 15 (19%) | 9 (11%) | 0 | 6 |
| 15 | CP | 78/82 (95%) | 53 (68%) | 15 (19%) | 10 (13%) | 0 | 4 |
| 16 | AQ | 78/83 (94%) | 56 (72%) | 17 (22%) | 5 (6%) | 1 | 14 |
| 16 | CQ | 79/83 (95%) | 56 (71%) | 17 (22%) | 6 (8%) | 1 | 10 |
| 17 | AR | 53/74 (72%) | 41 (77%) | 10 (19%) | 2 (4%) | 3 | 25 |
| 17 | CR | 53/74 (72%) | 41 (77%) | 10 (19%) | 2 (4%) | 3 | 25 |
| 18 | AS | 77/91 (85%) | 58 (75%) | 17 (22%) | 2 (3%) | 5 | 33 |
| 18 | CS | 78/91 (86%) | 58 (74%) | 18 (23%) | 2 (3%) | 5 | 33 |
| 19 | AT | 83/86 (96%) | 59 (71%) | 19 (23%) | 5 (6%) | 1 | 15 |
| 19 | CT | 83/86 (96%) | 59 (71%) | 19 (23%) | 5 (6%) | 1 | 15 |
| 20 | AB | 216/240 (90%) | 143 (66%) | 53 (24%) | 20 (9%) | 0 | 8 |
| 20 | CB | 216/240 (90%) | 148 (68%) | 46 (21%) | 22 (10%) | 0 | 7 |
| 21 | AU | 49/71 (69%) | 28 (57%) | 14 (29%) | 7 (14%) | 0 | 3 |
| 21 | CU | 49/71 (69%) | 28 (57%) | 14 (29%) | 7 (14%) | 0 | 3 |
| 24 | BV | 92/94 (98%) | 63 (68%) | 23 (25%) | 6 (6%) | 1 | 14 |
| 24 | DV | 92/94 (98%) | 62 (67%) | 24 (26%) | 6 (6%) | 1 | 14 |
| 25 | BC | 269/273 (98%) | 158 (59%) | 65 (24%) | 46 (17%) | 0 | 2 |
| 25 | DC | 269/273 (98%) | 158 (59%) | 65 (24%) | 46 (17%) | 0 | 2 |
| 26 | BD | 207/209 (99%) | 121 (58%) | 56 (27%) | 30 (14%) | 0 | 3 |
| 26 | DD | 207/209 (99%) | 123 (59%) | 52 (25%) | 32 (16%) | 0 | 3 |
| 27 | BE | 199/201 (99%) | 120 (60%) | 56 (28%) | 23 (12%) | 0 | 5 |
| 27 | DE | 199/201 (99%) | 120 (60%) | 56 (28%) | 23 (12%) | 0 | 5 |
| 28 | BF | 176/178 (99%) | 103 (58%) | 39 (22%) | 34 (19%) | 0 | 2 |
| 28 | DF | 176/178 (99%) | 101 (57%) | 41 (23%) | 34 (19%) | 0 | 2 |
| 29 | BG | 174/176 (99%) | 105 (60%) | 37 (21%) | 32 (18%) | 0 | 2 |
| 29 | DG | 174/176 (99%) | 105 (60%) | 36 (21%) | 33 (19%) | 0 | 2 |
| 30 | BH | 147/149 (99%) | 68 (46%) | 43 (29%) | 36 (24%) | 0 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|----------|----------|----------|-------------|----|
| 30 | DH | 147/149 (99%) | 88 (60%) | 32 (22%) | 27 (18%) | 0 | 2 |
| 31 | BJ | 140/142 (99%) | 85 (61%) | 39 (28%) | 16 (11%) | 0 | 6 |
| 31 | DJ | 140/142 (99%) | 83 (59%) | 40 (29%) | 17 (12%) | 0 | 5 |
| 32 | BK | 119/123 (97%) | 70 (59%) | 28 (24%) | 21 (18%) | 0 | 2 |
| 32 | DK | 119/123 (97%) | 69 (58%) | 27 (23%) | 23 (19%) | 0 | 2 |
| 33 | BL | 141/144 (98%) | 75 (53%) | 40 (28%) | 26 (18%) | 0 | 2 |
| 33 | DL | 141/144 (98%) | 75 (53%) | 40 (28%) | 26 (18%) | 0 | 2 |
| 34 | BM | 134/136 (98%) | 77 (58%) | 38 (28%) | 19 (14%) | 0 | 3 |
| 34 | DM | 134/136 (98%) | 78 (58%) | 35 (26%) | 21 (16%) | 0 | 2 |
| 35 | BN | 118/127 (93%) | 73 (62%) | 33 (28%) | 12 (10%) | 0 | 7 |
| 35 | DN | 118/127 (93%) | 73 (62%) | 32 (27%) | 13 (11%) | 0 | 6 |
| 36 | BO | 114/117 (97%) | 83 (73%) | 21 (18%) | 10 (9%) | 1 | 8 |
| 36 | DO | 114/117 (97%) | 83 (73%) | 20 (18%) | 11 (10%) | 0 | 8 |
| 37 | BP | 112/114 (98%) | 59 (53%) | 35 (31%) | 18 (16%) | 0 | 2 |
| 37 | DP | 112/114 (98%) | 58 (52%) | 36 (32%) | 18 (16%) | 0 | 2 |
| 38 | BQ | 115/117 (98%) | 79 (69%) | 27 (24%) | 9 (8%) | 1 | 10 |
| 38 | DQ | 115/117 (98%) | 75 (65%) | 32 (28%) | 8 (7%) | 1 | 12 |
| 39 | BR | 101/103 (98%) | 60 (59%) | 31 (31%) | 10 (10%) | 0 | 7 |
| 39 | DR | 101/103 (98%) | 61 (60%) | 29 (29%) | 11 (11%) | 0 | 6 |
| 40 | BS | 108/110 (98%) | 75 (69%) | 21 (19%) | 12 (11%) | 0 | 6 |
| 40 | DS | 108/110 (98%) | 75 (69%) | 20 (18%) | 13 (12%) | 0 | 5 |
| 41 | BT | 91/100 (91%) | 47 (52%) | 25 (28%) | 19 (21%) | 0 | 1 |
| 41 | DT | 91/100 (91%) | 47 (52%) | 23 (25%) | 21 (23%) | 0 | 1 |
| 42 | BU | 100/103 (97%) | 53 (53%) | 35 (35%) | 12 (12%) | 0 | 5 |
| 42 | DU | 100/103 (97%) | 51 (51%) | 35 (35%) | 14 (14%) | 0 | 3 |
| 43 | BW | 77/84 (92%) | 29 (38%) | 23 (30%) | 25 (32%) | 0 | 0 |
| 43 | DW | 77/84 (92%) | 29 (38%) | 22 (29%) | 26 (34%) | 0 | 0 |
| 44 | BX | 61/63 (97%) | 37 (61%) | 14 (23%) | 10 (16%) | 0 | 2 |
| 44 | DX | 61/63 (97%) | 37 (61%) | 14 (23%) | 10 (16%) | 0 | 2 |
| 45 | BY | 56/58 (97%) | 40 (71%) | 11 (20%) | 5 (9%) | 1 | 8 |
| 45 | DY | 56/58 (97%) | 40 (71%) | 11 (20%) | 5 (9%) | 1 | 8 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 46 | BZ | 75/78 (96%) | 47 (63%) | 20 (27%) | 8 (11%) | 0 | 6 |
| 46 | DZ | 75/78 (96%) | 48 (64%) | 19 (25%) | 8 (11%) | 0 | 6 |
| 47 | B0 | 54/56 (96%) | 33 (61%) | 16 (30%) | 5 (9%) | 0 | 8 |
| 47 | D0 | 54/56 (96%) | 33 (61%) | 16 (30%) | 5 (9%) | 0 | 8 |
| 48 | B1 | 48/54 (89%) | 34 (71%) | 12 (25%) | 2 (4%) | 3 | 23 |
| 48 | D1 | 48/54 (89%) | 34 (71%) | 12 (25%) | 2 (4%) | 3 | 23 |
| 49 | B2 | 44/46 (96%) | 31 (70%) | 9 (20%) | 4 (9%) | 1 | 8 |
| 49 | D2 | 44/46 (96%) | 30 (68%) | 8 (18%) | 6 (14%) | 0 | 4 |
| 50 | B3 | 62/64 (97%) | 41 (66%) | 15 (24%) | 6 (10%) | 0 | 7 |
| 50 | D3 | 62/64 (97%) | 42 (68%) | 14 (23%) | 6 (10%) | 0 | 7 |
| 51 | B4 | 36/38 (95%) | 21 (58%) | 10 (28%) | 5 (14%) | 0 | 3 |
| 51 | D4 | 36/38 (95%) | 21 (58%) | 9 (25%) | 6 (17%) | 0 | 2 |
| 52 | BI | 139/141 (99%) | 119 (86%) | 16 (12%) | 4 (3%) | 4 | 31 |
| 52 | DI | 139/141 (99%) | 115 (83%) | 19 (14%) | 5 (4%) | 3 | 26 |
| All | All | 11241/11918 (94%) | 7279 (65%) | 2673 (24%) | 1289 (12%) | 0 | 6 |

All (1289) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 112 | ALA |
| 2 | AC | 180 | ASP |
| 2 | AC | 205 | GLU |
| 4 | AE | 20 | VAL |
| 5 | AF | 98 | GLU |
| 6 | AG | 6 | ILE |
| 6 | AG | 14 | ASP |
| 8 | AI | 127 | SER |
| 9 | AJ | 36 | VAL |
| 9 | AJ | 57 | VAL |
| 10 | AK | 126 | ARG |
| 11 | AL | 13 | ARG |
| 11 | AL | 38 | THR |
| 11 | AL | 121 | PRO |
| 13 | AN | 50 | LEU |
| 14 | AO | 73 | ASP |
| 15 | AP | 44 | SER |
| 16 | AQ | 32 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AB | 22 | TRP |
| 20 | AB | 58 | LYS |
| 20 | AB | 94 | ARG |
| 20 | AB | 188 | THR |
| 25 | BC | 18 | VAL |
| 25 | BC | 53 | ILE |
| 25 | BC | 107 | LYS |
| 25 | BC | 109 | LEU |
| 25 | BC | 123 | ILE |
| 26 | BD | 9 | VAL |
| 26 | BD | 74 | GLU |
| 26 | BD | 93 | GLY |
| 26 | BD | 106 | LYS |
| 26 | BD | 112 | THR |
| 26 | BD | 118 | PHE |
| 26 | BD | 122 | VAL |
| 26 | BD | 169 | ARG |
| 26 | BD | 170 | VAL |
| 26 | BD | 172 | VAL |
| 27 | BE | 7 | ASP |
| 27 | BE | 62 | GLN |
| 27 | BE | 69 | ARG |
| 27 | BE | 79 | ARG |
| 27 | BE | 167 | VAL |
| 28 | BF | 32 | LYS |
| 28 | BF | 43 | ILE |
| 28 | BF | 77 | LYS |
| 28 | BF | 78 | ILE |
| 28 | BF | 92 | GLY |
| 28 | BF | 112 | ASP |
| 28 | BF | 135 | ILE |
| 28 | BF | 138 | PRO |
| 28 | BF | 140 | ILE |
| 28 | BF | 148 | VAL |
| 29 | BG | 9 | VAL |
| 29 | BG | 85 | LYS |
| 29 | BG | 91 | VAL |
| 29 | BG | 94 | ARG |
| 29 | BG | 117 | PRO |
| 29 | BG | 125 | PRO |
| 30 | BH | 3 | VAL |
| 30 | BH | 8 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BH | 10 | ALA |
| 30 | BH | 31 | VAL |
| 30 | BH | 32 | PRO |
| 30 | BH | 33 | GLN |
| 30 | BH | 60 | GLU |
| 30 | BH | 62 | LEU |
| 30 | BH | 65 | ALA |
| 30 | BH | 69 | ALA |
| 30 | BH | 125 | THR |
| 31 | BJ | 4 | PHE |
| 31 | BJ | 44 | TYR |
| 31 | BJ | 45 | THR |
| 31 | BJ | 73 | VAL |
| 32 | BK | 18 | ARG |
| 32 | BK | 31 | ARG |
| 32 | BK | 35 | VAL |
| 32 | BK | 89 | ASN |
| 32 | BK | 92 | GLU |
| 32 | BK | 119 | ALA |
| 32 | BK | 120 | PRO |
| 33 | BL | 36 | LYS |
| 33 | BL | 81 | ASP |
| 33 | BL | 89 | VAL |
| 33 | BL | 94 | THR |
| 33 | BL | 111 | ILE |
| 33 | BL | 116 | VAL |
| 34 | BM | 30 | SER |
| 34 | BM | 78 | LEU |
| 35 | BN | 11 | ASN |
| 35 | BN | 58 | ASP |
| 35 | BN | 82 | GLU |
| 35 | BN | 116 | VAL |
| 35 | BN | 117 | ASP |
| 36 | BO | 56 | LYS |
| 37 | BP | 20 | ARG |
| 37 | BP | 25 | VAL |
| 37 | BP | 50 | ARG |
| 37 | BP | 75 | THR |
| 37 | BP | 100 | ARG |
| 39 | BR | 7 | SER |
| 39 | BR | 70 | GLU |
| 40 | BS | 3 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | BS | 27 | LYS |
| 40 | BS | 42 | LYS |
| 40 | BS | 59 | GLU |
| 40 | BS | 61 | ASN |
| 41 | BT | 16 | VAL |
| 41 | BT | 39 | THR |
| 41 | BT | 58 | VAL |
| 41 | BT | 77 | ARG |
| 41 | BT | 88 | LYS |
| 42 | BU | 6 | ARG |
| 42 | BU | 38 | ILE |
| 42 | BU | 49 | PRO |
| 42 | BU | 50 | ALA |
| 43 | BW | 30 | VAL |
| 43 | BW | 36 | ILE |
| 43 | BW | 50 | VAL |
| 43 | BW | 59 | PHE |
| 43 | BW | 60 | ALA |
| 43 | BW | 62 | ALA |
| 44 | BX | 2 | LYS |
| 45 | BY | 56 | VAL |
| 46 | BZ | 33 | LEU |
| 47 | B0 | 42 | ILE |
| 47 | B0 | 48 | TYR |
| 49 | B2 | 44 | VAL |
| 52 | BI | 18 | ASN |
| 2 | CC | 112 | ALA |
| 2 | CC | 180 | ASP |
| 2 | CC | 205 | GLU |
| 4 | CE | 20 | VAL |
| 5 | CF | 41 | ASP |
| 5 | CF | 98 | GLU |
| 6 | CG | 14 | ASP |
| 8 | CI | 127 | SER |
| 9 | CJ | 36 | VAL |
| 9 | CJ | 57 | VAL |
| 10 | CK | 126 | ARG |
| 11 | CL | 13 | ARG |
| 11 | CL | 38 | THR |
| 11 | CL | 121 | PRO |
| 13 | CN | 50 | LEU |
| 14 | CO | 73 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | CP | 44 | SER |
| 16 | CQ | 32 | ILE |
| 16 | CQ | 82 | VAL |
| 20 | CB | 22 | TRP |
| 20 | CB | 58 | LYS |
| 20 | CB | 94 | ARG |
| 20 | CB | 188 | THR |
| 21 | CU | 23 | GLU |
| 25 | DC | 18 | VAL |
| 25 | DC | 53 | ILE |
| 25 | DC | 107 | LYS |
| 25 | DC | 109 | LEU |
| 25 | DC | 123 | ILE |
| 25 | DC | 162 | GLN |
| 26 | DD | 9 | VAL |
| 26 | DD | 74 | GLU |
| 26 | DD | 106 | LYS |
| 26 | DD | 112 | THR |
| 26 | DD | 118 | PHE |
| 26 | DD | 122 | VAL |
| 26 | DD | 169 | ARG |
| 26 | DD | 170 | VAL |
| 26 | DD | 172 | VAL |
| 27 | DE | 7 | ASP |
| 27 | DE | 62 | GLN |
| 27 | DE | 69 | ARG |
| 27 | DE | 79 | ARG |
| 27 | DE | 167 | VAL |
| 28 | DF | 32 | LYS |
| 28 | DF | 43 | ILE |
| 28 | DF | 77 | LYS |
| 28 | DF | 78 | ILE |
| 28 | DF | 80 | GLN |
| 28 | DF | 92 | GLY |
| 28 | DF | 112 | ASP |
| 28 | DF | 135 | ILE |
| 28 | DF | 138 | PRO |
| 28 | DF | 140 | ILE |
| 28 | DF | 148 | VAL |
| 29 | DG | 9 | VAL |
| 29 | DG | 85 | LYS |
| 29 | DG | 91 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | DG | 94 | ARG |
| 29 | DG | 117 | PRO |
| 29 | DG | 125 | PRO |
| 30 | DH | 3 | VAL |
| 30 | DH | 8 | LYS |
| 30 | DH | 10 | ALA |
| 30 | DH | 31 | VAL |
| 30 | DH | 32 | PRO |
| 30 | DH | 33 | GLN |
| 30 | DH | 86 | ASP |
| 30 | DH | 121 | VAL |
| 31 | DJ | 4 | PHE |
| 31 | DJ | 44 | TYR |
| 31 | DJ | 45 | THR |
| 31 | DJ | 73 | VAL |
| 32 | DK | 18 | ARG |
| 32 | DK | 31 | ARG |
| 32 | DK | 35 | VAL |
| 32 | DK | 89 | ASN |
| 32 | DK | 92 | GLU |
| 32 | DK | 119 | ALA |
| 32 | DK | 120 | PRO |
| 33 | DL | 36 | LYS |
| 33 | DL | 81 | ASP |
| 33 | DL | 89 | VAL |
| 33 | DL | 94 | THR |
| 33 | DL | 111 | ILE |
| 33 | DL | 116 | VAL |
| 34 | DM | 30 | SER |
| 34 | DM | 78 | LEU |
| 35 | DN | 11 | ASN |
| 35 | DN | 58 | ASP |
| 35 | DN | 82 | GLU |
| 35 | DN | 116 | VAL |
| 35 | DN | 117 | ASP |
| 36 | DO | 56 | LYS |
| 37 | DP | 25 | VAL |
| 37 | DP | 50 | ARG |
| 37 | DP | 75 | THR |
| 37 | DP | 100 | ARG |
| 39 | DR | 7 | SER |
| 39 | DR | 70 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | DS | 3 | THR |
| 40 | DS | 27 | LYS |
| 40 | DS | 42 | LYS |
| 40 | DS | 59 | GLU |
| 40 | DS | 61 | ASN |
| 41 | DT | 16 | VAL |
| 41 | DT | 39 | THR |
| 41 | DT | 58 | VAL |
| 41 | DT | 77 | ARG |
| 41 | DT | 88 | LYS |
| 42 | DU | 6 | ARG |
| 42 | DU | 38 | ILE |
| 42 | DU | 49 | PRO |
| 42 | DU | 50 | ALA |
| 42 | DU | 85 | ARG |
| 43 | DW | 30 | VAL |
| 43 | DW | 36 | ILE |
| 43 | DW | 50 | VAL |
| 43 | DW | 59 | PHE |
| 43 | DW | 60 | ALA |
| 43 | DW | 62 | ALA |
| 43 | DW | 70 | VAL |
| 44 | DX | 2 | LYS |
| 45 | DY | 2 | LYS |
| 45 | DY | 56 | VAL |
| 46 | DZ | 33 | LEU |
| 47 | D0 | 42 | ILE |
| 47 | D0 | 48 | TYR |
| 49 | D2 | 44 | VAL |
| 52 | DI | 5 | GLN |
| 52 | DI | 18 | ASN |
| 2 | AC | 14 | VAL |
| 2 | AC | 59 | PRO |
| 2 | AC | 100 | ILE |
| 2 | AC | 153 | SER |
| 3 | AD | 107 | GLY |
| 3 | AD | 191 | SER |
| 3 | AD | 192 | ALA |
| 5 | AF | 41 | ASP |
| 5 | AF | 92 | THR |
| 6 | AG | 5 | VAL |
| 7 | AH | 2 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AH | 66 | GLN |
| 7 | AH | 70 | VAL |
| 7 | AH | 82 | LEU |
| 7 | AH | 114 | ALA |
| 8 | AI | 8 | THR |
| 9 | AJ | 74 | VAL |
| 9 | AJ | 75 | ASP |
| 10 | AK | 124 | LYS |
| 11 | AL | 14 | LYS |
| 11 | AL | 42 | LYS |
| 11 | AL | 61 | GLU |
| 11 | AL | 117 | GLY |
| 12 | AM | 3 | ILE |
| 12 | AM | 47 | LEU |
| 12 | AM | 104 | ASN |
| 13 | AN | 2 | LYS |
| 13 | AN | 70 | HIS |
| 13 | AN | 71 | GLY |
| 14 | AO | 17 | ASP |
| 15 | AP | 52 | LEU |
| 16 | AQ | 81 | ALA |
| 19 | AT | 41 | GLY |
| 19 | AT | 65 | LEU |
| 20 | AB | 14 | HIS |
| 20 | AB | 19 | THR |
| 20 | AB | 121 | GLN |
| 20 | AB | 150 | ILE |
| 21 | AU | 23 | GLU |
| 21 | AU | 25 | ALA |
| 21 | AU | 34 | ARG |
| 21 | AU | 35 | GLU |
| 24 | BV | 25 | LYS |
| 25 | BC | 3 | VAL |
| 25 | BC | 93 | VAL |
| 25 | BC | 135 | PRO |
| 25 | BC | 140 | VAL |
| 25 | BC | 142 | ASN |
| 25 | BC | 151 | GLY |
| 25 | BC | 162 | GLN |
| 25 | BC | 222 | THR |
| 25 | BC | 232 | GLY |
| 25 | BC | 239 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BD | 24 | VAL |
| 26 | BD | 107 | VAL |
| 26 | BD | 119 | ALA |
| 26 | BD | 121 | THR |
| 26 | BD | 136 | ASN |
| 26 | BD | 184 | ARG |
| 26 | BD | 197 | THR |
| 27 | BE | 42 | GLY |
| 27 | BE | 45 | ALA |
| 27 | BE | 165 | HIS |
| 28 | BF | 11 | VAL |
| 28 | BF | 36 | ASN |
| 28 | BF | 80 | GLN |
| 28 | BF | 141 | ASP |
| 28 | BF | 149 | ARG |
| 29 | BG | 2 | ARG |
| 29 | BG | 32 | LEU |
| 29 | BG | 84 | LYS |
| 29 | BG | 89 | VAL |
| 29 | BG | 92 | GLY |
| 29 | BG | 107 | GLY |
| 30 | BH | 52 | ALA |
| 30 | BH | 59 | ALA |
| 30 | BH | 130 | VAL |
| 31 | BJ | 5 | THR |
| 31 | BJ | 41 | LYS |
| 31 | BJ | 43 | GLU |
| 31 | BJ | 81 | ILE |
| 31 | BJ | 124 | VAL |
| 31 | BJ | 129 | GLU |
| 32 | BK | 108 | ARG |
| 32 | BK | 113 | MET |
| 33 | BL | 3 | LEU |
| 33 | BL | 5 | THR |
| 33 | BL | 28 | GLY |
| 33 | BL | 29 | LYS |
| 33 | BL | 51 | GLU |
| 33 | BL | 52 | GLY |
| 33 | BL | 93 | ASN |
| 33 | BL | 113 | ALA |
| 34 | BM | 20 | LEU |
| 34 | BM | 36 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | BM | 59 | ARG |
| 34 | BM | 69 | PRO |
| 34 | BM | 79 | ALA |
| 35 | BN | 89 | SER |
| 35 | BN | 100 | CYS |
| 35 | BN | 101 | GLY |
| 36 | BO | 57 | ALA |
| 36 | BO | 79 | ALA |
| 36 | BO | 107 | ALA |
| 37 | BP | 32 | VAL |
| 37 | BP | 84 | SER |
| 37 | BP | 101 | GLU |
| 37 | BP | 108 | ARG |
| 38 | BQ | 87 | VAL |
| 38 | BQ | 91 | ARG |
| 39 | BR | 42 | ALA |
| 39 | BR | 49 | ILE |
| 39 | BR | 100 | GLY |
| 40 | BS | 25 | ARG |
| 40 | BS | 96 | ILE |
| 40 | BS | 109 | ASP |
| 41 | BT | 28 | ASN |
| 41 | BT | 35 | ALA |
| 41 | BT | 38 | ALA |
| 41 | BT | 69 | ARG |
| 42 | BU | 12 | VAL |
| 42 | BU | 85 | ARG |
| 42 | BU | 92 | VAL |
| 43 | BW | 12 | GLY |
| 43 | BW | 14 | ASP |
| 43 | BW | 23 | LYS |
| 43 | BW | 40 | ARG |
| 43 | BW | 61 | LYS |
| 43 | BW | 70 | VAL |
| 43 | BW | 76 | ARG |
| 43 | BW | 77 | LYS |
| 44 | BX | 10 | SER |
| 44 | BX | 36 | GLN |
| 45 | BY | 2 | LYS |
| 46 | BZ | 3 | ARG |
| 46 | BZ | 77 | LYS |
| 47 | B0 | 51 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | B1 | 4 | ILE |
| 49 | B2 | 42 | LEU |
| 50 | B3 | 31 | ILE |
| 52 | BI | 14 | ALA |
| 52 | BI | 23 | VAL |
| 52 | BI | 64 | ARG |
| 2 | CC | 14 | VAL |
| 2 | CC | 59 | PRO |
| 2 | CC | 100 | ILE |
| 3 | CD | 26 | ALA |
| 3 | CD | 107 | GLY |
| 3 | CD | 168 | THR |
| 3 | CD | 189 | ASP |
| 3 | CD | 191 | SER |
| 3 | CD | 192 | ALA |
| 5 | CF | 51 | ILE |
| 5 | CF | 92 | THR |
| 7 | CH | 2 | MET |
| 7 | CH | 66 | GLN |
| 7 | CH | 70 | VAL |
| 7 | CH | 82 | LEU |
| 8 | CI | 8 | THR |
| 9 | CJ | 74 | VAL |
| 9 | CJ | 75 | ASP |
| 10 | CK | 124 | LYS |
| 11 | CL | 14 | LYS |
| 11 | CL | 42 | LYS |
| 11 | CL | 61 | GLU |
| 11 | CL | 117 | GLY |
| 12 | CM | 3 | ILE |
| 12 | CM | 47 | LEU |
| 12 | CM | 104 | ASN |
| 13 | CN | 2 | LYS |
| 13 | CN | 70 | HIS |
| 13 | CN | 71 | GLY |
| 14 | CO | 17 | ASP |
| 15 | CP | 52 | LEU |
| 16 | CQ | 81 | ALA |
| 17 | CR | 20 | ILE |
| 19 | CT | 65 | LEU |
| 20 | CB | 14 | HIS |
| 20 | CB | 19 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CB | 121 | GLN |
| 20 | CB | 128 | LEU |
| 20 | CB | 131 | LYS |
| 20 | CB | 150 | ILE |
| 21 | CU | 25 | ALA |
| 21 | CU | 26 | GLY |
| 21 | CU | 34 | ARG |
| 21 | CU | 35 | GLU |
| 24 | DV | 25 | LYS |
| 25 | DC | 3 | VAL |
| 25 | DC | 52 | HIS |
| 25 | DC | 93 | VAL |
| 25 | DC | 135 | PRO |
| 25 | DC | 140 | VAL |
| 25 | DC | 142 | ASN |
| 25 | DC | 151 | GLY |
| 25 | DC | 222 | THR |
| 25 | DC | 232 | GLY |
| 25 | DC | 239 | PHE |
| 26 | DD | 24 | VAL |
| 26 | DD | 93 | GLY |
| 26 | DD | 107 | VAL |
| 26 | DD | 119 | ALA |
| 26 | DD | 121 | THR |
| 26 | DD | 136 | ASN |
| 26 | DD | 184 | ARG |
| 26 | DD | 197 | THR |
| 27 | DE | 42 | GLY |
| 27 | DE | 45 | ALA |
| 27 | DE | 165 | HIS |
| 28 | DF | 11 | VAL |
| 28 | DF | 36 | ASN |
| 28 | DF | 141 | ASP |
| 28 | DF | 142 | TYR |
| 28 | DF | 149 | ARG |
| 29 | DG | 2 | ARG |
| 29 | DG | 84 | LYS |
| 29 | DG | 89 | VAL |
| 29 | DG | 92 | GLY |
| 29 | DG | 107 | GLY |
| 29 | DG | 170 | THR |
| 30 | DH | 40 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 30 | DH | 96 | THR |
| 30 | DH | 102 | ALA |
| 30 | DH | 106 | ALA |
| 30 | DH | 109 | GLU |
| 30 | DH | 110 | VAL |
| 30 | DH | 113 | SER |
| 30 | DH | 148 | ALA |
| 31 | DJ | 5 | THR |
| 31 | DJ | 41 | LYS |
| 31 | DJ | 43 | GLU |
| 31 | DJ | 81 | ILE |
| 31 | DJ | 124 | VAL |
| 31 | DJ | 129 | GLU |
| 32 | DK | 108 | ARG |
| 32 | DK | 110 | GLU |
| 32 | DK | 113 | MET |
| 33 | DL | 3 | LEU |
| 33 | DL | 4 | ASN |
| 33 | DL | 5 | THR |
| 33 | DL | 28 | GLY |
| 33 | DL | 29 | LYS |
| 33 | DL | 51 | GLU |
| 33 | DL | 52 | GLY |
| 33 | DL | 93 | ASN |
| 33 | DL | 113 | ALA |
| 34 | DM | 20 | LEU |
| 34 | DM | 36 | VAL |
| 34 | DM | 59 | ARG |
| 34 | DM | 69 | PRO |
| 34 | DM | 79 | ALA |
| 34 | DM | 134 | THR |
| 35 | DN | 10 | LEU |
| 35 | DN | 89 | SER |
| 35 | DN | 100 | CYS |
| 35 | DN | 101 | GLY |
| 36 | DO | 57 | ALA |
| 36 | DO | 68 | LYS |
| 36 | DO | 79 | ALA |
| 36 | DO | 107 | ALA |
| 37 | DP | 20 | ARG |
| 37 | DP | 32 | VAL |
| 37 | DP | 84 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | DP | 101 | GLU |
| 37 | DP | 108 | ARG |
| 38 | DQ | 87 | VAL |
| 39 | DR | 42 | ALA |
| 39 | DR | 49 | ILE |
| 39 | DR | 100 | GLY |
| 40 | DS | 25 | ARG |
| 40 | DS | 96 | ILE |
| 40 | DS | 109 | ASP |
| 41 | DT | 19 | LYS |
| 41 | DT | 28 | ASN |
| 41 | DT | 35 | ALA |
| 41 | DT | 38 | ALA |
| 41 | DT | 69 | ARG |
| 42 | DU | 12 | VAL |
| 42 | DU | 92 | VAL |
| 43 | DW | 12 | GLY |
| 43 | DW | 14 | ASP |
| 43 | DW | 23 | LYS |
| 43 | DW | 40 | ARG |
| 43 | DW | 76 | ARG |
| 43 | DW | 77 | LYS |
| 44 | DX | 10 | SER |
| 44 | DX | 36 | GLN |
| 46 | DZ | 3 | ARG |
| 46 | DZ | 77 | LYS |
| 47 | D0 | 51 | ARG |
| 48 | D1 | 4 | ILE |
| 49 | D2 | 42 | LEU |
| 50 | D3 | 31 | ILE |
| 2 | AC | 81 | GLU |
| 2 | AC | 104 | GLU |
| 3 | AD | 24 | VAL |
| 3 | AD | 26 | ALA |
| 3 | AD | 31 | CYS |
| 3 | AD | 168 | THR |
| 3 | AD | 182 | LYS |
| 3 | AD | 189 | ASP |
| 4 | AE | 144 | GLU |
| 5 | AF | 51 | ILE |
| 8 | AI | 9 | GLY |
| 9 | AJ | 56 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AJ | 93 | ALA |
| 10 | AK | 88 | PRO |
| 10 | AK | 125 | LYS |
| 11 | AL | 23 | LEU |
| 11 | AL | 47 | ALA |
| 13 | AN | 21 | ALA |
| 14 | AO | 33 | ALA |
| 16 | AQ | 14 | ASP |
| 17 | AR | 20 | ILE |
| 19 | AT | 42 | ASP |
| 19 | AT | 67 | HIS |
| 20 | AB | 15 | PHE |
| 20 | AB | 18 | GLN |
| 20 | AB | 41 | ASN |
| 20 | AB | 76 | SER |
| 20 | AB | 127 | LYS |
| 20 | AB | 205 | ALA |
| 21 | AU | 22 | CYS |
| 21 | AU | 26 | GLY |
| 24 | BV | 71 | LYS |
| 25 | BC | 17 | LYS |
| 25 | BC | 34 | GLU |
| 25 | BC | 35 | LYS |
| 25 | BC | 37 | SER |
| 25 | BC | 52 | HIS |
| 25 | BC | 94 | LEU |
| 25 | BC | 122 | ALA |
| 25 | BC | 141 | HIS |
| 25 | BC | 145 | MET |
| 25 | BC | 190 | THR |
| 25 | BC | 200 | MET |
| 25 | BC | 250 | GLN |
| 25 | BC | 254 | LYS |
| 26 | BD | 127 | PHE |
| 26 | BD | 143 | PRO |
| 26 | BD | 145 | SER |
| 26 | BD | 159 | LYS |
| 26 | BD | 162 | ALA |
| 26 | BD | 194 | PRO |
| 27 | BE | 13 | THR |
| 27 | BE | 81 | GLY |
| 27 | BE | 86 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | BE | 97 | ASN |
| 27 | BE | 127 | GLU |
| 27 | BE | 166 | LYS |
| 28 | BF | 9 | ASP |
| 28 | BF | 28 | PRO |
| 28 | BF | 42 | ALA |
| 28 | BF | 81 | GLY |
| 28 | BF | 110 | ILE |
| 28 | BF | 125 | GLY |
| 28 | BF | 142 | TYR |
| 29 | BG | 11 | PRO |
| 29 | BG | 38 | ASP |
| 29 | BG | 61 | TRP |
| 29 | BG | 102 | ILE |
| 29 | BG | 170 | THR |
| 30 | BH | 7 | ASP |
| 30 | BH | 11 | ASN |
| 30 | BH | 66 | ASN |
| 30 | BH | 71 | LYS |
| 30 | BH | 77 | THR |
| 30 | BH | 83 | LYS |
| 30 | BH | 108 | VAL |
| 30 | BH | 122 | LEU |
| 31 | BJ | 14 | ASP |
| 31 | BJ | 72 | LYS |
| 31 | BJ | 111 | LYS |
| 32 | BK | 72 | PRO |
| 32 | BK | 101 | GLY |
| 32 | BK | 110 | GLU |
| 33 | BL | 4 | ASN |
| 33 | BL | 54 | GLN |
| 33 | BL | 82 | LEU |
| 34 | BM | 13 | HIS |
| 34 | BM | 60 | GLN |
| 34 | BM | 77 | PRO |
| 34 | BM | 134 | THR |
| 35 | BN | 10 | LEU |
| 35 | BN | 70 | THR |
| 35 | BN | 98 | LEU |
| 36 | BO | 9 | ARG |
| 36 | BO | 68 | LYS |
| 36 | BO | 95 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BO | 100 | HIS |
| 37 | BP | 64 | SER |
| 37 | BP | 104 | GLY |
| 37 | BP | 113 | LEU |
| 38 | BQ | 17 | LEU |
| 38 | BQ | 32 | ARG |
| 38 | BQ | 69 | ARG |
| 38 | BQ | 72 | GLY |
| 38 | BQ | 88 | GLU |
| 39 | BR | 24 | LYS |
| 39 | BR | 57 | GLY |
| 40 | BS | 60 | HIS |
| 40 | BS | 80 | PRO |
| 41 | BT | 10 | VAL |
| 41 | BT | 19 | LYS |
| 42 | BU | 16 | LYS |
| 42 | BU | 89 | GLY |
| 43 | BW | 9 | THR |
| 43 | BW | 13 | ARG |
| 43 | BW | 17 | ALA |
| 43 | BW | 82 | GLU |
| 44 | BX | 45 | GLN |
| 44 | BX | 62 | GLY |
| 46 | BZ | 35 | SER |
| 49 | B2 | 5 | PHE |
| 51 | B4 | 8 | LYS |
| 2 | CC | 81 | GLU |
| 2 | CC | 104 | GLU |
| 2 | CC | 153 | SER |
| 3 | CD | 24 | VAL |
| 3 | CD | 31 | CYS |
| 3 | CD | 182 | LYS |
| 4 | CE | 144 | GLU |
| 6 | CG | 3 | ARG |
| 6 | CG | 112 | ASP |
| 6 | CG | 151 | ALA |
| 7 | CH | 114 | ALA |
| 8 | CI | 9 | GLY |
| 8 | CI | 34 | LEU |
| 8 | CI | 106 | ASP |
| 9 | CJ | 56 | HIS |
| 9 | CJ | 93 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | CK | 71 | ASP |
| 10 | CK | 88 | PRO |
| 10 | CK | 125 | LYS |
| 11 | CL | 47 | ALA |
| 13 | CN | 21 | ALA |
| 14 | CO | 33 | ALA |
| 16 | CQ | 14 | ASP |
| 19 | CT | 41 | GLY |
| 19 | CT | 42 | ASP |
| 19 | CT | 67 | HIS |
| 20 | CB | 15 | PHE |
| 20 | CB | 18 | GLN |
| 20 | CB | 41 | ASN |
| 20 | CB | 76 | SER |
| 20 | CB | 120 | SER |
| 20 | CB | 130 | LYS |
| 20 | CB | 205 | ALA |
| 21 | CU | 22 | CYS |
| 24 | DV | 71 | LYS |
| 25 | DC | 17 | LYS |
| 25 | DC | 34 | GLU |
| 25 | DC | 35 | LYS |
| 25 | DC | 37 | SER |
| 25 | DC | 51 | ARG |
| 25 | DC | 94 | LEU |
| 25 | DC | 145 | MET |
| 25 | DC | 190 | THR |
| 25 | DC | 250 | GLN |
| 25 | DC | 254 | LYS |
| 26 | DD | 127 | PHE |
| 26 | DD | 143 | PRO |
| 26 | DD | 145 | SER |
| 26 | DD | 159 | LYS |
| 26 | DD | 162 | ALA |
| 26 | DD | 194 | PRO |
| 27 | DE | 13 | THR |
| 27 | DE | 81 | GLY |
| 27 | DE | 86 | ALA |
| 27 | DE | 97 | ASN |
| 27 | DE | 127 | GLU |
| 27 | DE | 166 | LYS |
| 28 | DF | 9 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | DF | 28 | PRO |
| 28 | DF | 42 | ALA |
| 28 | DF | 81 | GLY |
| 28 | DF | 125 | GLY |
| 29 | DG | 11 | PRO |
| 29 | DG | 32 | LEU |
| 29 | DG | 38 | ASP |
| 29 | DG | 61 | TRP |
| 29 | DG | 159 | LYS |
| 30 | DH | 7 | ASP |
| 30 | DH | 11 | ASN |
| 30 | DH | 12 | LEU |
| 30 | DH | 56 | ALA |
| 30 | DH | 88 | GLY |
| 31 | DJ | 14 | ASP |
| 31 | DJ | 72 | LYS |
| 31 | DJ | 111 | LYS |
| 32 | DK | 72 | PRO |
| 33 | DL | 82 | LEU |
| 34 | DM | 35 | ALA |
| 34 | DM | 60 | GLN |
| 34 | DM | 77 | PRO |
| 35 | DN | 98 | LEU |
| 36 | DO | 9 | ARG |
| 36 | DO | 95 | SER |
| 36 | DO | 100 | HIS |
| 37 | DP | 64 | SER |
| 38 | DQ | 69 | ARG |
| 38 | DQ | 72 | GLY |
| 38 | DQ | 88 | GLU |
| 38 | DQ | 91 | ARG |
| 39 | DR | 24 | LYS |
| 40 | DS | 60 | HIS |
| 40 | DS | 80 | PRO |
| 42 | DU | 5 | ARG |
| 42 | DU | 16 | LYS |
| 42 | DU | 89 | GLY |
| 43 | DW | 9 | THR |
| 43 | DW | 13 | ARG |
| 43 | DW | 17 | ALA |
| 43 | DW | 61 | LYS |
| 43 | DW | 82 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | DX | 62 | GLY |
| 45 | DY | 34 | THR |
| 46 | DZ | 35 | SER |
| 49 | D2 | 5 | PHE |
| 50 | D3 | 6 | VAL |
| 51 | D4 | 8 | LYS |
| 52 | DI | 23 | VAL |
| 2 | AC | 3 | LYS |
| 2 | AC | 166 | TRP |
| 3 | AD | 27 | ILE |
| 3 | AD | 167 | PRO |
| 5 | AF | 48 | ALA |
| 5 | AF | 89 | VAL |
| 6 | AG | 8 | GLN |
| 6 | AG | 112 | ASP |
| 8 | AI | 25 | GLY |
| 8 | AI | 34 | LEU |
| 8 | AI | 106 | ASP |
| 10 | AK | 71 | ASP |
| 10 | AK | 107 | THR |
| 11 | AL | 24 | GLU |
| 11 | AL | 33 | CYS |
| 11 | AL | 122 | LYS |
| 12 | AM | 15 | VAL |
| 13 | AN | 34 | ASN |
| 13 | AN | 48 | GLN |
| 13 | AN | 61 | ASN |
| 14 | AO | 75 | ALA |
| 16 | AQ | 35 | LYS |
| 20 | AB | 86 | CYS |
| 20 | AB | 128 | LEU |
| 20 | AB | 211 | LEU |
| 21 | AU | 9 | GLU |
| 25 | BC | 51 | ARG |
| 25 | BC | 59 | GLN |
| 25 | BC | 64 | VAL |
| 25 | BC | 92 | LEU |
| 25 | BC | 131 | MET |
| 25 | BC | 189 | ALA |
| 25 | BC | 196 | ASN |
| 26 | BD | 31 | ALA |
| 27 | BE | 92 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BF | 82 | TYR |
| 28 | BF | 103 | ILE |
| 28 | BF | 106 | ALA |
| 28 | BF | 124 | ARG |
| 29 | BG | 45 | ALA |
| 29 | BG | 83 | THR |
| 29 | BG | 100 | ASN |
| 29 | BG | 111 | PRO |
| 30 | BH | 9 | VAL |
| 30 | BH | 12 | LEU |
| 30 | BH | 73 | ASN |
| 30 | BH | 97 | ARG |
| 30 | BH | 109 | GLU |
| 30 | BH | 118 | PRO |
| 30 | BH | 146 | VAL |
| 31 | BJ | 26 | GLY |
| 31 | BJ | 58 | ASN |
| 32 | BK | 14 | SER |
| 32 | BK | 54 | LYS |
| 32 | BK | 90 | ASN |
| 32 | BK | 94 | PRO |
| 33 | BL | 12 | SER |
| 33 | BL | 15 | ALA |
| 33 | BL | 19 | LEU |
| 33 | BL | 53 | GLY |
| 34 | BM | 27 | SER |
| 34 | BM | 35 | ALA |
| 34 | BM | 55 | ARG |
| 34 | BM | 75 | GLU |
| 34 | BM | 106 | ASP |
| 35 | BN | 112 | TYR |
| 36 | BO | 99 | TYR |
| 37 | BP | 65 | ASN |
| 39 | BR | 98 | ILE |
| 41 | BT | 8 | LEU |
| 41 | BT | 11 | LEU |
| 41 | BT | 37 | ASP |
| 41 | BT | 86 | THR |
| 43 | BW | 21 | GLY |
| 43 | BW | 34 | SER |
| 43 | BW | 75 | ASN |
| 44 | BX | 16 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | BX | 37 | LEU |
| 44 | BX | 58 | ASN |
| 45 | BY | 4 | ILE |
| 45 | BY | 34 | THR |
| 46 | BZ | 22 | LEU |
| 46 | BZ | 34 | HIS |
| 48 | B1 | 36 | LYS |
| 50 | B3 | 6 | VAL |
| 50 | B3 | 20 | GLY |
| 50 | B3 | 50 | SER |
| 50 | B3 | 58 | ILE |
| 50 | B3 | 59 | ALA |
| 51 | B4 | 4 | ARG |
| 2 | CC | 3 | LYS |
| 2 | CC | 166 | TRP |
| 3 | CD | 18 | LEU |
| 3 | CD | 22 | SER |
| 3 | CD | 27 | ILE |
| 3 | CD | 59 | LYS |
| 3 | CD | 82 | LYS |
| 3 | CD | 167 | PRO |
| 5 | CF | 48 | ALA |
| 5 | CF | 89 | VAL |
| 7 | CH | 30 | LYS |
| 8 | CI | 25 | GLY |
| 9 | CJ | 13 | PHE |
| 10 | CK | 107 | THR |
| 11 | CL | 23 | LEU |
| 11 | CL | 24 | GLU |
| 11 | CL | 33 | CYS |
| 11 | CL | 122 | LYS |
| 13 | CN | 34 | ASN |
| 13 | CN | 57 | SER |
| 13 | CN | 61 | ASN |
| 15 | CP | 17 | TYR |
| 15 | CP | 54 | LEU |
| 16 | CQ | 35 | LYS |
| 20 | CB | 38 | HIS |
| 20 | CB | 86 | CYS |
| 21 | CU | 9 | GLU |
| 24 | DV | 44 | HIS |
| 25 | DC | 59 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DC | 64 | VAL |
| 25 | DC | 92 | LEU |
| 25 | DC | 122 | ALA |
| 25 | DC | 131 | MET |
| 25 | DC | 141 | HIS |
| 25 | DC | 150 | GLY |
| 25 | DC | 161 | VAL |
| 25 | DC | 189 | ALA |
| 25 | DC | 196 | ASN |
| 25 | DC | 200 | MET |
| 26 | DD | 31 | ALA |
| 26 | DD | 75 | ALA |
| 27 | DE | 92 | HIS |
| 28 | DF | 20 | ASN |
| 28 | DF | 41 | GLU |
| 28 | DF | 82 | TYR |
| 28 | DF | 103 | ILE |
| 28 | DF | 106 | ALA |
| 28 | DF | 110 | ILE |
| 29 | DG | 45 | ALA |
| 29 | DG | 78 | VAL |
| 29 | DG | 83 | THR |
| 29 | DG | 100 | ASN |
| 29 | DG | 102 | ILE |
| 29 | DG | 111 | PRO |
| 29 | DG | 151 | ARG |
| 30 | DH | 9 | VAL |
| 30 | DH | 92 | GLY |
| 32 | DK | 14 | SER |
| 32 | DK | 16 | ALA |
| 32 | DK | 54 | LYS |
| 32 | DK | 90 | ASN |
| 32 | DK | 94 | PRO |
| 33 | DL | 15 | ALA |
| 33 | DL | 19 | LEU |
| 33 | DL | 53 | GLY |
| 33 | DL | 54 | GLN |
| 34 | DM | 13 | HIS |
| 34 | DM | 26 | VAL |
| 34 | DM | 27 | SER |
| 34 | DM | 55 | ARG |
| 34 | DM | 87 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DM | 106 | ASP |
| 35 | DN | 70 | THR |
| 36 | DO | 99 | TYR |
| 37 | DP | 65 | ASN |
| 37 | DP | 104 | GLY |
| 37 | DP | 113 | LEU |
| 38 | DQ | 17 | LEU |
| 40 | DS | 21 | ALA |
| 41 | DT | 8 | LEU |
| 41 | DT | 11 | LEU |
| 41 | DT | 18 | GLU |
| 41 | DT | 29 | THR |
| 41 | DT | 37 | ASP |
| 41 | DT | 64 | LYS |
| 41 | DT | 86 | THR |
| 43 | DW | 21 | GLY |
| 43 | DW | 34 | SER |
| 43 | DW | 75 | ASN |
| 44 | DX | 16 | THR |
| 44 | DX | 45 | GLN |
| 44 | DX | 58 | ASN |
| 45 | DY | 4 | ILE |
| 46 | DZ | 22 | LEU |
| 46 | DZ | 34 | HIS |
| 47 | D0 | 19 | ASP |
| 48 | D1 | 36 | LYS |
| 50 | D3 | 50 | SER |
| 50 | D3 | 59 | ALA |
| 51 | D4 | 4 | ARG |
| 51 | D4 | 23 | ILE |
| 2 | AC | 107 | LYS |
| 2 | AC | 145 | ALA |
| 2 | AC | 189 | HIS |
| 3 | AD | 18 | LEU |
| 3 | AD | 22 | SER |
| 3 | AD | 59 | LYS |
| 4 | AE | 43 | GLY |
| 4 | AE | 56 | PRO |
| 5 | AF | 85 | ILE |
| 5 | AF | 95 | ALA |
| 6 | AG | 7 | GLY |
| 7 | AH | 30 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AJ | 13 | PHE |
| 9 | AJ | 62 | ARG |
| 10 | AK | 14 | GLN |
| 10 | AK | 119 | GLY |
| 11 | AL | 83 | GLY |
| 13 | AN | 57 | SER |
| 13 | AN | 67 | GLY |
| 15 | AP | 17 | TYR |
| 15 | AP | 28 | ARG |
| 15 | AP | 54 | LEU |
| 16 | AQ | 31 | PRO |
| 17 | AR | 33 | THR |
| 20 | AB | 24 | PRO |
| 24 | BV | 44 | HIS |
| 24 | BV | 54 | ALA |
| 25 | BC | 5 | CYS |
| 25 | BC | 36 | ASN |
| 25 | BC | 105 | ALA |
| 25 | BC | 150 | GLY |
| 25 | BC | 161 | VAL |
| 25 | BC | 237 | ARG |
| 26 | BD | 75 | ALA |
| 26 | BD | 109 | VAL |
| 26 | BD | 131 | ASP |
| 27 | BE | 4 | VAL |
| 27 | BE | 12 | LEU |
| 27 | BE | 46 | GLN |
| 27 | BE | 59 | PRO |
| 27 | BE | 129 | PRO |
| 28 | BF | 20 | ASN |
| 28 | BF | 41 | GLU |
| 28 | BF | 156 | THR |
| 29 | BG | 78 | VAL |
| 29 | BG | 97 | VAL |
| 29 | BG | 151 | ARG |
| 29 | BG | 157 | LYS |
| 29 | BG | 159 | LYS |
| 29 | BG | 168 | VAL |
| 30 | BH | 14 | SER |
| 30 | BH | 16 | GLY |
| 30 | BH | 81 | ALA |
| 30 | BH | 95 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | BJ | 13 | ARG |
| 32 | BK | 3 | GLN |
| 32 | BK | 16 | ALA |
| 32 | BK | 17 | ARG |
| 32 | BK | 93 | GLN |
| 33 | BL | 41 | ARG |
| 33 | BL | 66 | PHE |
| 33 | BL | 86 | GLU |
| 34 | BM | 73 | ILE |
| 34 | BM | 87 | GLY |
| 36 | BO | 8 | ILE |
| 37 | BP | 59 | THR |
| 38 | BQ | 27 | ARG |
| 39 | BR | 46 | GLU |
| 41 | BT | 18 | GLU |
| 41 | BT | 29 | THR |
| 42 | BU | 37 | GLY |
| 43 | BW | 56 | HIS |
| 44 | BX | 9 | LYS |
| 46 | BZ | 18 | ARG |
| 47 | B0 | 19 | ASP |
| 47 | B0 | 54 | ILE |
| 49 | B2 | 45 | SER |
| 51 | B4 | 16 | ILE |
| 51 | B4 | 23 | ILE |
| 2 | CC | 83 | VAL |
| 2 | CC | 107 | LYS |
| 2 | CC | 145 | ALA |
| 2 | CC | 167 | TYR |
| 4 | CE | 43 | GLY |
| 5 | CF | 55 | HIS |
| 5 | CF | 85 | ILE |
| 5 | CF | 95 | ALA |
| 8 | CI | 55 | ASP |
| 9 | CJ | 62 | ARG |
| 10 | CK | 119 | GLY |
| 12 | CM | 15 | VAL |
| 13 | CN | 48 | GLN |
| 13 | CN | 67 | GLY |
| 14 | CO | 75 | ALA |
| 16 | CQ | 31 | PRO |
| 17 | CR | 33 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | CS | 27 | LYS |
| 20 | CB | 24 | PRO |
| 20 | CB | 211 | LEU |
| 24 | DV | 45 | ASP |
| 24 | DV | 54 | ALA |
| 25 | DC | 5 | CYS |
| 25 | DC | 36 | ASN |
| 25 | DC | 55 | GLY |
| 25 | DC | 65 | ASP |
| 25 | DC | 77 | VAL |
| 25 | DC | 105 | ALA |
| 26 | DD | 109 | VAL |
| 26 | DD | 131 | ASP |
| 26 | DD | 156 | PHE |
| 26 | DD | 173 | GLN |
| 27 | DE | 12 | LEU |
| 27 | DE | 37 | ALA |
| 27 | DE | 46 | GLN |
| 27 | DE | 59 | PRO |
| 28 | DF | 69 | ALA |
| 28 | DF | 124 | ARG |
| 28 | DF | 156 | THR |
| 29 | DG | 97 | VAL |
| 29 | DG | 157 | LYS |
| 29 | DG | 168 | VAL |
| 30 | DH | 16 | GLY |
| 30 | DH | 91 | PHE |
| 30 | DH | 107 | GLY |
| 31 | DJ | 13 | ARG |
| 31 | DJ | 26 | GLY |
| 31 | DJ | 58 | ASN |
| 32 | DK | 17 | ARG |
| 32 | DK | 45 | GLU |
| 32 | DK | 46 | ALA |
| 32 | DK | 73 | ASP |
| 32 | DK | 93 | GLN |
| 32 | DK | 101 | GLY |
| 33 | DL | 12 | SER |
| 33 | DL | 30 | THR |
| 33 | DL | 41 | ARG |
| 33 | DL | 66 | PHE |
| 33 | DL | 86 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DM | 66 | ARG |
| 34 | DM | 73 | ILE |
| 34 | DM | 75 | GLU |
| 35 | DN | 107 | ASN |
| 35 | DN | 112 | TYR |
| 36 | DO | 8 | ILE |
| 36 | DO | 53 | THR |
| 37 | DP | 59 | THR |
| 38 | DQ | 27 | ARG |
| 39 | DR | 57 | GLY |
| 39 | DR | 82 | HIS |
| 39 | DR | 98 | ILE |
| 42 | DU | 24 | VAL |
| 43 | DW | 29 | SER |
| 44 | DX | 9 | LYS |
| 44 | DX | 37 | LEU |
| 46 | DZ | 18 | ARG |
| 47 | D0 | 54 | ILE |
| 49 | D2 | 45 | SER |
| 50 | D3 | 20 | GLY |
| 50 | D3 | 58 | ILE |
| 52 | DI | 6 | ALA |
| 52 | DI | 14 | ALA |
| 2 | AC | 83 | VAL |
| 2 | AC | 167 | TYR |
| 3 | AD | 82 | LYS |
| 5 | AF | 55 | HIS |
| 5 | AF | 94 | HIS |
| 5 | AF | 99 | ALA |
| 8 | AI | 55 | ASP |
| 18 | AS | 27 | LYS |
| 18 | AS | 53 | GLY |
| 20 | AB | 123 | GLY |
| 24 | BV | 45 | ASP |
| 24 | BV | 84 | PRO |
| 25 | BC | 65 | ASP |
| 26 | BD | 173 | GLN |
| 27 | BE | 37 | ALA |
| 27 | BE | 83 | VAL |
| 28 | BF | 88 | VAL |
| 29 | BG | 155 | PRO |
| 32 | BK | 73 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | BP | 4 | ILE |
| 39 | BR | 9 | GLY |
| 40 | BS | 21 | ALA |
| 40 | BS | 29 | VAL |
| 41 | BT | 55 | VAL |
| 41 | BT | 71 | GLY |
| 4 | CE | 56 | PRO |
| 5 | CF | 94 | HIS |
| 7 | CH | 71 | VAL |
| 10 | CK | 16 | SER |
| 11 | CL | 83 | GLY |
| 15 | CP | 24 | SER |
| 15 | CP | 28 | ARG |
| 18 | CS | 53 | GLY |
| 24 | DV | 84 | PRO |
| 25 | DC | 4 | LYS |
| 27 | DE | 83 | VAL |
| 27 | DE | 129 | PRO |
| 28 | DF | 12 | VAL |
| 28 | DF | 88 | VAL |
| 29 | DG | 60 | GLY |
| 29 | DG | 155 | PRO |
| 30 | DH | 29 | PHE |
| 33 | DL | 62 | PRO |
| 37 | DP | 4 | ILE |
| 38 | DQ | 32 | ARG |
| 39 | DR | 9 | GLY |
| 40 | DS | 18 | ARG |
| 40 | DS | 29 | VAL |
| 41 | DT | 10 | VAL |
| 41 | DT | 55 | VAL |
| 42 | DU | 37 | GLY |
| 42 | DU | 90 | LYS |
| 43 | DW | 46 | ALA |
| 49 | D2 | 2 | LYS |
| 49 | D2 | 19 | ARG |
| 51 | D4 | 11 | CYS |
| 51 | D4 | 16 | ILE |
| 6 | AG | 15 | PRO |
| 9 | AJ | 41 | PRO |
| 9 | AJ | 42 | LEU |
| 15 | AP | 42 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AT | 3 | ILE |
| 20 | AB | 28 | PRO |
| 25 | BC | 55 | GLY |
| 25 | BC | 77 | VAL |
| 27 | BE | 96 | VAL |
| 28 | BF | 12 | VAL |
| 30 | BH | 61 | VAL |
| 30 | BH | 103 | VAL |
| 33 | BL | 62 | PRO |
| 34 | BM | 26 | VAL |
| 37 | BP | 63 | ILE |
| 42 | BU | 24 | VAL |
| 43 | BW | 53 | GLY |
| 45 | BY | 50 | VAL |
| 51 | B4 | 3 | VAL |
| 6 | CG | 15 | PRO |
| 8 | CI | 71 | ILE |
| 9 | CJ | 42 | LEU |
| 15 | CP | 33 | ILE |
| 15 | CP | 42 | ILE |
| 25 | DC | 158 | GLY |
| 28 | DF | 145 | VAL |
| 37 | DP | 63 | ILE |
| 41 | DT | 71 | GLY |
| 45 | DY | 50 | VAL |
| 51 | D4 | 3 | VAL |
| 6 | AG | 92 | PRO |
| 7 | AH | 71 | VAL |
| 7 | AH | 128 | VAL |
| 8 | AI | 71 | ILE |
| 25 | BC | 158 | GLY |
| 25 | BC | 246 | PRO |
| 28 | BF | 136 | ILE |
| 28 | BF | 145 | VAL |
| 29 | BG | 60 | GLY |
| 4 | CE | 133 | ILE |
| 6 | CG | 92 | PRO |
| 9 | CJ | 41 | PRO |
| 15 | CP | 49 | GLY |
| 19 | CT | 3 | ILE |
| 20 | CB | 28 | PRO |
| 25 | DC | 246 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | DD | 60 | VAL |
| 27 | DE | 4 | VAL |
| 27 | DE | 96 | VAL |
| 28 | DF | 136 | ILE |
| 43 | DW | 22 | VAL |
| 43 | DW | 53 | GLY |
| 14 | AO | 28 | VAL |
| 15 | AP | 33 | ILE |
| 29 | BG | 16 | VAL |
| 29 | BG | 152 | ARG |
| 30 | BH | 78 | VAL |
| 37 | BP | 91 | VAL |
| 43 | BW | 22 | VAL |
| 46 | BZ | 64 | ILE |
| 4 | CE | 132 | PRO |
| 7 | CH | 125 | ILE |
| 7 | CH | 128 | VAL |
| 14 | CO | 28 | VAL |
| 26 | DD | 178 | VAL |
| 29 | DG | 16 | VAL |
| 29 | DG | 152 | ARG |
| 34 | DM | 72 | PRO |
| 37 | DP | 91 | VAL |
| 43 | DW | 37 | VAL |
| 46 | DZ | 64 | ILE |
| 7 | AH | 125 | ILE |
| 11 | AL | 15 | VAL |
| 15 | AP | 37 | GLY |
| 15 | AP | 49 | GLY |
| 26 | BD | 60 | VAL |
| 26 | BD | 178 | VAL |
| 29 | BG | 139 | VAL |
| 33 | BL | 139 | GLY |
| 37 | BP | 83 | ILE |
| 42 | BU | 82 | VAL |
| 43 | BW | 37 | VAL |
| 44 | BX | 46 | VAL |
| 11 | CL | 15 | VAL |
| 15 | CP | 20 | VAL |
| 29 | DG | 139 | VAL |
| 37 | DP | 83 | ILE |
| 39 | DR | 101 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DU | 82 | VAL |
| 44 | DX | 11 | VAL |
| 2 | AC | 80 | GLY |
| 28 | BF | 150 | GLY |
| 38 | BQ | 39 | ILE |
| 2 | CC | 80 | GLY |
| 26 | DD | 163 | GLY |
| 29 | DG | 90 | GLY |
| 31 | DJ | 22 | GLY |
| 32 | DK | 43 | ILE |
| 41 | DT | 57 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AC | 170/189 (90%) | 144 (85%) | 26 (15%) | 2 | 17 |
| 2 | CC | 170/189 (90%) | 145 (85%) | 25 (15%) | 3 | 18 |
| 3 | AD | 172/172 (100%) | 148 (86%) | 24 (14%) | 3 | 19 |
| 3 | CD | 172/172 (100%) | 149 (87%) | 23 (13%) | 4 | 21 |
| 4 | AE | 113/125 (90%) | 100 (88%) | 13 (12%) | 5 | 26 |
| 4 | CE | 113/125 (90%) | 98 (87%) | 15 (13%) | 4 | 21 |
| 5 | AF | 87/116 (75%) | 76 (87%) | 11 (13%) | 4 | 22 |
| 5 | CF | 87/116 (75%) | 75 (86%) | 12 (14%) | 3 | 20 |
| 6 | AG | 123/146 (84%) | 108 (88%) | 15 (12%) | 5 | 23 |
| 6 | CG | 125/146 (86%) | 108 (86%) | 17 (14%) | 3 | 20 |
| 7 | AH | 104/104 (100%) | 96 (92%) | 8 (8%) | 13 | 42 |
| 7 | CH | 104/104 (100%) | 96 (92%) | 8 (8%) | 13 | 42 |
| 8 | AI | 105/106 (99%) | 94 (90%) | 11 (10%) | 7 | 31 |
| 8 | CI | 105/106 (99%) | 93 (89%) | 12 (11%) | 5 | 26 |
| 9 | AJ | 86/90 (96%) | 79 (92%) | 7 (8%) | 11 | 41 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 9 | CJ | 86/90 (96%) | 80 (93%) | 6 (7%) | 15 | 46 |
| 10 | AK | 90/98 (92%) | 77 (86%) | 13 (14%) | 3 | 18 |
| 10 | CK | 90/98 (92%) | 77 (86%) | 13 (14%) | 3 | 18 |
| 11 | AL | 103/103 (100%) | 85 (82%) | 18 (18%) | 2 | 10 |
| 11 | CL | 103/103 (100%) | 84 (82%) | 19 (18%) | 1 | 8 |
| 12 | AM | 92/95 (97%) | 82 (89%) | 10 (11%) | 6 | 29 |
| 12 | CM | 91/95 (96%) | 82 (90%) | 9 (10%) | 8 | 33 |
| 13 | AN | 79/83 (95%) | 67 (85%) | 12 (15%) | 3 | 17 |
| 13 | CN | 79/83 (95%) | 67 (85%) | 12 (15%) | 3 | 17 |
| 14 | AO | 76/77 (99%) | 69 (91%) | 7 (9%) | 9 | 36 |
| 14 | CO | 76/77 (99%) | 70 (92%) | 6 (8%) | 12 | 41 |
| 15 | AP | 65/65 (100%) | 57 (88%) | 8 (12%) | 4 | 23 |
| 15 | CP | 65/65 (100%) | 57 (88%) | 8 (12%) | 4 | 23 |
| 16 | AQ | 74/77 (96%) | 65 (88%) | 9 (12%) | 5 | 23 |
| 16 | CQ | 75/77 (97%) | 65 (87%) | 10 (13%) | 4 | 21 |
| 17 | AR | 48/64 (75%) | 46 (96%) | 2 (4%) | 30 | 63 |
| 17 | CR | 48/64 (75%) | 46 (96%) | 2 (4%) | 30 | 63 |
| 18 | AS | 70/78 (90%) | 52 (74%) | 18 (26%) | 0 | 3 |
| 18 | CS | 71/78 (91%) | 53 (75%) | 18 (25%) | 0 | 3 |
| 19 | AT | 65/65 (100%) | 53 (82%) | 12 (18%) | 1 | 8 |
| 19 | CT | 65/65 (100%) | 53 (82%) | 12 (18%) | 1 | 8 |
| 20 | AB | 180/198 (91%) | 152 (84%) | 28 (16%) | 2 | 16 |
| 20 | CB | 180/198 (91%) | 150 (83%) | 30 (17%) | 2 | 12 |
| 21 | AU | 44/61 (72%) | 35 (80%) | 9 (20%) | 1 | 6 |
| 21 | CU | 44/61 (72%) | 35 (80%) | 9 (20%) | 1 | 6 |
| 24 | BV | 78/78 (100%) | 68 (87%) | 10 (13%) | 4 | 22 |
| 24 | DV | 78/78 (100%) | 69 (88%) | 9 (12%) | 5 | 26 |
| 25 | BC | 216/218 (99%) | 178 (82%) | 38 (18%) | 2 | 10 |
| 25 | DC | 216/218 (99%) | 175 (81%) | 41 (19%) | 1 | 8 |
| 26 | BD | 164/164 (100%) | 140 (85%) | 24 (15%) | 3 | 18 |
| 26 | DD | 164/164 (100%) | 140 (85%) | 24 (15%) | 3 | 18 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 27 | BE | 165/165 (100%) | 146 (88%) | 19 (12%) | 5 | 26 |
| 27 | DE | 165/165 (100%) | 146 (88%) | 19 (12%) | 5 | 26 |
| 28 | BF | 149/149 (100%) | 114 (76%) | 35 (24%) | 1 | 4 |
| 28 | DF | 149/149 (100%) | 115 (77%) | 34 (23%) | 1 | 4 |
| 29 | BG | 137/137 (100%) | 116 (85%) | 21 (15%) | 2 | 17 |
| 29 | DG | 137/137 (100%) | 116 (85%) | 21 (15%) | 2 | 17 |
| 30 | BH | 114/114 (100%) | 77 (68%) | 37 (32%) | 0 | 2 |
| 30 | DH | 114/114 (100%) | 93 (82%) | 21 (18%) | 1 | 8 |
| 31 | BJ | 116/116 (100%) | 98 (84%) | 18 (16%) | 2 | 16 |
| 31 | DJ | 116/116 (100%) | 98 (84%) | 18 (16%) | 2 | 16 |
| 32 | BK | 102/104 (98%) | 79 (78%) | 23 (22%) | 1 | 4 |
| 32 | DK | 102/104 (98%) | 79 (78%) | 23 (22%) | 1 | 4 |
| 33 | BL | 102/103 (99%) | 89 (87%) | 13 (13%) | 4 | 22 |
| 33 | DL | 102/103 (99%) | 90 (88%) | 12 (12%) | 5 | 25 |
| 34 | BM | 109/109 (100%) | 88 (81%) | 21 (19%) | 1 | 7 |
| 34 | DM | 109/109 (100%) | 88 (81%) | 21 (19%) | 1 | 7 |
| 35 | BN | 100/103 (97%) | 82 (82%) | 18 (18%) | 1 | 9 |
| 35 | DN | 100/103 (97%) | 81 (81%) | 19 (19%) | 1 | 8 |
| 36 | BO | 86/87 (99%) | 69 (80%) | 17 (20%) | 1 | 7 |
| 36 | DO | 86/87 (99%) | 69 (80%) | 17 (20%) | 1 | 7 |
| 37 | BP | 99/99 (100%) | 80 (81%) | 19 (19%) | 1 | 7 |
| 37 | DP | 99/99 (100%) | 81 (82%) | 18 (18%) | 1 | 9 |
| 38 | BQ | 89/89 (100%) | 79 (89%) | 10 (11%) | 6 | 27 |
| 38 | DQ | 89/89 (100%) | 79 (89%) | 10 (11%) | 6 | 27 |
| 39 | BR | 84/84 (100%) | 68 (81%) | 16 (19%) | 1 | 8 |
| 39 | DR | 84/84 (100%) | 70 (83%) | 14 (17%) | 2 | 12 |
| 40 | BS | 93/93 (100%) | 81 (87%) | 12 (13%) | 4 | 22 |
| 40 | DS | 93/93 (100%) | 82 (88%) | 11 (12%) | 5 | 25 |
| 41 | BT | 80/84 (95%) | 62 (78%) | 18 (22%) | 1 | 4 |
| 41 | DT | 80/84 (95%) | 62 (78%) | 18 (22%) | 1 | 4 |
| 42 | BU | 83/84 (99%) | 67 (81%) | 16 (19%) | 1 | 7 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-------------|----|
| 42 | DU | 83/84 (99%) | 67 (81%) | 16 (19%) | 1 | 7 |
| 43 | BW | 59/62 (95%) | 42 (71%) | 17 (29%) | 0 | 2 |
| 43 | DW | 59/62 (95%) | 42 (71%) | 17 (29%) | 0 | 2 |
| 44 | BX | 55/55 (100%) | 42 (76%) | 13 (24%) | 1 | 4 |
| 44 | DX | 55/55 (100%) | 42 (76%) | 13 (24%) | 1 | 4 |
| 45 | BY | 48/48 (100%) | 40 (83%) | 8 (17%) | 2 | 12 |
| 45 | DY | 48/48 (100%) | 40 (83%) | 8 (17%) | 2 | 12 |
| 46 | BZ | 67/68 (98%) | 54 (81%) | 13 (19%) | 1 | 7 |
| 46 | DZ | 67/68 (98%) | 53 (79%) | 14 (21%) | 1 | 6 |
| 47 | B0 | 47/47 (100%) | 39 (83%) | 8 (17%) | 2 | 12 |
| 47 | D0 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 | 17 |
| 48 | B1 | 45/48 (94%) | 40 (89%) | 5 (11%) | 6 | 28 |
| 48 | D1 | 45/48 (94%) | 41 (91%) | 4 (9%) | 9 | 37 |
| 49 | B2 | 38/38 (100%) | 32 (84%) | 6 (16%) | 2 | 15 |
| 49 | D2 | 38/38 (100%) | 32 (84%) | 6 (16%) | 2 | 15 |
| 50 | B3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 8 | 33 |
| 50 | D3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 8 | 33 |
| 51 | B4 | 34/34 (100%) | 32 (94%) | 2 (6%) | 19 | 53 |
| 51 | D4 | 34/34 (100%) | 32 (94%) | 2 (6%) | 19 | 53 |
| 52 | BI | 109/109 (100%) | 108 (99%) | 1 (1%) | 78 | 90 |
| 52 | DI | 109/109 (100%) | 103 (94%) | 6 (6%) | 21 | 54 |
| All | All | 9333/9704 (96%) | 7895 (85%) | 1438 (15%) | 2 | 16 |

All (1438) 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 | 18 | ASN |
| 2 | AC | 20 | THR |
| 2 | AC | 27 | GLU |
| 2 | AC | 35 | ASP |
| 2 | AC | 41 | TYR |
| 2 | AC | 48 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 62 | SER |
| 2 | AC | 69 | THR |
| 2 | AC | 87 | ARG |
| 2 | AC | 88 | LYS |
| 2 | AC | 113 | LYS |
| 2 | AC | 128 | MET |
| 2 | AC | 131 | ARG |
| 2 | AC | 138 | GLN |
| 2 | AC | 163 | ARG |
| 2 | AC | 166 | TRP |
| 2 | AC | 168 | ARG |
| 2 | AC | 171 | ARG |
| 2 | AC | 174 | LEU |
| 2 | AC | 175 | HIS |
| 2 | AC | 180 | ASP |
| 2 | AC | 184 | ASN |
| 2 | AC | 206 | ILE |
| 3 | AD | 4 | LEU |
| 3 | AD | 7 | LYS |
| 3 | AD | 18 | LEU |
| 3 | AD | 25 | ARG |
| 3 | AD | 28 | ASP |
| 3 | AD | 39 | GLN |
| 3 | AD | 47 | LEU |
| 3 | AD | 49 | ASP |
| 3 | AD | 55 | ARG |
| 3 | AD | 82 | LYS |
| 3 | AD | 87 | GLU |
| 3 | AD | 94 | GLU |
| 3 | AD | 114 | ARG |
| 3 | AD | 117 | VAL |
| 3 | AD | 125 | ASN |
| 3 | AD | 135 | GLN |
| 3 | AD | 146 | GLU |
| 3 | AD | 147 | LYS |
| 3 | AD | 160 | LEU |
| 3 | AD | 162 | GLU |
| 3 | AD | 168 | THR |
| 3 | AD | 189 | ASP |
| 3 | AD | 190 | LEU |
| 3 | AD | 195 | ASN |
| 4 | AE | 19 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AE | 23 | THR |
| 4 | AE | 44 | ARG |
| 4 | AE | 45 | VAL |
| 4 | AE | 55 | VAL |
| 4 | AE | 72 | ASN |
| 4 | AE | 81 | GLN |
| 4 | AE | 92 | ARG |
| 4 | AE | 105 | ILE |
| 4 | AE | 123 | LEU |
| 4 | AE | 127 | TYR |
| 4 | AE | 151 | MET |
| 4 | AE | 156 | ARG |
| 5 | AF | 6 | ILE |
| 5 | AF | 39 | LEU |
| 5 | AF | 51 | ILE |
| 5 | AF | 55 | HIS |
| 5 | AF | 60 | VAL |
| 5 | AF | 62 | MET |
| 5 | AF | 69 | GLU |
| 5 | AF | 82 | ASP |
| 5 | AF | 86 | ARG |
| 5 | AF | 94 | HIS |
| 5 | AF | 98 | GLU |
| 6 | AG | 3 | ARG |
| 6 | AG | 5 | VAL |
| 6 | AG | 10 | LYS |
| 6 | AG | 21 | LEU |
| 6 | AG | 49 | LEU |
| 6 | AG | 51 | GLN |
| 6 | AG | 55 | LYS |
| 6 | AG | 62 | GLU |
| 6 | AG | 67 | ASN |
| 6 | AG | 78 | ARG |
| 6 | AG | 89 | GLU |
| 6 | AG | 94 | ARG |
| 6 | AG | 96 | ASN |
| 6 | AG | 105 | GLU |
| 6 | AG | 113 | LYS |
| 7 | AH | 2 | MET |
| 7 | AH | 30 | LYS |
| 7 | AH | 55 | LYS |
| 7 | AH | 61 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AH | 72 | GLU |
| 7 | AH | 82 | LEU |
| 7 | AH | 105 | THR |
| 7 | AH | 113 | ARG |
| 8 | AI | 36 | GLN |
| 8 | AI | 45 | MET |
| 8 | AI | 59 | LYS |
| 8 | AI | 62 | LEU |
| 8 | AI | 87 | MET |
| 8 | AI | 93 | LEU |
| 8 | AI | 96 | GLU |
| 8 | AI | 105 | ARG |
| 8 | AI | 109 | GLN |
| 8 | AI | 112 | ARG |
| 8 | AI | 114 | LYS |
| 9 | AJ | 15 | HIS |
| 9 | AJ | 47 | GLU |
| 9 | AJ | 69 | THR |
| 9 | AJ | 77 | VAL |
| 9 | AJ | 78 | GLU |
| 9 | AJ | 88 | MET |
| 9 | AJ | 97 | ASP |
| 10 | AK | 22 | ILE |
| 10 | AK | 31 | VAL |
| 10 | AK | 34 | THR |
| 10 | AK | 51 | PHE |
| 10 | AK | 55 | ARG |
| 10 | AK | 64 | VAL |
| 10 | AK | 76 | TYR |
| 10 | AK | 82 | GLU |
| 10 | AK | 83 | VAL |
| 10 | AK | 107 | THR |
| 10 | AK | 115 | ILE |
| 10 | AK | 118 | ASN |
| 10 | AK | 121 | ARG |
| 11 | AL | 13 | ARG |
| 11 | AL | 14 | LYS |
| 11 | AL | 15 | VAL |
| 11 | AL | 17 | LYS |
| 11 | AL | 18 | SER |
| 11 | AL | 19 | ASN |
| 11 | AL | 28 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | AL | 35 | ARG |
| 11 | AL | 38 | THR |
| 11 | AL | 40 | THR |
| 11 | AL | 43 | LYS |
| 11 | AL | 61 | GLU |
| 11 | AL | 63 | THR |
| 11 | AL | 95 | HIS |
| 11 | AL | 107 | LYS |
| 11 | AL | 113 | ARG |
| 11 | AL | 119 | LYS |
| 11 | AL | 122 | LYS |
| 12 | AM | 2 | ARG |
| 12 | AM | 16 | ILE |
| 12 | AM | 28 | ARG |
| 12 | AM | 41 | ASP |
| 12 | AM | 43 | LYS |
| 12 | AM | 71 | GLU |
| 12 | AM | 80 | MET |
| 12 | AM | 82 | LEU |
| 12 | AM | 88 | LEU |
| 12 | AM | 102 | LYS |
| 13 | AN | 11 | LYS |
| 13 | AN | 19 | TYR |
| 13 | AN | 20 | PHE |
| 13 | AN | 25 | GLU |
| 13 | AN | 27 | LYS |
| 13 | AN | 41 | TRP |
| 13 | AN | 48 | GLN |
| 13 | AN | 49 | THR |
| 13 | AN | 50 | LEU |
| 13 | AN | 53 | ASP |
| 13 | AN | 58 | ARG |
| 13 | AN | 65 | GLN |
| 14 | AO | 17 | ASP |
| 14 | AO | 39 | GLN |
| 14 | AO | 53 | ARG |
| 14 | AO | 65 | LEU |
| 14 | AO | 69 | LEU |
| 14 | AO | 87 | ARG |
| 14 | AO | 88 | ARG |
| 15 | AP | 12 | LYS |
| 15 | AP | 23 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AP | 26 | ASN |
| 15 | AP | 28 | ARG |
| 15 | AP | 45 | GLU |
| 15 | AP | 51 | ARG |
| 15 | AP | 55 | ASP |
| 15 | AP | 68 | SER |
| 16 | AQ | 3 | LYS |
| 16 | AQ | 4 | ILE |
| 16 | AQ | 7 | LEU |
| 16 | AQ | 8 | GLN |
| 16 | AQ | 39 | ARG |
| 16 | AQ | 41 | THR |
| 16 | AQ | 56 | ASP |
| 16 | AQ | 60 | ILE |
| 16 | AQ | 80 | LYS |
| 17 | AR | 23 | LYS |
| 17 | AR | 38 | ILE |
| 18 | AS | 2 | ARG |
| 18 | AS | 4 | LEU |
| 18 | AS | 6 | LYS |
| 18 | AS | 10 | ILE |
| 18 | AS | 13 | HIS |
| 18 | AS | 20 | LYS |
| 18 | AS | 23 | GLU |
| 18 | AS | 26 | ASP |
| 18 | AS | 27 | LYS |
| 18 | AS | 28 | LYS |
| 18 | AS | 32 | THR |
| 18 | AS | 35 | ARG |
| 18 | AS | 38 | THR |
| 18 | AS | 42 | ASN |
| 18 | AS | 47 | THR |
| 18 | AS | 60 | PHE |
| 18 | AS | 64 | GLU |
| 18 | AS | 77 | ARG |
| 19 | AT | 3 | ILE |
| 19 | AT | 4 | LYS |
| 19 | AT | 35 | TYR |
| 19 | AT | 43 | LYS |
| 19 | AT | 51 | ASN |
| 19 | AT | 52 | GLU |
| 19 | AT | 53 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AT | 57 | VAL |
| 19 | AT | 67 | HIS |
| 19 | AT | 68 | LYS |
| 19 | AT | 74 | HIS |
| 19 | AT | 84 | LYS |
| 20 | AB | 31 | PHE |
| 20 | AB | 35 | ASN |
| 20 | AB | 46 | VAL |
| 20 | AB | 49 | PHE |
| 20 | AB | 57 | ASN |
| 20 | AB | 62 | ARG |
| 20 | AB | 67 | LEU |
| 20 | AB | 72 | LYS |
| 20 | AB | 87 | ASP |
| 20 | AB | 88 | GLN |
| 20 | AB | 94 | ARG |
| 20 | AB | 95 | TRP |
| 20 | AB | 104 | LYS |
| 20 | AB | 113 | LEU |
| 20 | AB | 115 | ASP |
| 20 | AB | 116 | LEU |
| 20 | AB | 117 | GLU |
| 20 | AB | 124 | THR |
| 20 | AB | 125 | PHE |
| 20 | AB | 127 | LYS |
| 20 | AB | 128 | LEU |
| 20 | AB | 145 | ASN |
| 20 | AB | 160 | LEU |
| 20 | AB | 176 | ASN |
| 20 | AB | 196 | ASP |
| 20 | AB | 199 | ILE |
| 20 | AB | 202 | ASN |
| 20 | AB | 212 | TYR |
| 21 | AU | 11 | PHE |
| 21 | AU | 15 | LEU |
| 21 | AU | 16 | ARG |
| 21 | AU | 22 | CYS |
| 21 | AU | 24 | LYS |
| 21 | AU | 32 | ARG |
| 21 | AU | 34 | ARG |
| 21 | AU | 38 | GLU |
| 21 | AU | 44 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | BV | 24 | ASN |
| 24 | BV | 40 | ILE |
| 24 | BV | 42 | LEU |
| 24 | BV | 51 | GLN |
| 24 | BV | 53 | LYS |
| 24 | BV | 66 | ASP |
| 24 | BV | 68 | LYS |
| 24 | BV | 69 | GLU |
| 24 | BV | 70 | ILE |
| 24 | BV | 86 | LEU |
| 25 | BC | 4 | LYS |
| 25 | BC | 6 | LYS |
| 25 | BC | 8 | THR |
| 25 | BC | 9 | SER |
| 25 | BC | 12 | ARG |
| 25 | BC | 37 | SER |
| 25 | BC | 43 | ASN |
| 25 | BC | 45 | ASN |
| 25 | BC | 47 | ARG |
| 25 | BC | 52 | HIS |
| 25 | BC | 62 | ARG |
| 25 | BC | 65 | ASP |
| 25 | BC | 67 | LYS |
| 25 | BC | 89 | ASN |
| 25 | BC | 90 | ILE |
| 25 | BC | 109 | LEU |
| 25 | BC | 123 | ILE |
| 25 | BC | 128 | THR |
| 25 | BC | 134 | ILE |
| 25 | BC | 142 | ASN |
| 25 | BC | 152 | GLN |
| 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 | 193 | GLU |
| 25 | BC | 203 | VAL |
| 25 | BC | 224 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BC | 239 | PHE |
| 25 | BC | 249 | VAL |
| 25 | BC | 252 | LYS |
| 25 | BC | 257 | ARG |
| 25 | BC | 266 | ILE |
| 25 | BC | 269 | ARG |
| 26 | BD | 13 | ARG |
| 26 | BD | 33 | ARG |
| 26 | BD | 35 | THR |
| 26 | BD | 36 | GLN |
| 26 | BD | 45 | TYR |
| 26 | BD | 46 | ARG |
| 26 | BD | 56 | LYS |
| 26 | BD | 74 | GLU |
| 26 | BD | 79 | LEU |
| 26 | BD | 81 | GLU |
| 26 | BD | 84 | LEU |
| 26 | BD | 88 | GLU |
| 26 | BD | 91 | THR |
| 26 | BD | 114 | LYS |
| 26 | BD | 123 | LYS |
| 26 | BD | 124 | ARG |
| 26 | BD | 131 | ASP |
| 26 | BD | 142 | VAL |
| 26 | BD | 148 | GLN |
| 26 | BD | 151 | THR |
| 26 | BD | 154 | LYS |
| 26 | BD | 157 | LYS |
| 26 | BD | 170 | VAL |
| 26 | BD | 172 | VAL |
| 27 | BE | 3 | LEU |
| 27 | BE | 5 | LEU |
| 27 | BE | 7 | ASP |
| 27 | BE | 14 | VAL |
| 27 | BE | 21 | ARG |
| 27 | BE | 58 | LYS |
| 27 | BE | 60 | TRP |
| 27 | BE | 61 | ARG |
| 27 | BE | 62 | GLN |
| 27 | BE | 63 | LYS |
| 27 | BE | 67 | ARG |
| 27 | BE | 78 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | BE | 111 | GLU |
| 27 | BE | 118 | LEU |
| 27 | BE | 122 | GLU |
| 27 | BE | 147 | LEU |
| 27 | BE | 152 | GLU |
| 27 | BE | 159 | LEU |
| 27 | BE | 163 | ASN |
| 28 | BF | 3 | LEU |
| 28 | BF | 13 | LYS |
| 28 | BF | 29 | ARG |
| 28 | BF | 32 | LYS |
| 28 | BF | 47 | LYS |
| 28 | BF | 48 | LEU |
| 28 | BF | 50 | ASP |
| 28 | BF | 56 | LEU |
| 28 | BF | 62 | GLN |
| 28 | BF | 76 | PHE |
| 28 | BF | 96 | TRP |
| 28 | BF | 97 | GLU |
| 28 | BF | 100 | GLU |
| 28 | BF | 102 | LEU |
| 28 | BF | 103 | ILE |
| 28 | BF | 109 | ARG |
| 28 | BF | 111 | ARG |
| 28 | BF | 112 | ASP |
| 28 | BF | 121 | PHE |
| 28 | BF | 126 | ASN |
| 28 | BF | 129 | MET |
| 28 | BF | 133 | GLU |
| 28 | BF | 134 | GLN |
| 28 | BF | 137 | PHE |
| 28 | BF | 138 | PRO |
| 28 | BF | 139 | GLU |
| 28 | BF | 146 | ASP |
| 28 | BF | 147 | ARG |
| 28 | BF | 149 | ARG |
| 28 | BF | 151 | LEU |
| 28 | BF | 162 | ASP |
| 28 | BF | 168 | LEU |
| 28 | BF | 173 | ASP |
| 28 | BF | 174 | PHE |
| 28 | BF | 177 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | BG | 5 | LYS |
| 29 | BG | 17 | LYS |
| 29 | BG | 24 | THR |
| 29 | BG | 26 | LYS |
| 29 | BG | 29 | ASN |
| 29 | BG | 34 | ARG |
| 29 | BG | 54 | ARG |
| 29 | BG | 55 | ASP |
| 29 | BG | 68 | ARG |
| 29 | BG | 70 | LEU |
| 29 | BG | 74 | MET |
| 29 | BG | 84 | LYS |
| 29 | BG | 85 | LYS |
| 29 | BG | 94 | ARG |
| 29 | BG | 106 | LEU |
| 29 | BG | 120 | ILE |
| 29 | BG | 132 | LEU |
| 29 | BG | 138 | GLN |
| 29 | BG | 152 | ARG |
| 29 | BG | 162 | ARG |
| 29 | BG | 166 | GLU |
| 30 | BH | 3 | VAL |
| 30 | BH | 15 | LEU |
| 30 | BH | 25 | TYR |
| 30 | BH | 28 | ASN |
| 30 | BH | 32 | PRO |
| 30 | BH | 33 | GLN |
| 30 | BH | 43 | ASN |
| 30 | BH | 44 | ILE |
| 30 | BH | 47 | PHE |
| 30 | BH | 50 | ARG |
| 30 | BH | 53 | GLU |
| 30 | BH | 57 | LYS |
| 30 | BH | 62 | LEU |
| 30 | BH | 66 | ASN |
| 30 | BH | 68 | ARG |
| 30 | BH | 71 | LYS |
| 30 | BH | 73 | ASN |
| 30 | BH | 75 | LEU |
| 30 | BH | 89 | LYS |
| 30 | BH | 93 | SER |
| 30 | BH | 98 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BH | 99 | ILE |
| 30 | BH | 101 | ASP |
| 30 | BH | 103 | VAL |
| 30 | BH | 104 | THR |
| 30 | BH | 108 | VAL |
| 30 | BH | 109 | GLU |
| 30 | BH | 110 | VAL |
| 30 | BH | 112 | LYS |
| 30 | BH | 115 | VAL |
| 30 | BH | 116 | ARG |
| 30 | BH | 130 | VAL |
| 30 | BH | 133 | GLN |
| 30 | BH | 135 | HIS |
| 30 | BH | 139 | PHE |
| 30 | BH | 141 | LYS |
| 30 | BH | 147 | VAL |
| 31 | BJ | 2 | LYS |
| 31 | BJ | 3 | THR |
| 31 | BJ | 12 | LYS |
| 31 | BJ | 28 | LEU |
| 31 | BJ | 36 | LEU |
| 31 | BJ | 39 | LYS |
| 31 | BJ | 43 | GLU |
| 31 | BJ | 44 | TYR |
| 31 | BJ | 54 | ILE |
| 31 | BJ | 65 | THR |
| 31 | BJ | 71 | ASP |
| 31 | BJ | 73 | VAL |
| 31 | BJ | 89 | PHE |
| 31 | BJ | 95 | ARG |
| 31 | BJ | 103 | ILE |
| 31 | BJ | 106 | LYS |
| 31 | BJ | 111 | LYS |
| 31 | BJ | 120 | ARG |
| 32 | BK | 2 | ILE |
| 32 | BK | 6 | THR |
| 32 | BK | 8 | LEU |
| 32 | BK | 9 | ASN |
| 32 | BK | 21 | CYS |
| 32 | BK | 32 | TYR |
| 32 | BK | 47 | ILE |
| 32 | BK | 53 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BK | 54 | LYS |
| 32 | BK | 58 | LEU |
| 32 | BK | 64 | ARG |
| 32 | BK | 66 | LYS |
| 32 | BK | 72 | PRO |
| 32 | BK | 79 | PHE |
| 32 | BK | 80 | ASP |
| 32 | BK | 86 | LEU |
| 32 | BK | 87 | LEU |
| 32 | BK | 88 | ASN |
| 32 | BK | 103 | VAL |
| 32 | BK | 104 | THR |
| 32 | BK | 105 | ARG |
| 32 | BK | 111 | LYS |
| 32 | BK | 120 | PRO |
| 33 | BL | 4 | ASN |
| 33 | BL | 6 | LEU |
| 33 | BL | 27 | LEU |
| 33 | BL | 47 | ARG |
| 33 | BL | 60 | ARG |
| 33 | BL | 69 | ARG |
| 33 | BL | 92 | LEU |
| 33 | BL | 93 | ASN |
| 33 | BL | 95 | LEU |
| 33 | BL | 118 | THR |
| 33 | BL | 125 | LEU |
| 33 | BL | 126 | ARG |
| 33 | BL | 128 | THR |
| 34 | BM | 20 | LEU |
| 34 | BM | 25 | ASP |
| 34 | BM | 40 | ARG |
| 34 | BM | 55 | ARG |
| 34 | BM | 60 | GLN |
| 34 | BM | 63 | ILE |
| 34 | BM | 65 | ILE |
| 34 | BM | 70 | ASP |
| 34 | BM | 78 | LEU |
| 34 | BM | 81 | ARG |
| 34 | BM | 82 | MET |
| 34 | BM | 88 | ASN |
| 34 | BM | 93 | VAL |
| 34 | BM | 95 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | BM | 108 | VAL |
| 34 | BM | 110 | GLU |
| 34 | BM | 111 | GLU |
| 34 | BM | 114 | ARG |
| 34 | BM | 115 | GLU |
| 34 | BM | 131 | VAL |
| 34 | BM | 136 | MET |
| 35 | BN | 1 | MET |
| 35 | BN | 2 | ARG |
| 35 | BN | 11 | ASN |
| 35 | BN | 18 | GLN |
| 35 | BN | 28 | LEU |
| 35 | BN | 29 | VAL |
| 35 | BN | 35 | LYS |
| 35 | BN | 48 | VAL |
| 35 | BN | 62 | ASN |
| 35 | BN | 69 | ARG |
| 35 | BN | 71 | ARG |
| 35 | BN | 82 | GLU |
| 35 | BN | 86 | ARG |
| 35 | BN | 98 | LEU |
| 35 | BN | 107 | ASN |
| 35 | BN | 112 | TYR |
| 35 | BN | 118 | ARG |
| 35 | BN | 120 | GLU |
| 36 | BO | 2 | ASP |
| 36 | BO | 7 | ARG |
| 36 | BO | 9 | ARG |
| 36 | BO | 17 | LYS |
| 36 | BO | 19 | GLN |
| 36 | BO | 20 | GLU |
| 36 | BO | 21 | LEU |
| 36 | BO | 31 | THR |
| 36 | BO | 62 | LEU |
| 36 | BO | 69 | ASP |
| 36 | BO | 78 | VAL |
| 36 | BO | 80 | GLU |
| 36 | BO | 88 | LYS |
| 36 | BO | 98 | GLN |
| 36 | BO | 100 | HIS |
| 36 | BO | 106 | LEU |
| 36 | BO | 116 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 37 | BP | 3 | ILE |
| 37 | BP | 5 | LYS |
| 37 | BP | 6 | GLN |
| 37 | BP | 19 | PHE |
| 37 | BP | 25 | VAL |
| 37 | BP | 32 | VAL |
| 37 | BP | 33 | GLU |
| 37 | BP | 43 | GLU |
| 37 | BP | 61 | ARG |
| 37 | BP | 65 | ASN |
| 37 | BP | 72 | VAL |
| 37 | BP | 80 | VAL |
| 37 | BP | 83 | ILE |
| 37 | BP | 99 | LEU |
| 37 | BP | 100 | ARG |
| 37 | BP | 101 | GLU |
| 37 | BP | 111 | GLU |
| 37 | BP | 112 | ARG |
| 37 | BP | 113 | LEU |
| 38 | BQ | 5 | ARG |
| 38 | BQ | 15 | LYS |
| 38 | BQ | 50 | ARG |
| 38 | BQ | 57 | ARG |
| 38 | BQ | 63 | ARG |
| 38 | BQ | 79 | ILE |
| 38 | BQ | 83 | LYS |
| 38 | BQ | 88 | GLU |
| 38 | BQ | 96 | ASP |
| 38 | BQ | 111 | LYS |
| 39 | BR | 2 | TYR |
| 39 | BR | 10 | LYS |
| 39 | BR | 22 | LEU |
| 39 | BR | 37 | GLU |
| 39 | BR | 39 | LEU |
| 39 | BR | 43 | ASN |
| 39 | BR | 48 | LYS |
| 39 | BR | 55 | ASP |
| 39 | BR | 70 | GLU |
| 39 | BR | 71 | LYS |
| 39 | BR | 72 | VAL |
| 39 | BR | 76 | LYS |
| 39 | BR | 82 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BR | 86 | GLN |
| 39 | BR | 96 | VAL |
| 39 | BR | 99 | THR |
| 40 | BS | 6 | LYS |
| 40 | BS | 28 | LYS |
| 40 | BS | 37 | THR |
| 40 | BS | 57 | ASN |
| 40 | BS | 61 | ASN |
| 40 | BS | 62 | ASP |
| 40 | BS | 66 | ILE |
| 40 | BS | 84 | ARG |
| 40 | BS | 86 | MET |
| 40 | BS | 88 | ARG |
| 40 | BS | 99 | ARG |
| 40 | BS | 110 | ARG |
| 41 | BT | 2 | ILE |
| 41 | BT | 3 | ARG |
| 41 | BT | 4 | GLU |
| 41 | BT | 6 | ARG |
| 41 | BT | 9 | LYS |
| 41 | BT | 11 | LEU |
| 41 | BT | 12 | ARG |
| 41 | BT | 24 | MET |
| 41 | BT | 29 | THR |
| 41 | BT | 32 | LEU |
| 41 | BT | 34 | VAL |
| 41 | BT | 39 | THR |
| 41 | BT | 64 | LYS |
| 41 | BT | 68 | LYS |
| 41 | BT | 69 | ARG |
| 41 | BT | 70 | HIS |
| 41 | BT | 76 | ARG |
| 41 | BT | 81 | LYS |
| 42 | BU | 11 | ILE |
| 42 | BU | 13 | LEU |
| 42 | BU | 20 | LYS |
| 42 | BU | 26 | ASN |
| 42 | BU | 39 | ASN |
| 42 | BU | 51 | LEU |
| 42 | BU | 53 | GLN |
| 42 | BU | 60 | LYS |
| 42 | BU | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BU | 73 | ASN |
| 42 | BU | 78 | LYS |
| 42 | BU | 81 | ARG |
| 42 | BU | 84 | PHE |
| 42 | BU | 85 | ARG |
| 42 | BU | 88 | ASP |
| 42 | BU | 102 | ILE |
| 43 | BW | 10 | ARG |
| 43 | BW | 16 | GLU |
| 43 | BW | 19 | ARG |
| 43 | BW | 23 | LYS |
| 43 | BW | 38 | ARG |
| 43 | BW | 39 | GLN |
| 43 | BW | 40 | ARG |
| 43 | BW | 44 | PHE |
| 43 | BW | 45 | HIS |
| 43 | BW | 50 | VAL |
| 43 | BW | 61 | LYS |
| 43 | BW | 63 | ASP |
| 43 | BW | 68 | PHE |
| 43 | BW | 76 | ARG |
| 43 | BW | 77 | LYS |
| 43 | BW | 82 | GLU |
| 43 | BW | 84 | GLU |
| 44 | BX | 1 | MET |
| 44 | BX | 15 | ASN |
| 44 | BX | 16 | THR |
| 44 | BX | 21 | LEU |
| 44 | BX | 24 | GLU |
| 44 | BX | 25 | GLN |
| 44 | BX | 28 | LEU |
| 44 | BX | 29 | ARG |
| 44 | BX | 36 | GLN |
| 44 | BX | 37 | LEU |
| 44 | BX | 41 | HIS |
| 44 | BX | 48 | ARG |
| 44 | BX | 59 | GLU |
| 45 | BY | 2 | LYS |
| 45 | BY | 8 | GLN |
| 45 | BY | 9 | THR |
| 45 | BY | 15 | ARG |
| 45 | BY | 23 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | BY | 30 | ARG |
| 45 | BY | 37 | ARG |
| 45 | BY | 57 | GLU |
| 46 | BZ | 13 | VAL |
| 46 | BZ | 14 | THR |
| 46 | BZ | 22 | LEU |
| 46 | BZ | 27 | ARG |
| 46 | BZ | 28 | ARG |
| 46 | BZ | 37 | ARG |
| 46 | BZ | 41 | GLU |
| 46 | BZ | 46 | PHE |
| 46 | BZ | 48 | THR |
| 46 | BZ | 50 | ARG |
| 46 | BZ | 59 | ILE |
| 46 | BZ | 65 | ASP |
| 46 | BZ | 74 | ARG |
| 47 | B0 | 18 | HIS |
| 47 | B0 | 27 | LEU |
| 47 | B0 | 37 | HIS |
| 47 | B0 | 38 | LEU |
| 47 | B0 | 41 | HIS |
| 47 | B0 | 45 | ASP |
| 47 | B0 | 51 | ARG |
| 47 | B0 | 56 | LYS |
| 48 | B1 | 8 | ILE |
| 48 | B1 | 9 | LYS |
| 48 | B1 | 34 | GLU |
| 48 | B1 | 35 | LEU |
| 48 | B1 | 42 | VAL |
| 49 | B2 | 3 | ARG |
| 49 | B2 | 19 | ARG |
| 49 | B2 | 28 | ARG |
| 49 | B2 | 33 | ARG |
| 49 | B2 | 39 | ARG |
| 49 | B2 | 42 | LEU |
| 50 | B3 | 7 | ARG |
| 50 | B3 | 27 | ASN |
| 50 | B3 | 31 | ILE |
| 50 | B3 | 46 | LYS |
| 50 | B3 | 58 | ILE |
| 51 | B4 | 9 | LYS |
| 51 | B4 | 10 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | BI | 96 | LYS |
| 2 | CC | 2 | GLN |
| 2 | CC | 13 | ILE |
| 2 | CC | 17 | TRP |
| 2 | CC | 18 | ASN |
| 2 | CC | 20 | THR |
| 2 | CC | 27 | GLU |
| 2 | CC | 35 | ASP |
| 2 | CC | 41 | TYR |
| 2 | CC | 48 | LYS |
| 2 | CC | 62 | SER |
| 2 | CC | 69 | THR |
| 2 | CC | 87 | ARG |
| 2 | CC | 88 | LYS |
| 2 | CC | 113 | LYS |
| 2 | CC | 128 | MET |
| 2 | CC | 131 | ARG |
| 2 | CC | 138 | GLN |
| 2 | CC | 163 | ARG |
| 2 | CC | 166 | TRP |
| 2 | CC | 168 | ARG |
| 2 | CC | 171 | ARG |
| 2 | CC | 175 | HIS |
| 2 | CC | 180 | ASP |
| 2 | CC | 184 | ASN |
| 2 | CC | 206 | ILE |
| 3 | CD | 4 | LEU |
| 3 | CD | 7 | LYS |
| 3 | CD | 18 | LEU |
| 3 | CD | 25 | ARG |
| 3 | CD | 28 | ASP |
| 3 | CD | 39 | GLN |
| 3 | CD | 47 | LEU |
| 3 | CD | 49 | ASP |
| 3 | CD | 55 | ARG |
| 3 | CD | 82 | LYS |
| 3 | CD | 87 | GLU |
| 3 | CD | 94 | GLU |
| 3 | CD | 114 | ARG |
| 3 | CD | 117 | VAL |
| 3 | CD | 125 | ASN |
| 3 | CD | 135 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CD | 146 | GLU |
| 3 | CD | 147 | LYS |
| 3 | CD | 160 | LEU |
| 3 | CD | 162 | GLU |
| 3 | CD | 168 | THR |
| 3 | CD | 190 | LEU |
| 3 | CD | 195 | ASN |
| 4 | CE | 9 | GLU |
| 4 | CE | 19 | ARG |
| 4 | CE | 23 | THR |
| 4 | CE | 44 | ARG |
| 4 | CE | 45 | VAL |
| 4 | CE | 55 | VAL |
| 4 | CE | 71 | ILE |
| 4 | CE | 72 | ASN |
| 4 | CE | 81 | GLN |
| 4 | CE | 92 | ARG |
| 4 | CE | 105 | ILE |
| 4 | CE | 123 | LEU |
| 4 | CE | 127 | TYR |
| 4 | CE | 151 | MET |
| 4 | CE | 156 | ARG |
| 5 | CF | 6 | ILE |
| 5 | CF | 39 | LEU |
| 5 | CF | 51 | ILE |
| 5 | CF | 55 | HIS |
| 5 | CF | 60 | VAL |
| 5 | CF | 62 | MET |
| 5 | CF | 64 | VAL |
| 5 | CF | 69 | GLU |
| 5 | CF | 82 | ASP |
| 5 | CF | 86 | ARG |
| 5 | CF | 94 | HIS |
| 5 | CF | 98 | GLU |
| 6 | CG | 2 | ARG |
| 6 | CG | 3 | ARG |
| 6 | CG | 8 | GLN |
| 6 | CG | 10 | LYS |
| 6 | CG | 21 | LEU |
| 6 | CG | 49 | LEU |
| 6 | CG | 51 | GLN |
| 6 | CG | 55 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | CG | 62 | GLU |
| 6 | CG | 67 | ASN |
| 6 | CG | 78 | ARG |
| 6 | CG | 89 | GLU |
| 6 | CG | 94 | ARG |
| 6 | CG | 96 | ASN |
| 6 | CG | 105 | GLU |
| 6 | CG | 113 | LYS |
| 6 | CG | 125 | ASP |
| 7 | CH | 2 | MET |
| 7 | CH | 30 | LYS |
| 7 | CH | 55 | LYS |
| 7 | CH | 61 | THR |
| 7 | CH | 72 | GLU |
| 7 | CH | 82 | LEU |
| 7 | CH | 105 | THR |
| 7 | CH | 113 | ARG |
| 8 | CI | 36 | GLN |
| 8 | CI | 45 | MET |
| 8 | CI | 59 | LYS |
| 8 | CI | 62 | LEU |
| 8 | CI | 87 | MET |
| 8 | CI | 93 | LEU |
| 8 | CI | 94 | ARG |
| 8 | CI | 96 | GLU |
| 8 | CI | 105 | ARG |
| 8 | CI | 109 | GLN |
| 8 | CI | 112 | ARG |
| 8 | CI | 114 | LYS |
| 9 | CJ | 15 | HIS |
| 9 | CJ | 47 | GLU |
| 9 | CJ | 69 | THR |
| 9 | CJ | 77 | VAL |
| 9 | CJ | 78 | GLU |
| 9 | CJ | 88 | MET |
| 10 | CK | 22 | ILE |
| 10 | CK | 31 | VAL |
| 10 | CK | 34 | THR |
| 10 | CK | 51 | PHE |
| 10 | CK | 55 | ARG |
| 10 | CK | 64 | VAL |
| 10 | CK | 76 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | CK | 82 | GLU |
| 10 | CK | 83 | VAL |
| 10 | CK | 107 | THR |
| 10 | CK | 115 | ILE |
| 10 | CK | 118 | ASN |
| 10 | CK | 121 | ARG |
| 11 | CL | 13 | ARG |
| 11 | CL | 14 | LYS |
| 11 | CL | 15 | VAL |
| 11 | CL | 17 | LYS |
| 11 | CL | 18 | SER |
| 11 | CL | 19 | ASN |
| 11 | CL | 28 | GLN |
| 11 | CL | 33 | CYS |
| 11 | CL | 35 | ARG |
| 11 | CL | 38 | THR |
| 11 | CL | 40 | THR |
| 11 | CL | 43 | LYS |
| 11 | CL | 61 | GLU |
| 11 | CL | 63 | THR |
| 11 | CL | 95 | HIS |
| 11 | CL | 102 | ASP |
| 11 | CL | 107 | LYS |
| 11 | CL | 119 | LYS |
| 11 | CL | 122 | LYS |
| 12 | CM | 2 | ARG |
| 12 | CM | 16 | ILE |
| 12 | CM | 28 | ARG |
| 12 | CM | 41 | ASP |
| 12 | CM | 43 | LYS |
| 12 | CM | 71 | GLU |
| 12 | CM | 80 | MET |
| 12 | CM | 88 | LEU |
| 12 | CM | 102 | LYS |
| 13 | CN | 11 | LYS |
| 13 | CN | 19 | TYR |
| 13 | CN | 20 | PHE |
| 13 | CN | 25 | GLU |
| 13 | CN | 27 | LYS |
| 13 | CN | 41 | TRP |
| 13 | CN | 48 | GLN |
| 13 | CN | 49 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | CN | 50 | LEU |
| 13 | CN | 53 | ASP |
| 13 | CN | 58 | ARG |
| 13 | CN | 65 | GLN |
| 14 | CO | 17 | ASP |
| 14 | CO | 53 | ARG |
| 14 | CO | 65 | LEU |
| 14 | CO | 69 | LEU |
| 14 | CO | 87 | ARG |
| 14 | CO | 88 | ARG |
| 15 | CP | 12 | LYS |
| 15 | CP | 23 | ASP |
| 15 | CP | 26 | ASN |
| 15 | CP | 28 | ARG |
| 15 | CP | 45 | GLU |
| 15 | CP | 51 | ARG |
| 15 | CP | 55 | ASP |
| 15 | CP | 68 | SER |
| 16 | CQ | 3 | LYS |
| 16 | CQ | 4 | ILE |
| 16 | CQ | 7 | LEU |
| 16 | CQ | 8 | GLN |
| 16 | CQ | 39 | ARG |
| 16 | CQ | 41 | THR |
| 16 | CQ | 56 | ASP |
| 16 | CQ | 60 | ILE |
| 16 | CQ | 80 | LYS |
| 16 | CQ | 83 | LEU |
| 17 | CR | 23 | LYS |
| 17 | CR | 38 | ILE |
| 18 | CS | 2 | ARG |
| 18 | CS | 4 | LEU |
| 18 | CS | 6 | LYS |
| 18 | CS | 10 | ILE |
| 18 | CS | 13 | HIS |
| 18 | CS | 20 | LYS |
| 18 | CS | 23 | GLU |
| 18 | CS | 26 | ASP |
| 18 | CS | 27 | LYS |
| 18 | CS | 28 | LYS |
| 18 | CS | 32 | THR |
| 18 | CS | 35 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | CS | 38 | THR |
| 18 | CS | 42 | ASN |
| 18 | CS | 47 | THR |
| 18 | CS | 60 | PHE |
| 18 | CS | 64 | GLU |
| 18 | CS | 77 | ARG |
| 19 | CT | 3 | ILE |
| 19 | CT | 4 | LYS |
| 19 | CT | 35 | TYR |
| 19 | CT | 43 | LYS |
| 19 | CT | 51 | ASN |
| 19 | CT | 52 | GLU |
| 19 | CT | 53 | MET |
| 19 | CT | 57 | VAL |
| 19 | CT | 67 | HIS |
| 19 | CT | 68 | LYS |
| 19 | CT | 74 | HIS |
| 19 | CT | 84 | LYS |
| 20 | CB | 8 | MET |
| 20 | CB | 31 | PHE |
| 20 | CB | 35 | ASN |
| 20 | CB | 46 | VAL |
| 20 | CB | 49 | PHE |
| 20 | CB | 57 | ASN |
| 20 | CB | 62 | ARG |
| 20 | CB | 67 | LEU |
| 20 | CB | 72 | LYS |
| 20 | CB | 87 | ASP |
| 20 | CB | 88 | GLN |
| 20 | CB | 94 | ARG |
| 20 | CB | 95 | TRP |
| 20 | CB | 104 | LYS |
| 20 | CB | 113 | LEU |
| 20 | CB | 115 | ASP |
| 20 | CB | 116 | LEU |
| 20 | CB | 117 | GLU |
| 20 | CB | 121 | GLN |
| 20 | CB | 126 | ASP |
| 20 | CB | 127 | LYS |
| 20 | CB | 130 | LYS |
| 20 | CB | 134 | LEU |
| 20 | CB | 145 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CB | 160 | LEU |
| 20 | CB | 176 | ASN |
| 20 | CB | 196 | ASP |
| 20 | CB | 199 | ILE |
| 20 | CB | 202 | ASN |
| 20 | CB | 212 | TYR |
| 21 | CU | 11 | PHE |
| 21 | CU | 15 | LEU |
| 21 | CU | 16 | ARG |
| 21 | CU | 22 | CYS |
| 21 | CU | 24 | LYS |
| 21 | CU | 32 | ARG |
| 21 | CU | 34 | ARG |
| 21 | CU | 38 | GLU |
| 21 | CU | 44 | ARG |
| 24 | DV | 24 | ASN |
| 24 | DV | 40 | ILE |
| 24 | DV | 42 | LEU |
| 24 | DV | 51 | GLN |
| 24 | DV | 53 | LYS |
| 24 | DV | 68 | LYS |
| 24 | DV | 69 | GLU |
| 24 | DV | 70 | ILE |
| 24 | DV | 86 | LEU |
| 25 | DC | 4 | LYS |
| 25 | DC | 5 | CYS |
| 25 | DC | 8 | THR |
| 25 | DC | 9 | SER |
| 25 | DC | 12 | ARG |
| 25 | DC | 37 | SER |
| 25 | DC | 43 | ASN |
| 25 | DC | 45 | ASN |
| 25 | DC | 47 | ARG |
| 25 | DC | 52 | HIS |
| 25 | DC | 62 | ARG |
| 25 | DC | 63 | ILE |
| 25 | DC | 65 | ASP |
| 25 | DC | 67 | LYS |
| 25 | DC | 89 | ASN |
| 25 | DC | 90 | ILE |
| 25 | DC | 109 | LEU |
| 25 | DC | 123 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DC | 128 | THR |
| 25 | DC | 134 | ILE |
| 25 | DC | 142 | ASN |
| 25 | DC | 152 | GLN |
| 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 | 193 | GLU |
| 25 | DC | 203 | VAL |
| 25 | DC | 212 | TRP |
| 25 | DC | 224 | MET |
| 25 | DC | 239 | PHE |
| 25 | DC | 249 | VAL |
| 25 | DC | 252 | LYS |
| 25 | DC | 255 | LYS |
| 25 | DC | 257 | ARG |
| 25 | DC | 266 | ILE |
| 25 | DC | 269 | ARG |
| 26 | DD | 13 | ARG |
| 26 | DD | 33 | ARG |
| 26 | DD | 35 | THR |
| 26 | DD | 36 | GLN |
| 26 | DD | 45 | TYR |
| 26 | DD | 46 | ARG |
| 26 | DD | 56 | LYS |
| 26 | DD | 74 | GLU |
| 26 | DD | 79 | LEU |
| 26 | DD | 81 | GLU |
| 26 | DD | 84 | LEU |
| 26 | DD | 88 | GLU |
| 26 | DD | 91 | THR |
| 26 | DD | 114 | LYS |
| 26 | DD | 123 | LYS |
| 26 | DD | 124 | ARG |
| 26 | DD | 131 | ASP |
| 26 | DD | 142 | VAL |
| 26 | DD | 148 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | DD | 151 | THR |
| 26 | DD | 154 | LYS |
| 26 | DD | 157 | LYS |
| 26 | DD | 170 | VAL |
| 26 | DD | 172 | VAL |
| 27 | DE | 3 | LEU |
| 27 | DE | 5 | LEU |
| 27 | DE | 7 | ASP |
| 27 | DE | 14 | VAL |
| 27 | DE | 21 | ARG |
| 27 | DE | 48 | THR |
| 27 | DE | 58 | LYS |
| 27 | DE | 60 | TRP |
| 27 | DE | 61 | ARG |
| 27 | DE | 62 | GLN |
| 27 | DE | 63 | LYS |
| 27 | DE | 67 | ARG |
| 27 | DE | 78 | TRP |
| 27 | DE | 111 | GLU |
| 27 | DE | 118 | LEU |
| 27 | DE | 122 | GLU |
| 27 | DE | 147 | LEU |
| 27 | DE | 152 | GLU |
| 27 | DE | 159 | LEU |
| 28 | DF | 3 | LEU |
| 28 | DF | 13 | LYS |
| 28 | DF | 29 | ARG |
| 28 | DF | 32 | LYS |
| 28 | DF | 47 | LYS |
| 28 | DF | 48 | LEU |
| 28 | DF | 50 | ASP |
| 28 | DF | 56 | LEU |
| 28 | DF | 62 | GLN |
| 28 | DF | 76 | PHE |
| 28 | DF | 96 | TRP |
| 28 | DF | 97 | GLU |
| 28 | DF | 102 | LEU |
| 28 | DF | 103 | ILE |
| 28 | DF | 109 | ARG |
| 28 | DF | 111 | ARG |
| 28 | DF | 112 | ASP |
| 28 | DF | 121 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | DF | 126 | ASN |
| 28 | DF | 129 | MET |
| 28 | DF | 133 | GLU |
| 28 | DF | 134 | GLN |
| 28 | DF | 137 | PHE |
| 28 | DF | 138 | PRO |
| 28 | DF | 139 | GLU |
| 28 | DF | 146 | ASP |
| 28 | DF | 147 | ARG |
| 28 | DF | 149 | ARG |
| 28 | DF | 151 | LEU |
| 28 | DF | 162 | ASP |
| 28 | DF | 168 | LEU |
| 28 | DF | 173 | ASP |
| 28 | DF | 174 | PHE |
| 28 | DF | 177 | ARG |
| 29 | DG | 5 | LYS |
| 29 | DG | 17 | LYS |
| 29 | DG | 24 | THR |
| 29 | DG | 26 | LYS |
| 29 | DG | 29 | ASN |
| 29 | DG | 34 | ARG |
| 29 | DG | 54 | ARG |
| 29 | DG | 55 | ASP |
| 29 | DG | 68 | ARG |
| 29 | DG | 70 | LEU |
| 29 | DG | 74 | MET |
| 29 | DG | 84 | LYS |
| 29 | DG | 85 | LYS |
| 29 | DG | 94 | ARG |
| 29 | DG | 106 | LEU |
| 29 | DG | 120 | ILE |
| 29 | DG | 132 | LEU |
| 29 | DG | 138 | GLN |
| 29 | DG | 152 | ARG |
| 29 | DG | 162 | ARG |
| 29 | DG | 166 | GLU |
| 30 | DH | 3 | VAL |
| 30 | DH | 15 | LEU |
| 30 | DH | 25 | TYR |
| 30 | DH | 28 | ASN |
| 30 | DH | 32 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DH | 33 | GLN |
| 30 | DH | 46 | PHE |
| 30 | DH | 50 | ARG |
| 30 | DH | 68 | ARG |
| 30 | DH | 83 | LYS |
| 30 | DH | 94 | ILE |
| 30 | DH | 97 | ARG |
| 30 | DH | 101 | ASP |
| 30 | DH | 112 | LYS |
| 30 | DH | 122 | LEU |
| 30 | DH | 124 | THR |
| 30 | DH | 129 | GLU |
| 30 | DH | 134 | VAL |
| 30 | DH | 137 | GLU |
| 30 | DH | 141 | LYS |
| 30 | DH | 149 | GLU |
| 31 | DJ | 2 | LYS |
| 31 | DJ | 3 | THR |
| 31 | DJ | 12 | LYS |
| 31 | DJ | 28 | LEU |
| 31 | DJ | 31 | GLU |
| 31 | DJ | 36 | LEU |
| 31 | DJ | 39 | LYS |
| 31 | DJ | 43 | GLU |
| 31 | DJ | 44 | TYR |
| 31 | DJ | 54 | ILE |
| 31 | DJ | 65 | THR |
| 31 | DJ | 73 | VAL |
| 31 | DJ | 89 | PHE |
| 31 | DJ | 95 | ARG |
| 31 | DJ | 103 | ILE |
| 31 | DJ | 106 | LYS |
| 31 | DJ | 111 | LYS |
| 31 | DJ | 120 | ARG |
| 32 | DK | 2 | ILE |
| 32 | DK | 6 | THR |
| 32 | DK | 8 | LEU |
| 32 | DK | 9 | ASN |
| 32 | DK | 21 | CYS |
| 32 | DK | 32 | TYR |
| 32 | DK | 47 | ILE |
| 32 | DK | 53 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DK | 54 | LYS |
| 32 | DK | 58 | LEU |
| 32 | DK | 64 | ARG |
| 32 | DK | 66 | LYS |
| 32 | DK | 72 | PRO |
| 32 | DK | 79 | PHE |
| 32 | DK | 80 | ASP |
| 32 | DK | 86 | LEU |
| 32 | DK | 87 | LEU |
| 32 | DK | 88 | ASN |
| 32 | DK | 103 | VAL |
| 32 | DK | 104 | THR |
| 32 | DK | 105 | ARG |
| 32 | DK | 111 | LYS |
| 32 | DK | 120 | PRO |
| 33 | DL | 4 | ASN |
| 33 | DL | 6 | LEU |
| 33 | DL | 27 | LEU |
| 33 | DL | 47 | ARG |
| 33 | DL | 60 | ARG |
| 33 | DL | 69 | ARG |
| 33 | DL | 92 | LEU |
| 33 | DL | 93 | ASN |
| 33 | DL | 95 | LEU |
| 33 | DL | 118 | THR |
| 33 | DL | 125 | LEU |
| 33 | DL | 126 | ARG |
| 34 | DM | 20 | LEU |
| 34 | DM | 25 | ASP |
| 34 | DM | 40 | ARG |
| 34 | DM | 55 | ARG |
| 34 | DM | 60 | GLN |
| 34 | DM | 63 | ILE |
| 34 | DM | 65 | ILE |
| 34 | DM | 70 | ASP |
| 34 | DM | 78 | LEU |
| 34 | DM | 81 | ARG |
| 34 | DM | 82 | MET |
| 34 | DM | 88 | ASN |
| 34 | DM | 93 | VAL |
| 34 | DM | 95 | LEU |
| 34 | DM | 108 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DM | 110 | GLU |
| 34 | DM | 111 | GLU |
| 34 | DM | 114 | ARG |
| 34 | DM | 115 | GLU |
| 34 | DM | 131 | VAL |
| 34 | DM | 136 | MET |
| 35 | DN | 1 | MET |
| 35 | DN | 2 | ARG |
| 35 | DN | 11 | ASN |
| 35 | DN | 18 | GLN |
| 35 | DN | 28 | LEU |
| 35 | DN | 29 | VAL |
| 35 | DN | 35 | LYS |
| 35 | DN | 48 | VAL |
| 35 | DN | 51 | LEU |
| 35 | DN | 62 | ASN |
| 35 | DN | 69 | ARG |
| 35 | DN | 71 | ARG |
| 35 | DN | 82 | GLU |
| 35 | DN | 86 | ARG |
| 35 | DN | 98 | LEU |
| 35 | DN | 107 | ASN |
| 35 | DN | 112 | TYR |
| 35 | DN | 118 | ARG |
| 35 | DN | 120 | GLU |
| 36 | DO | 7 | ARG |
| 36 | DO | 9 | ARG |
| 36 | DO | 17 | LYS |
| 36 | DO | 19 | GLN |
| 36 | DO | 20 | GLU |
| 36 | DO | 21 | LEU |
| 36 | DO | 31 | THR |
| 36 | DO | 62 | LEU |
| 36 | DO | 69 | ASP |
| 36 | DO | 78 | VAL |
| 36 | DO | 80 | GLU |
| 36 | DO | 88 | LYS |
| 36 | DO | 91 | SER |
| 36 | DO | 98 | GLN |
| 36 | DO | 100 | HIS |
| 36 | DO | 106 | LEU |
| 36 | DO | 116 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | DP | 3 | ILE |
| 37 | DP | 5 | LYS |
| 37 | DP | 6 | GLN |
| 37 | DP | 19 | PHE |
| 37 | DP | 25 | VAL |
| 37 | DP | 32 | VAL |
| 37 | DP | 33 | GLU |
| 37 | DP | 61 | ARG |
| 37 | DP | 65 | ASN |
| 37 | DP | 72 | VAL |
| 37 | DP | 80 | VAL |
| 37 | DP | 83 | ILE |
| 37 | DP | 99 | LEU |
| 37 | DP | 100 | ARG |
| 37 | DP | 101 | GLU |
| 37 | DP | 111 | GLU |
| 37 | DP | 112 | ARG |
| 37 | DP | 113 | LEU |
| 38 | DQ | 5 | ARG |
| 38 | DQ | 15 | LYS |
| 38 | DQ | 50 | ARG |
| 38 | DQ | 57 | ARG |
| 38 | DQ | 63 | ARG |
| 38 | DQ | 79 | ILE |
| 38 | DQ | 83 | LYS |
| 38 | DQ | 88 | GLU |
| 38 | DQ | 96 | ASP |
| 38 | DQ | 111 | LYS |
| 39 | DR | 2 | TYR |
| 39 | DR | 10 | LYS |
| 39 | DR | 22 | LEU |
| 39 | DR | 25 | LEU |
| 39 | DR | 37 | GLU |
| 39 | DR | 39 | LEU |
| 39 | DR | 43 | ASN |
| 39 | DR | 55 | ASP |
| 39 | DR | 70 | GLU |
| 39 | DR | 72 | VAL |
| 39 | DR | 76 | LYS |
| 39 | DR | 86 | GLN |
| 39 | DR | 96 | VAL |
| 39 | DR | 99 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | DS | 6 | LYS |
| 40 | DS | 28 | LYS |
| 40 | DS | 37 | THR |
| 40 | DS | 57 | ASN |
| 40 | DS | 61 | ASN |
| 40 | DS | 62 | ASP |
| 40 | DS | 66 | ILE |
| 40 | DS | 84 | ARG |
| 40 | DS | 86 | MET |
| 40 | DS | 88 | ARG |
| 40 | DS | 110 | ARG |
| 41 | DT | 2 | ILE |
| 41 | DT | 3 | ARG |
| 41 | DT | 4 | GLU |
| 41 | DT | 6 | ARG |
| 41 | DT | 9 | LYS |
| 41 | DT | 11 | LEU |
| 41 | DT | 12 | ARG |
| 41 | DT | 24 | MET |
| 41 | DT | 29 | THR |
| 41 | DT | 32 | LEU |
| 41 | DT | 34 | VAL |
| 41 | DT | 39 | THR |
| 41 | DT | 64 | LYS |
| 41 | DT | 68 | LYS |
| 41 | DT | 69 | ARG |
| 41 | DT | 70 | HIS |
| 41 | DT | 76 | ARG |
| 41 | DT | 81 | LYS |
| 42 | DU | 11 | ILE |
| 42 | DU | 13 | LEU |
| 42 | DU | 20 | LYS |
| 42 | DU | 26 | ASN |
| 42 | DU | 39 | ASN |
| 42 | DU | 51 | LEU |
| 42 | DU | 53 | GLN |
| 42 | DU | 60 | LYS |
| 42 | DU | 65 | GLN |
| 42 | DU | 73 | ASN |
| 42 | DU | 78 | LYS |
| 42 | DU | 81 | ARG |
| 42 | DU | 84 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DU | 85 | ARG |
| 42 | DU | 88 | ASP |
| 42 | DU | 102 | ILE |
| 43 | DW | 10 | ARG |
| 43 | DW | 11 | ASN |
| 43 | DW | 16 | GLU |
| 43 | DW | 19 | ARG |
| 43 | DW | 23 | LYS |
| 43 | DW | 38 | ARG |
| 43 | DW | 39 | GLN |
| 43 | DW | 40 | ARG |
| 43 | DW | 44 | PHE |
| 43 | DW | 45 | HIS |
| 43 | DW | 50 | VAL |
| 43 | DW | 63 | ASP |
| 43 | DW | 68 | PHE |
| 43 | DW | 76 | ARG |
| 43 | DW | 77 | LYS |
| 43 | DW | 82 | GLU |
| 43 | DW | 84 | GLU |
| 44 | DX | 1 | MET |
| 44 | DX | 15 | ASN |
| 44 | DX | 16 | THR |
| 44 | DX | 21 | LEU |
| 44 | DX | 24 | GLU |
| 44 | DX | 25 | GLN |
| 44 | DX | 28 | LEU |
| 44 | DX | 29 | ARG |
| 44 | DX | 36 | GLN |
| 44 | DX | 37 | LEU |
| 44 | DX | 41 | HIS |
| 44 | DX | 48 | ARG |
| 44 | DX | 59 | GLU |
| 45 | DY | 2 | LYS |
| 45 | DY | 8 | GLN |
| 45 | DY | 9 | THR |
| 45 | DY | 15 | ARG |
| 45 | DY | 23 | LEU |
| 45 | DY | 30 | ARG |
| 45 | DY | 37 | ARG |
| 45 | DY | 57 | GLU |
| 46 | DZ | 13 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | DZ | 14 | THR |
| 46 | DZ | 22 | LEU |
| 46 | DZ | 27 | ARG |
| 46 | DZ | 28 | ARG |
| 46 | DZ | 37 | ARG |
| 46 | DZ | 41 | GLU |
| 46 | DZ | 46 | PHE |
| 46 | DZ | 48 | THR |
| 46 | DZ | 50 | ARG |
| 46 | DZ | 59 | ILE |
| 46 | DZ | 65 | ASP |
| 46 | DZ | 70 | GLU |
| 46 | DZ | 74 | ARG |
| 47 | D0 | 27 | LEU |
| 47 | D0 | 37 | HIS |
| 47 | D0 | 38 | LEU |
| 47 | D0 | 41 | HIS |
| 47 | D0 | 45 | ASP |
| 47 | D0 | 51 | ARG |
| 47 | D0 | 56 | LYS |
| 48 | D1 | 8 | ILE |
| 48 | D1 | 9 | LYS |
| 48 | D1 | 35 | LEU |
| 48 | D1 | 42 | VAL |
| 49 | D2 | 3 | ARG |
| 49 | D2 | 19 | ARG |
| 49 | D2 | 28 | ARG |
| 49 | D2 | 33 | ARG |
| 49 | D2 | 39 | ARG |
| 49 | D2 | 42 | LEU |
| 50 | D3 | 7 | ARG |
| 50 | D3 | 27 | ASN |
| 50 | D3 | 31 | ILE |
| 50 | D3 | 46 | LYS |
| 50 | D3 | 58 | ILE |
| 51 | D4 | 9 | LYS |
| 51 | D4 | 10 | LEU |
| 52 | DI | 2 | LYS |
| 52 | DI | 54 | ILE |
| 52 | DI | 91 | LYS |
| 52 | DI | 99 | LYS |
| 52 | DI | 121 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | DI | 140 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (346) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 2 | GLN |
| 2 | AC | 7 | ASN |
| 2 | AC | 31 | ASN |
| 2 | AC | 68 | HIS |
| 2 | AC | 139 | ASN |
| 3 | AD | 35 | GLN |
| 3 | AD | 39 | GLN |
| 3 | AD | 53 | GLN |
| 3 | AD | 70 | GLN |
| 3 | AD | 88 | ASN |
| 3 | AD | 115 | GLN |
| 3 | AD | 135 | GLN |
| 3 | AD | 195 | ASN |
| 4 | AE | 18 | ASN |
| 4 | AE | 72 | ASN |
| 4 | AE | 81 | GLN |
| 4 | AE | 131 | ASN |
| 5 | AF | 46 | GLN |
| 6 | AG | 27 | ASN |
| 6 | AG | 67 | ASN |
| 6 | AG | 121 | ASN |
| 6 | AG | 129 | ASN |
| 6 | AG | 141 | HIS |
| 7 | AH | 3 | GLN |
| 7 | AH | 75 | GLN |
| 7 | AH | 117 | GLN |
| 8 | AI | 30 | ASN |
| 8 | AI | 31 | GLN |
| 8 | AI | 36 | GLN |
| 8 | AI | 80 | HIS |
| 8 | AI | 109 | GLN |
| 9 | AJ | 15 | HIS |
| 9 | AJ | 20 | GLN |
| 9 | AJ | 56 | HIS |
| 9 | AJ | 70 | HIS |
| 10 | AK | 14 | GLN |
| 10 | AK | 28 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | AK | 39 | ASN |
| 10 | AK | 118 | ASN |
| 11 | AL | 5 | GLN |
| 11 | AL | 28 | GLN |
| 11 | AL | 45 | ASN |
| 11 | AL | 71 | HIS |
| 12 | AM | 7 | ASN |
| 13 | AN | 34 | ASN |
| 13 | AN | 48 | GLN |
| 13 | AN | 61 | ASN |
| 14 | AO | 27 | GLN |
| 14 | AO | 36 | ASN |
| 14 | AO | 39 | GLN |
| 14 | AO | 61 | GLN |
| 15 | AP | 9 | HIS |
| 15 | AP | 29 | ASN |
| 15 | AP | 40 | ASN |
| 16 | AQ | 50 | ASN |
| 17 | AR | 53 | GLN |
| 17 | AR | 73 | HIS |
| 18 | AS | 42 | ASN |
| 18 | AS | 56 | HIS |
| 18 | AS | 68 | HIS |
| 19 | AT | 67 | HIS |
| 19 | AT | 74 | HIS |
| 20 | AB | 14 | HIS |
| 20 | AB | 23 | ASN |
| 20 | AB | 35 | ASN |
| 20 | AB | 38 | HIS |
| 20 | AB | 41 | ASN |
| 20 | AB | 119 | GLN |
| 20 | AB | 145 | ASN |
| 20 | AB | 169 | HIS |
| 20 | AB | 202 | ASN |
| 24 | BV | 44 | HIS |
| 24 | BV | 51 | GLN |
| 24 | BV | 80 | HIS |
| 25 | BC | 43 | ASN |
| 25 | BC | 45 | ASN |
| 25 | BC | 59 | GLN |
| 25 | BC | 85 | ASN |
| 25 | BC | 114 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BC | 133 | ASN |
| 25 | BC | 152 | GLN |
| 25 | BC | 162 | GLN |
| 25 | BC | 196 | ASN |
| 26 | BD | 32 | ASN |
| 26 | BD | 36 | GLN |
| 26 | BD | 49 | GLN |
| 26 | BD | 126 | ASN |
| 26 | BD | 136 | ASN |
| 26 | BD | 148 | GLN |
| 26 | BD | 173 | GLN |
| 27 | BE | 29 | HIS |
| 27 | BE | 30 | GLN |
| 27 | BE | 62 | GLN |
| 27 | BE | 90 | GLN |
| 27 | BE | 94 | GLN |
| 27 | BE | 195 | GLN |
| 28 | BF | 26 | GLN |
| 28 | BF | 36 | ASN |
| 28 | BF | 51 | ASN |
| 28 | BF | 62 | GLN |
| 28 | BF | 80 | GLN |
| 28 | BF | 134 | GLN |
| 29 | BG | 29 | ASN |
| 29 | BG | 63 | GLN |
| 29 | BG | 87 | GLN |
| 29 | BG | 103 | ASN |
| 29 | BG | 127 | GLN |
| 30 | BH | 28 | ASN |
| 30 | BH | 66 | ASN |
| 30 | BH | 73 | ASN |
| 31 | BJ | 130 | HIS |
| 31 | BJ | 138 | GLN |
| 32 | BK | 5 | GLN |
| 32 | BK | 13 | ASN |
| 32 | BK | 89 | ASN |
| 33 | BL | 4 | ASN |
| 33 | BL | 54 | GLN |
| 33 | BL | 104 | GLN |
| 34 | BM | 17 | ASN |
| 34 | BM | 60 | GLN |
| 34 | BM | 88 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | BN | 11 | ASN |
| 35 | BN | 62 | ASN |
| 35 | BN | 107 | ASN |
| 36 | BO | 19 | GLN |
| 36 | BO | 29 | HIS |
| 36 | BO | 38 | GLN |
| 36 | BO | 61 | GLN |
| 36 | BO | 104 | GLN |
| 37 | BP | 11 | GLN |
| 37 | BP | 40 | GLN |
| 37 | BP | 74 | GLN |
| 37 | BP | 76 | HIS |
| 37 | BP | 114 | ASN |
| 38 | BQ | 51 | GLN |
| 38 | BQ | 71 | ASN |
| 38 | BQ | 80 | ASN |
| 39 | BR | 6 | GLN |
| 39 | BR | 82 | HIS |
| 39 | BR | 86 | GLN |
| 40 | BS | 61 | ASN |
| 41 | BT | 48 | GLN |
| 41 | BT | 59 | ASN |
| 41 | BT | 72 | GLN |
| 41 | BT | 91 | GLN |
| 41 | BT | 92 | ASN |
| 42 | BU | 26 | ASN |
| 42 | BU | 65 | GLN |
| 42 | BU | 68 | ASN |
| 42 | BU | 73 | ASN |
| 43 | BW | 11 | ASN |
| 43 | BW | 39 | GLN |
| 43 | BW | 49 | ASN |
| 43 | BW | 56 | HIS |
| 43 | BW | 75 | ASN |
| 44 | BX | 20 | ASN |
| 44 | BX | 25 | GLN |
| 44 | BX | 27 | ASN |
| 44 | BX | 31 | GLN |
| 44 | BX | 58 | ASN |
| 45 | BY | 33 | HIS |
| 45 | BY | 48 | ASN |
| 46 | BZ | 6 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | BZ | 23 | ASN |
| 46 | BZ | 36 | HIS |
| 47 | B0 | 3 | GLN |
| 49 | B2 | 6 | GLN |
| 49 | B2 | 29 | GLN |
| 50 | B3 | 42 | HIS |
| 51 | B4 | 35 | GLN |
| 52 | BI | 11 | GLN |
| 52 | BI | 29 | GLN |
| 52 | BI | 33 | ASN |
| 52 | BI | 93 | ASN |
| 2 | CC | 2 | GLN |
| 2 | CC | 7 | ASN |
| 2 | CC | 31 | ASN |
| 2 | CC | 68 | HIS |
| 2 | CC | 139 | ASN |
| 3 | CD | 35 | GLN |
| 3 | CD | 39 | GLN |
| 3 | CD | 53 | GLN |
| 3 | CD | 70 | GLN |
| 3 | CD | 135 | GLN |
| 3 | CD | 195 | ASN |
| 4 | CE | 18 | ASN |
| 4 | CE | 72 | ASN |
| 4 | CE | 81 | GLN |
| 4 | CE | 131 | ASN |
| 5 | CF | 46 | GLN |
| 6 | CG | 27 | ASN |
| 6 | CG | 67 | ASN |
| 6 | CG | 121 | ASN |
| 6 | CG | 129 | ASN |
| 6 | CG | 141 | HIS |
| 7 | CH | 3 | GLN |
| 7 | CH | 117 | GLN |
| 8 | CI | 30 | ASN |
| 8 | CI | 31 | GLN |
| 8 | CI | 36 | GLN |
| 8 | CI | 80 | HIS |
| 8 | CI | 109 | GLN |
| 9 | CJ | 15 | HIS |
| 9 | CJ | 20 | GLN |
| 9 | CJ | 35 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | CJ | 56 | HIS |
| 9 | CJ | 70 | HIS |
| 10 | CK | 14 | GLN |
| 10 | CK | 28 | ASN |
| 10 | CK | 39 | ASN |
| 10 | CK | 118 | ASN |
| 11 | CL | 5 | GLN |
| 11 | CL | 28 | GLN |
| 11 | CL | 45 | ASN |
| 11 | CL | 71 | HIS |
| 12 | CM | 7 | ASN |
| 13 | CN | 34 | ASN |
| 13 | CN | 48 | GLN |
| 13 | CN | 61 | ASN |
| 14 | CO | 27 | GLN |
| 14 | CO | 36 | ASN |
| 14 | CO | 39 | GLN |
| 14 | CO | 61 | GLN |
| 15 | CP | 9 | HIS |
| 15 | CP | 29 | ASN |
| 15 | CP | 40 | ASN |
| 16 | CQ | 50 | ASN |
| 17 | CR | 53 | GLN |
| 17 | CR | 73 | HIS |
| 18 | CS | 42 | ASN |
| 18 | CS | 56 | HIS |
| 18 | CS | 68 | HIS |
| 19 | CT | 67 | HIS |
| 19 | CT | 74 | HIS |
| 20 | CB | 14 | HIS |
| 20 | CB | 23 | ASN |
| 20 | CB | 35 | ASN |
| 20 | CB | 41 | ASN |
| 20 | CB | 119 | GLN |
| 20 | CB | 121 | GLN |
| 20 | CB | 145 | ASN |
| 20 | CB | 169 | HIS |
| 20 | CB | 202 | ASN |
| 24 | DV | 44 | HIS |
| 24 | DV | 51 | GLN |
| 24 | DV | 80 | HIS |
| 24 | DV | 88 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DC | 43 | ASN |
| 25 | DC | 45 | ASN |
| 25 | DC | 59 | GLN |
| 25 | DC | 85 | ASN |
| 25 | DC | 114 | GLN |
| 25 | DC | 133 | ASN |
| 25 | DC | 152 | GLN |
| 25 | DC | 162 | GLN |
| 25 | DC | 196 | ASN |
| 26 | DD | 32 | ASN |
| 26 | DD | 36 | GLN |
| 26 | DD | 49 | GLN |
| 26 | DD | 126 | ASN |
| 26 | DD | 136 | ASN |
| 26 | DD | 148 | GLN |
| 26 | DD | 173 | GLN |
| 27 | DE | 30 | GLN |
| 27 | DE | 62 | GLN |
| 27 | DE | 90 | GLN |
| 27 | DE | 195 | GLN |
| 28 | DF | 26 | GLN |
| 28 | DF | 36 | ASN |
| 28 | DF | 51 | ASN |
| 28 | DF | 62 | GLN |
| 28 | DF | 80 | GLN |
| 28 | DF | 134 | GLN |
| 29 | DG | 29 | ASN |
| 29 | DG | 87 | GLN |
| 29 | DG | 103 | ASN |
| 29 | DG | 127 | GLN |
| 29 | DG | 142 | GLN |
| 30 | DH | 28 | ASN |
| 30 | DH | 43 | ASN |
| 30 | DH | 66 | ASN |
| 30 | DH | 133 | GLN |
| 31 | DJ | 130 | HIS |
| 31 | DJ | 138 | GLN |
| 32 | DK | 5 | GLN |
| 32 | DK | 13 | ASN |
| 32 | DK | 89 | ASN |
| 33 | DL | 4 | ASN |
| 33 | DL | 54 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | DL | 104 | GLN |
| 34 | DM | 17 | ASN |
| 34 | DM | 60 | GLN |
| 34 | DM | 88 | ASN |
| 35 | DN | 11 | ASN |
| 35 | DN | 23 | ASN |
| 35 | DN | 62 | ASN |
| 35 | DN | 107 | ASN |
| 36 | DO | 19 | GLN |
| 36 | DO | 38 | GLN |
| 36 | DO | 61 | GLN |
| 36 | DO | 100 | HIS |
| 36 | DO | 104 | GLN |
| 37 | DP | 11 | GLN |
| 37 | DP | 40 | GLN |
| 37 | DP | 74 | GLN |
| 37 | DP | 76 | HIS |
| 37 | DP | 114 | ASN |
| 38 | DQ | 51 | GLN |
| 38 | DQ | 71 | ASN |
| 38 | DQ | 80 | ASN |
| 39 | DR | 6 | GLN |
| 39 | DR | 82 | HIS |
| 39 | DR | 86 | GLN |
| 40 | DS | 57 | ASN |
| 40 | DS | 61 | ASN |
| 41 | DT | 48 | GLN |
| 41 | DT | 72 | GLN |
| 41 | DT | 91 | GLN |
| 41 | DT | 92 | ASN |
| 42 | DU | 26 | ASN |
| 42 | DU | 65 | GLN |
| 42 | DU | 68 | ASN |
| 42 | DU | 73 | ASN |
| 43 | DW | 11 | ASN |
| 43 | DW | 39 | GLN |
| 43 | DW | 49 | ASN |
| 43 | DW | 56 | HIS |
| 43 | DW | 75 | ASN |
| 44 | DX | 20 | ASN |
| 44 | DX | 25 | GLN |
| 44 | DX | 27 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | DX | 31 | GLN |
| 44 | DX | 58 | ASN |
| 45 | DY | 33 | HIS |
| 45 | DY | 48 | ASN |
| 46 | DZ | 6 | GLN |
| 46 | DZ | 23 | ASN |
| 46 | DZ | 36 | HIS |
| 47 | D0 | 3 | GLN |
| 49 | D2 | 6 | GLN |
| 49 | D2 | 29 | GLN |
| 50 | D3 | 42 | HIS |
| 51 | D4 | 35 | GLN |
| 52 | DI | 5 | GLN |
| 52 | DI | 11 | GLN |
| 52 | DI | 33 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1529/1542 (99%) | 257 (16%) | 27 (1%) |
| 1 | CA | 1529/1542 (99%) | 240 (15%) | 27 (1%) |
| 22 | BA | 116/120 (96%) | 22 (18%) | 0 |
| 22 | DA | 116/120 (96%) | 22 (18%) | 0 |
| 23 | BB | 2837/2904 (97%) | 460 (16%) | 17 (0%) |
| 23 | DB | 2837/2904 (97%) | 460 (16%) | 21 (0%) |
| All | All | 8964/9132 (98%) | 1461 (16%) | 92 (1%) |

All (1461) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 6 | G |
| 1 | AA | 9 | G |
| 1 | AA | 14 | U |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 52 | C |
| 1 | AA | 54 | C |
| 1 | AA | 55 | A |
| 1 | AA | 61 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 65 | A |
| 1 | AA | 70 | U |
| 1 | AA | 71 | A |
| 1 | AA | 72 | A |
| 1 | AA | 75 | G |
| 1 | AA | 76 | G |
| 1 | AA | 79 | G |
| 1 | AA | 80 | A |
| 1 | AA | 81 | A |
| 1 | AA | 82 | 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 | 90 | C |
| 1 | AA | 92 | U |
| 1 | AA | 93 | U |
| 1 | AA | 94 | G |
| 1 | AA | 95 | C |
| 1 | AA | 121 | U |
| 1 | AA | 130 | A |
| 1 | AA | 131 | A |
| 1 | AA | 164 | G |
| 1 | AA | 177 | G |
| 1 | AA | 182 | A |
| 1 | AA | 183 | C |
| 1 | AA | 197 | A |
| 1 | AA | 206 | C |
| 1 | AA | 209 | U |
| 1 | AA | 210 | C |
| 1 | AA | 233 | C |
| 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 |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 256 | U |
| 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 | 321 | A |
| 1 | AA | 328 | C |
| 1 | AA | 329 | A |
| 1 | AA | 330 | C |
| 1 | AA | 332 | 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 | 384 | G |
| 1 | AA | 392 | C |
| 1 | AA | 397 | A |
| 1 | AA | 398 | U |
| 1 | AA | 406 | G |
| 1 | AA | 408 | A |
| 1 | AA | 411 | A |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 415 | A |
| 1 | AA | 421 | U |
| 1 | AA | 422 | C |
| 1 | AA | 429 | U |
| 1 | AA | 430 | A |
| 1 | AA | 435 | A |
| 1 | AA | 438 | U |
| 1 | AA | 460 | A |
| 1 | AA | 461 | A |
| 1 | AA | 462 | G |
| 1 | AA | 463 | U |
| 1 | AA | 464 | U |
| 1 | AA | 465 | A |
| 1 | AA | 466 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 467 | U |
| 1 | AA | 468 | A |
| 1 | AA | 479 | U |
| 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 | 512 | U |
| 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 | 596 | A |
| 1 | AA | 633 | G |
| 1 | AA | 653 | U |
| 1 | AA | 661 | G |
| 1 | AA | 665 | A |
| 1 | AA | 687 | A |
| 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 | 785 | G |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 812 | G |
| 1 | AA | 815 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 817 | C |
| 1 | AA | 818 | G |
| 1 | AA | 819 | A |
| 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 | 846 | G |
| 1 | AA | 847 | G |
| 1 | AA | 849 | G |
| 1 | AA | 914 | A |
| 1 | AA | 926 | G |
| 1 | AA | 927 | G |
| 1 | AA | 931 | C |
| 1 | AA | 933 | G |
| 1 | AA | 934 | C |
| 1 | AA | 935 | A |
| 1 | AA | 960 | U |
| 1 | AA | 961 | U |
| 1 | AA | 966 | G |
| 1 | AA | 968 | A |
| 1 | AA | 969 | A |
| 1 | AA | 974 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 984 | C |
| 1 | AA | 991 | U |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 1003 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1010 | U |
| 1 | AA | 1019 | A |
| 1 | AA | 1020 | G |
| 1 | AA | 1028 | C |
| 1 | AA | 1030 | U |
| 1 | AA | 1031 | C |
| 1 | AA | 1034 | G |
| 1 | AA | 1035 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1041 | G |
| 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 | 1101 | A |
| 1 | AA | 1136 | C |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1146 | A |
| 1 | AA | 1159 | U |
| 1 | AA | 1167 | A |
| 1 | AA | 1168 | U |
| 1 | AA | 1174 | G |
| 1 | AA | 1179 | A |
| 1 | AA | 1181 | G |
| 1 | AA | 1184 | G |
| 1 | AA | 1196 | A |
| 1 | AA | 1197 | A |
| 1 | AA | 1202 | U |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1214 | C |
| 1 | AA | 1225 | A |
| 1 | AA | 1226 | C |
| 1 | AA | 1227 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1250 | A |
| 1 | AA | 1256 | A |
| 1 | AA | 1261 | A |
| 1 | AA | 1278 | G |
| 1 | AA | 1279 | G |
| 1 | AA | 1280 | A |
| 1 | AA | 1281 | C |
| 1 | AA | 1285 | A |
| 1 | AA | 1286 | U |
| 1 | AA | 1287 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1297 | G |
| 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 | 1323 | G |
| 1 | AA | 1336 | C |
| 1 | AA | 1362 | A |
| 1 | AA | 1363 | A |
| 1 | AA | 1364 | U |
| 1 | AA | 1398 | A |
| 1 | AA | 1400 | C |
| 1 | AA | 1401 | G |
| 1 | AA | 1410 | A |
| 1 | AA | 1432 | G |
| 1 | AA | 1446 | A |
| 1 | AA | 1448 | C |
| 1 | AA | 1452 | C |
| 1 | AA | 1475 | G |
| 1 | AA | 1490 | U |
| 1 | AA | 1491 | G |
| 1 | AA | 1492 | A |
| 1 | AA | 1493 | A |
| 1 | AA | 1494 | G |
| 1 | AA | 1497 | G |
| 1 | AA | 1503 | A |
| 1 | AA | 1506 | U |
| 1 | AA | 1517 | G |
| 1 | AA | 1520 | C |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 1 | AA | 1533 | C |
| 1 | AA | 1534 | A |
| 22 | BA | 11 | C |
| 22 | BA | 12 | C |
| 22 | BA | 13 | G |
| 22 | BA | 16 | G |
| 22 | BA | 26 | C |
| 22 | BA | 29 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 30 | C |
| 22 | BA | 35 | C |
| 22 | BA | 42 | C |
| 22 | BA | 44 | G |
| 22 | BA | 57 | A |
| 22 | BA | 66 | A |
| 22 | BA | 67 | G |
| 22 | BA | 74 | U |
| 22 | BA | 88 | C |
| 22 | BA | 90 | C |
| 22 | BA | 96 | G |
| 22 | BA | 99 | A |
| 22 | BA | 108 | A |
| 22 | BA | 109 | A |
| 22 | BA | 112 | G |
| 22 | BA | 116 | G |
| 23 | BB | 2 | G |
| 23 | BB | 34 | U |
| 23 | BB | 46 | G |
| 23 | BB | 51 | G |
| 23 | BB | 63 | A |
| 23 | BB | 71 | A |
| 23 | BB | 74 | A |
| 23 | BB | 75 | G |
| 23 | BB | 84 | A |
| 23 | BB | 91 | A |
| 23 | BB | 98 | G |
| 23 | BB | 100 | U |
| 23 | BB | 101 | A |
| 23 | BB | 102 | U |
| 23 | BB | 118 | A |
| 23 | BB | 119 | A |
| 23 | BB | 120 | U |
| 23 | BB | 125 | A |
| 23 | BB | 126 | A |
| 23 | BB | 128 | C |
| 23 | BB | 138 | U |
| 23 | BB | 139 | U |
| 23 | BB | 140 | C |
| 23 | BB | 141 | G |
| 23 | BB | 142 | A |
| 23 | BB | 160 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 215 | G |
| 23 | BB | 216 | A |
| 23 | BB | 221 | A |
| 23 | BB | 222 | A |
| 23 | BB | 230 | G |
| 23 | BB | 233 | A |
| 23 | BB | 241 | A |
| 23 | BB | 248 | G |
| 23 | BB | 252 | G |
| 23 | BB | 255 | A |
| 23 | BB | 265 | A |
| 23 | BB | 266 | G |
| 23 | BB | 267 | C |
| 23 | BB | 268 | C |
| 23 | BB | 271 | G |
| 23 | BB | 277 | G |
| 23 | BB | 279 | A |
| 23 | BB | 280 | U |
| 23 | BB | 281 | C |
| 23 | BB | 299 | A |
| 23 | BB | 311 | A |
| 23 | BB | 323 | C |
| 23 | BB | 329 | G |
| 23 | BB | 330 | A |
| 23 | BB | 331 | C |
| 23 | BB | 333 | G |
| 23 | BB | 343 | C |
| 23 | BB | 346 | A |
| 23 | BB | 353 | C |
| 23 | BB | 355 | U |
| 23 | BB | 364 | C |
| 23 | BB | 367 | G |
| 23 | BB | 371 | A |
| 23 | BB | 372 | G |
| 23 | BB | 386 | G |
| 23 | BB | 387 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | BB | 395 | U |
| 23 | BB | 396 | G |
| 23 | BB | 411 | G |
| 23 | BB | 412 | A |
| 23 | BB | 424 | G |
| 23 | BB | 444 | C |
| 23 | BB | 456 | C |
| 23 | BB | 457 | A |
| 23 | BB | 473 | G |
| 23 | BB | 479 | A |
| 23 | BB | 480 | A |
| 23 | BB | 481 | G |
| 23 | BB | 490 | C |
| 23 | BB | 491 | G |
| 23 | BB | 502 | A |
| 23 | BB | 504 | A |
| 23 | BB | 505 | A |
| 23 | BB | 508 | A |
| 23 | BB | 512 | G |
| 23 | BB | 527 | C |
| 23 | BB | 531 | C |
| 23 | BB | 532 | A |
| 23 | BB | 533 | G |
| 23 | BB | 544 | C |
| 23 | BB | 546 | U |
| 23 | BB | 548 | G |
| 23 | BB | 549 | G |
| 23 | BB | 550 | C |
| 23 | BB | 563 | A |
| 23 | BB | 573 | U |
| 23 | BB | 575 | A |
| 23 | BB | 586 | A |
| 23 | BB | 588 | U |
| 23 | BB | 603 | A |
| 23 | BB | 613 | A |
| 23 | BB | 614 | A |
| 23 | BB | 615 | U |
| 23 | BB | 616 | A |
| 23 | BB | 627 | A |
| 23 | BB | 637 | A |
| 23 | BB | 645 | C |
| 23 | BB | 646 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | BB | 647 | G |
| 23 | BB | 654 | A |
| 23 | BB | 655 | A |
| 23 | BB | 671 | C |
| 23 | BB | 686 | U |
| 23 | BB | 699 | A |
| 23 | BB | 717 | C |
| 23 | BB | 718 | A |
| 23 | BB | 719 | C |
| 23 | BB | 727 | A |
| 23 | BB | 730 | A |
| 23 | BB | 743 | A |
| 23 | BB | 746 | U |
| 23 | BB | 747 | U |
| 23 | BB | 775 | G |
| 23 | BB | 782 | A |
| 23 | BB | 783 | A |
| 23 | BB | 784 | G |
| 23 | BB | 785 | G |
| 23 | BB | 789 | A |
| 23 | BB | 798 | G |
| 23 | BB | 805 | G |
| 23 | BB | 811 | U |
| 23 | BB | 812 | C |
| 23 | BB | 819 | A |
| 23 | BB | 827 | U |
| 23 | BB | 828 | U |
| 23 | BB | 846 | U |
| 23 | BB | 847 | U |
| 23 | BB | 859 | G |
| 23 | BB | 869 | G |
| 23 | BB | 874 | G |
| 23 | BB | 876 | C |
| 23 | BB | 899 | A |
| 23 | BB | 910 | A |
| 23 | BB | 912 | C |
| 23 | BB | 919 | U |
| 23 | BB | 931 | U |
| 23 | BB | 932 | U |
| 23 | BB | 933 | A |
| 23 | BB | 941 | A |
| 23 | BB | 946 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 961 | C |
| 23 | BB | 974 | G |
| 23 | BB | 982 | C |
| 23 | BB | 983 | 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 | 1025 | G |
| 23 | BB | 1033 | U |
| 23 | BB | 1043 | C |
| 23 | BB | 1046 | A |
| 23 | BB | 1047 | G |
| 23 | BB | 1056 | G |
| 23 | BB | 1062 | G |
| 23 | BB | 1070 | A |
| 23 | BB | 1088 | A |
| 23 | BB | 1090 | A |
| 23 | BB | 1110 | G |
| 23 | BB | 1111 | A |
| 23 | BB | 1112 | G |
| 23 | BB | 1132 | U |
| 23 | BB | 1133 | A |
| 23 | BB | 1134 | A |
| 23 | BB | 1135 | C |
| 23 | BB | 1136 | G |
| 23 | BB | 1139 | G |
| 23 | BB | 1142 | A |
| 23 | BB | 1156 | A |
| 23 | BB | 1171 | G |
| 23 | BB | 1172 | C |
| 23 | BB | 1173 | U |
| 23 | BB | 1174 | U |
| 23 | BB | 1176 | U |
| 23 | BB | 1177 | G |
| 23 | BB | 1181 | U |
| 23 | BB | 1186 | G |
| 23 | BB | 1194 | A |
| 23 | BB | 1205 | A |
| 23 | BB | 1211 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 1212 | G |
| 23 | BB | 1218 | G |
| 23 | BB | 1237 | A |
| 23 | BB | 1241 | A |
| 23 | BB | 1242 | U |
| 23 | BB | 1248 | G |
| 23 | BB | 1249 | U |
| 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 | 1275 | A |
| 23 | BB | 1276 | A |
| 23 | BB | 1301 | A |
| 23 | BB | 1325 | U |
| 23 | BB | 1337 | G |
| 23 | BB | 1341 | G |
| 23 | BB | 1352 | U |
| 23 | BB | 1365 | A |
| 23 | BB | 1368 | G |
| 23 | BB | 1371 | G |
| 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 | 1420 | A |
| 23 | BB | 1426 | G |
| 23 | BB | 1427 | A |
| 23 | BB | 1428 | C |
| 23 | BB | 1434 | A |
| 23 | BB | 1451 | C |
| 23 | BB | 1453 | A |
| 23 | BB | 1454 | C |
| 23 | BB | 1458 | U |
| 23 | BB | 1459 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 1460 | U |
| 23 | BB | 1461 | C |
| 23 | BB | 1470 | A |
| 23 | BB | 1475 | G |
| 23 | BB | 1476 | U |
| 23 | BB | 1477 | A |
| 23 | BB | 1482 | G |
| 23 | BB | 1490 | A |
| 23 | BB | 1493 | C |
| 23 | BB | 1494 | A |
| 23 | BB | 1504 | A |
| 23 | BB | 1507 | C |
| 23 | BB | 1508 | A |
| 23 | BB | 1509 | A |
| 23 | BB | 1510 | G |
| 23 | BB | 1519 | G |
| 23 | BB | 1524 | G |
| 23 | BB | 1535 | A |
| 23 | BB | 1537 | G |
| 23 | BB | 1540 | G |
| 23 | BB | 1552 | A |
| 23 | BB | 1558 | C |
| 23 | BB | 1559 | U |
| 23 | BB | 1560 | G |
| 23 | BB | 1569 | A |
| 23 | BB | 1578 | U |
| 23 | BB | 1583 | A |
| 23 | BB | 1584 | U |
| 23 | BB | 1585 | C |
| 23 | BB | 1608 | A |
| 23 | BB | 1610 | A |
| 23 | BB | 1613 | G |
| 23 | BB | 1616 | A |
| 23 | BB | 1619 | G |
| 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 | 1714 | U |
| 23 | BB | 1715 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 1722 | A |
| 23 | BB | 1723 | G |
| 23 | BB | 1729 | U |
| 23 | BB | 1730 | C |
| 23 | BB | 1733 | G |
| 23 | BB | 1738 | G |
| 23 | BB | 1756 | G |
| 23 | BB | 1758 | U |
| 23 | BB | 1764 | C |
| 23 | BB | 1772 | A |
| 23 | BB | 1773 | A |
| 23 | BB | 1800 | C |
| 23 | BB | 1816 | C |
| 23 | BB | 1829 | A |
| 23 | BB | 1857 | G |
| 23 | BB | 1870 | C |
| 23 | BB | 1906 | G |
| 23 | BB | 1913 | A |
| 23 | BB | 1914 | C |
| 23 | BB | 1919 | A |
| 23 | BB | 1926 | U |
| 23 | BB | 1929 | G |
| 23 | BB | 1930 | G |
| 23 | BB | 1938 | A |
| 23 | BB | 1939 | U |
| 23 | BB | 1940 | U |
| 23 | BB | 1955 | U |
| 23 | BB | 1966 | A |
| 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 | 1996 | C |
| 23 | BB | 1997 | C |
| 23 | BB | 2022 | U |
| 23 | BB | 2023 | C |
| 23 | BB | 2031 | 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 | 2093 | G |
| 23 | BB | 2102 | G |
| 23 | BB | 2103 | C |
| 23 | BB | 2104 | C |
| 23 | BB | 2105 | U |
| 23 | BB | 2109 | U |
| 23 | BB | 2140 | G |
| 23 | BB | 2144 | G |
| 23 | BB | 2145 | C |
| 23 | BB | 2147 | A |
| 23 | BB | 2148 | G |
| 23 | BB | 2149 | U |
| 23 | BB | 2152 | G |
| 23 | BB | 2153 | C |
| 23 | BB | 2157 | G |
| 23 | BB | 2181 | U |
| 23 | BB | 2183 | A |
| 23 | BB | 2185 | U |
| 23 | BB | 2187 | U |
| 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 | 2266 | A |
| 23 | BB | 2272 | U |
| 23 | BB | 2283 | C |
| 23 | BB | 2287 | A |
| 23 | BB | 2288 | A |
| 23 | BB | 2305 | U |
| 23 | BB | 2307 | G |
| 23 | BB | 2308 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 2309 | A |
| 23 | BB | 2311 | A |
| 23 | BB | 2319 | G |
| 23 | BB | 2321 | U |
| 23 | BB | 2322 | A |
| 23 | BB | 2324 | U |
| 23 | BB | 2325 | G |
| 23 | BB | 2333 | A |
| 23 | BB | 2334 | U |
| 23 | BB | 2335 | A |
| 23 | BB | 2336 | A |
| 23 | BB | 2345 | G |
| 23 | BB | 2347 | C |
| 23 | BB | 2353 | G |
| 23 | BB | 2357 | G |
| 23 | BB | 2358 | A |
| 23 | BB | 2361 | G |
| 23 | BB | 2383 | G |
| 23 | BB | 2385 | C |
| 23 | BB | 2392 | A |
| 23 | BB | 2396 | G |
| 23 | BB | 2402 | U |
| 23 | BB | 2406 | A |
| 23 | BB | 2423 | U |
| 23 | BB | 2426 | A |
| 23 | BB | 2427 | C |
| 23 | BB | 2429 | G |
| 23 | BB | 2430 | A |
| 23 | BB | 2431 | U |
| 23 | BB | 2435 | A |
| 23 | BB | 2441 | U |
| 23 | BB | 2446 | G |
| 23 | BB | 2448 | A |
| 23 | BB | 2472 | G |
| 23 | BB | 2474 | U |
| 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 | 2529 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 2530 | A |
| 23 | BB | 2531 | A |
| 23 | BB | 2535 | G |
| 23 | BB | 2554 | U |
| 23 | BB | 2556 | C |
| 23 | BB | 2566 | A |
| 23 | BB | 2567 | G |
| 23 | BB | 2573 | C |
| 23 | BB | 2574 | G |
| 23 | BB | 2586 | U |
| 23 | BB | 2602 | A |
| 23 | BB | 2609 | U |
| 23 | BB | 2613 | U |
| 23 | BB | 2621 | G |
| 23 | BB | 2629 | U |
| 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 | 2726 | A |
| 23 | BB | 2739 | U |
| 23 | BB | 2744 | G |
| 23 | BB | 2750 | A |
| 23 | BB | 2751 | G |
| 23 | BB | 2752 | C |
| 23 | BB | 2753 | A |
| 23 | BB | 2756 | U |
| 23 | BB | 2757 | A |
| 23 | BB | 2760 | C |
| 23 | BB | 2765 | A |
| 23 | BB | 2778 | A |
| 23 | BB | 2790 | U |
| 23 | BB | 2791 | G |
| 23 | BB | 2792 | A |
| 23 | BB | 2798 | U |
| 23 | BB | 2799 | A |
| 23 | BB | 2800 | A |
| 23 | BB | 2801 | G |
| 23 | BB | 2808 | G |
| 23 | BB | 2809 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 2820 | A |
| 23 | BB | 2821 | A |
| 23 | BB | 2832 | U |
| 23 | BB | 2834 | G |
| 23 | BB | 2836 | U |
| 23 | BB | 2850 | A |
| 23 | BB | 2861 | U |
| 23 | BB | 2867 | G |
| 23 | BB | 2872 | A |
| 23 | BB | 2873 | A |
| 23 | BB | 2883 | A |
| 23 | BB | 2886 | A |
| 23 | BB | 2901 | C |
| 23 | BB | 2903 | U |
| 1 | CA | 6 | G |
| 1 | CA | 9 | G |
| 1 | CA | 14 | U |
| 1 | CA | 32 | A |
| 1 | CA | 39 | G |
| 1 | CA | 47 | C |
| 1 | CA | 48 | C |
| 1 | CA | 52 | C |
| 1 | CA | 54 | C |
| 1 | CA | 55 | A |
| 1 | CA | 68 | G |
| 1 | CA | 71 | A |
| 1 | CA | 83 | C |
| 1 | CA | 84 | U |
| 1 | CA | 85 | U |
| 1 | CA | 86 | G |
| 1 | CA | 87 | C |
| 1 | CA | 91 | U |
| 1 | CA | 121 | U |
| 1 | CA | 130 | A |
| 1 | CA | 131 | A |
| 1 | CA | 149 | A |
| 1 | CA | 164 | G |
| 1 | CA | 177 | G |
| 1 | CA | 182 | A |
| 1 | CA | 183 | C |
| 1 | CA | 197 | A |
| 1 | CA | 206 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 209 | U |
| 1 | CA | 210 | C |
| 1 | CA | 233 | C |
| 1 | CA | 239 | U |
| 1 | CA | 240 | G |
| 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 | 256 | U |
| 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 | 321 | A |
| 1 | CA | 328 | C |
| 1 | CA | 329 | A |
| 1 | CA | 330 | C |
| 1 | CA | 332 | 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 | 384 | G |
| 1 | CA | 392 | C |
| 1 | CA | 397 | A |
| 1 | CA | 398 | U |
| 1 | CA | 406 | G |
| 1 | CA | 408 | A |
| 1 | CA | 411 | A |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 415 | A |
| 1 | CA | 421 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 422 | C |
| 1 | CA | 429 | U |
| 1 | CA | 430 | A |
| 1 | CA | 435 | A |
| 1 | CA | 438 | U |
| 1 | CA | 460 | A |
| 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 | 479 | U |
| 1 | CA | 484 | G |
| 1 | CA | 485 | U |
| 1 | CA | 486 | U |
| 1 | CA | 493 | A |
| 1 | CA | 500 | G |
| 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 | 596 | A |
| 1 | CA | 633 | G |
| 1 | CA | 653 | U |
| 1 | CA | 661 | G |
| 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 |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 747 | A |
| 1 | CA | 748 | G |
| 1 | CA | 755 | G |
| 1 | CA | 777 | A |
| 1 | CA | 781 | A |
| 1 | CA | 782 | A |
| 1 | CA | 785 | G |
| 1 | CA | 793 | U |
| 1 | CA | 794 | A |
| 1 | CA | 812 | G |
| 1 | CA | 815 | A |
| 1 | CA | 817 | C |
| 1 | CA | 818 | G |
| 1 | CA | 819 | A |
| 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 | 846 | G |
| 1 | CA | 847 | G |
| 1 | CA | 849 | G |
| 1 | CA | 914 | 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 | 966 | G |
| 1 | CA | 968 | A |
| 1 | CA | 969 | A |
| 1 | CA | 974 | A |
| 1 | CA | 975 | A |
| 1 | CA | 976 | G |
| 1 | CA | 977 | A |
| 1 | CA | 984 | C |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |
| 1 | CA | 993 | G |
| 1 | CA | 1003 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1004 | A |
| 1 | CA | 1010 | U |
| 1 | CA | 1011 | C |
| 1 | CA | 1019 | A |
| 1 | CA | 1020 | G |
| 1 | CA | 1028 | C |
| 1 | CA | 1030 | U |
| 1 | CA | 1031 | C |
| 1 | CA | 1034 | G |
| 1 | CA | 1035 | A |
| 1 | CA | 1041 | G |
| 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 | 1094 | G |
| 1 | CA | 1101 | A |
| 1 | CA | 1136 | C |
| 1 | CA | 1137 | C |
| 1 | CA | 1138 | G |
| 1 | CA | 1139 | G |
| 1 | CA | 1146 | A |
| 1 | CA | 1159 | U |
| 1 | CA | 1167 | A |
| 1 | CA | 1168 | U |
| 1 | CA | 1174 | G |
| 1 | CA | 1179 | A |
| 1 | CA | 1181 | G |
| 1 | CA | 1184 | G |
| 1 | CA | 1196 | A |
| 1 | CA | 1197 | A |
| 1 | CA | 1202 | U |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1214 | C |
| 1 | CA | 1225 | A |
| 1 | CA | 1226 | C |
| 1 | CA | 1227 | A |
| 1 | CA | 1238 | A |
| 1 | CA | 1240 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1250 | A |
| 1 | CA | 1256 | A |
| 1 | CA | 1261 | A |
| 1 | CA | 1278 | G |
| 1 | CA | 1279 | G |
| 1 | CA | 1280 | A |
| 1 | CA | 1281 | C |
| 1 | CA | 1285 | A |
| 1 | CA | 1286 | U |
| 1 | CA | 1287 | A |
| 1 | CA | 1297 | G |
| 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 | 1323 | G |
| 1 | CA | 1336 | C |
| 1 | CA | 1362 | A |
| 1 | CA | 1363 | A |
| 1 | CA | 1364 | U |
| 1 | CA | 1388 | C |
| 1 | CA | 1398 | A |
| 1 | CA | 1400 | C |
| 1 | CA | 1401 | G |
| 1 | CA | 1432 | G |
| 1 | CA | 1446 | A |
| 1 | CA | 1448 | C |
| 1 | CA | 1452 | C |
| 1 | CA | 1490 | U |
| 1 | CA | 1491 | G |
| 1 | CA | 1492 | A |
| 1 | CA | 1493 | A |
| 1 | CA | 1494 | G |
| 1 | CA | 1497 | G |
| 1 | CA | 1503 | A |
| 1 | CA | 1506 | U |
| 1 | CA | 1517 | G |
| 1 | CA | 1520 | C |
| 1 | CA | 1529 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1530 | G |
| 1 | CA | 1534 | A |
| 22 | DA | 11 | C |
| 22 | DA | 12 | C |
| 22 | DA | 13 | G |
| 22 | DA | 16 | G |
| 22 | DA | 26 | C |
| 22 | DA | 29 | A |
| 22 | DA | 30 | C |
| 22 | DA | 35 | C |
| 22 | DA | 42 | C |
| 22 | DA | 44 | G |
| 22 | DA | 57 | A |
| 22 | DA | 66 | A |
| 22 | DA | 67 | G |
| 22 | DA | 88 | C |
| 22 | DA | 90 | C |
| 22 | DA | 96 | G |
| 22 | DA | 99 | A |
| 22 | DA | 108 | A |
| 22 | DA | 109 | A |
| 22 | DA | 112 | G |
| 22 | DA | 116 | G |
| 22 | DA | 118 | C |
| 23 | DB | 34 | U |
| 23 | DB | 46 | G |
| 23 | DB | 51 | G |
| 23 | DB | 63 | A |
| 23 | DB | 71 | A |
| 23 | DB | 74 | A |
| 23 | DB | 75 | G |
| 23 | DB | 84 | A |
| 23 | DB | 91 | A |
| 23 | DB | 98 | G |
| 23 | DB | 100 | U |
| 23 | DB | 101 | A |
| 23 | DB | 102 | U |
| 23 | DB | 118 | A |
| 23 | DB | 119 | A |
| 23 | DB | 120 | U |
| 23 | DB | 125 | A |
| 23 | DB | 126 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | DB | 128 | C |
| 23 | DB | 135 | U |
| 23 | DB | 139 | U |
| 23 | DB | 140 | C |
| 23 | DB | 141 | G |
| 23 | DB | 143 | C |
| 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 | 223 | A |
| 23 | DB | 230 | G |
| 23 | DB | 233 | A |
| 23 | DB | 241 | A |
| 23 | DB | 242 | G |
| 23 | DB | 248 | G |
| 23 | DB | 252 | G |
| 23 | DB | 255 | A |
| 23 | DB | 265 | A |
| 23 | DB | 266 | G |
| 23 | DB | 267 | C |
| 23 | DB | 268 | C |
| 23 | DB | 271 | G |
| 23 | DB | 276 | U |
| 23 | DB | 277 | G |
| 23 | DB | 278 | A |
| 23 | DB | 282 | A |
| 23 | DB | 284 | U |
| 23 | DB | 288 | U |
| 23 | DB | 289 | G |
| 23 | DB | 299 | A |
| 23 | DB | 311 | A |
| 23 | DB | 323 | C |
| 23 | DB | 329 | G |
| 23 | DB | 330 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | DB | 331 | C |
| 23 | DB | 333 | G |
| 23 | DB | 343 | C |
| 23 | DB | 346 | A |
| 23 | DB | 349 | U |
| 23 | DB | 353 | C |
| 23 | DB | 354 | A |
| 23 | DB | 358 | U |
| 23 | DB | 362 | A |
| 23 | DB | 367 | G |
| 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 | 411 | G |
| 23 | DB | 412 | A |
| 23 | DB | 424 | G |
| 23 | DB | 444 | C |
| 23 | DB | 456 | C |
| 23 | DB | 457 | A |
| 23 | DB | 473 | G |
| 23 | DB | 479 | A |
| 23 | DB | 480 | A |
| 23 | DB | 481 | G |
| 23 | DB | 490 | C |
| 23 | DB | 491 | G |
| 23 | DB | 502 | A |
| 23 | DB | 504 | A |
| 23 | DB | 505 | A |
| 23 | DB | 508 | A |
| 23 | DB | 512 | G |
| 23 | DB | 527 | C |
| 23 | DB | 531 | C |
| 23 | DB | 532 | A |
| 23 | DB | 533 | G |
| 23 | DB | 544 | C |
| 23 | DB | 545 | U |
| 23 | DB | 546 | U |
| 23 | DB | 548 | G |
| 23 | DB | 549 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | DB | 550 | C |
| 23 | DB | 563 | A |
| 23 | DB | 573 | U |
| 23 | DB | 575 | A |
| 23 | DB | 586 | A |
| 23 | DB | 588 | U |
| 23 | DB | 603 | A |
| 23 | DB | 613 | A |
| 23 | DB | 614 | A |
| 23 | DB | 615 | U |
| 23 | DB | 616 | A |
| 23 | DB | 627 | 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 | 699 | A |
| 23 | DB | 717 | C |
| 23 | DB | 718 | A |
| 23 | DB | 719 | C |
| 23 | DB | 727 | A |
| 23 | DB | 730 | A |
| 23 | DB | 743 | A |
| 23 | DB | 746 | U |
| 23 | DB | 747 | U |
| 23 | DB | 775 | G |
| 23 | DB | 782 | A |
| 23 | DB | 783 | A |
| 23 | DB | 784 | G |
| 23 | DB | 785 | G |
| 23 | DB | 789 | A |
| 23 | DB | 798 | G |
| 23 | DB | 805 | G |
| 23 | DB | 806 | C |
| 23 | DB | 811 | U |
| 23 | DB | 812 | C |
| 23 | DB | 819 | A |
| 23 | DB | 827 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DB | 828 | U |
| 23 | DB | 846 | U |
| 23 | DB | 847 | U |
| 23 | DB | 859 | G |
| 23 | DB | 869 | G |
| 23 | DB | 874 | G |
| 23 | DB | 877 | A |
| 23 | DB | 878 | A |
| 23 | DB | 899 | A |
| 23 | DB | 910 | A |
| 23 | DB | 912 | C |
| 23 | DB | 919 | U |
| 23 | DB | 931 | U |
| 23 | DB | 932 | U |
| 23 | DB | 933 | A |
| 23 | DB | 941 | A |
| 23 | DB | 946 | C |
| 23 | DB | 961 | C |
| 23 | DB | 974 | G |
| 23 | DB | 982 | C |
| 23 | DB | 983 | 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 | 1025 | G |
| 23 | DB | 1033 | U |
| 23 | DB | 1046 | A |
| 23 | DB | 1047 | G |
| 23 | DB | 1070 | A |
| 23 | DB | 1088 | A |
| 23 | DB | 1090 | A |
| 23 | DB | 1098 | A |
| 23 | DB | 1110 | G |
| 23 | DB | 1111 | A |
| 23 | DB | 1112 | G |
| 23 | DB | 1116 | G |
| 23 | DB | 1118 | C |
| 23 | DB | 1132 | U |
| 23 | DB | 1133 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DB | 1134 | A |
| 23 | DB | 1135 | C |
| 23 | DB | 1136 | G |
| 23 | DB | 1139 | G |
| 23 | DB | 1142 | A |
| 23 | DB | 1156 | A |
| 23 | DB | 1172 | C |
| 23 | DB | 1173 | U |
| 23 | DB | 1174 | U |
| 23 | DB | 1176 | U |
| 23 | DB | 1186 | G |
| 23 | DB | 1194 | A |
| 23 | DB | 1205 | A |
| 23 | DB | 1211 | C |
| 23 | DB | 1212 | G |
| 23 | DB | 1218 | G |
| 23 | DB | 1237 | A |
| 23 | DB | 1241 | A |
| 23 | DB | 1242 | U |
| 23 | DB | 1248 | G |
| 23 | DB | 1249 | U |
| 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 | 1275 | A |
| 23 | DB | 1276 | A |
| 23 | DB | 1301 | A |
| 23 | DB | 1324 | G |
| 23 | DB | 1325 | U |
| 23 | DB | 1337 | G |
| 23 | DB | 1341 | G |
| 23 | DB | 1352 | U |
| 23 | DB | 1365 | A |
| 23 | DB | 1368 | G |
| 23 | DB | 1379 | U |
| 23 | DB | 1383 | A |
| 23 | DB | 1384 | A |
| 23 | DB | 1386 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DB | 1396 | U |
| 23 | DB | 1397 | U |
| 23 | DB | 1416 | G |
| 23 | DB | 1419 | A |
| 23 | DB | 1420 | A |
| 23 | DB | 1426 | G |
| 23 | DB | 1428 | C |
| 23 | DB | 1434 | A |
| 23 | DB | 1451 | C |
| 23 | DB | 1453 | A |
| 23 | DB | 1454 | C |
| 23 | DB | 1458 | U |
| 23 | DB | 1459 | G |
| 23 | DB | 1460 | U |
| 23 | DB | 1461 | C |
| 23 | DB | 1470 | A |
| 23 | DB | 1475 | G |
| 23 | DB | 1476 | U |
| 23 | DB | 1477 | A |
| 23 | DB | 1482 | G |
| 23 | DB | 1490 | A |
| 23 | DB | 1493 | C |
| 23 | DB | 1494 | A |
| 23 | DB | 1504 | A |
| 23 | DB | 1507 | C |
| 23 | DB | 1508 | A |
| 23 | DB | 1509 | A |
| 23 | DB | 1510 | G |
| 23 | DB | 1519 | G |
| 23 | DB | 1524 | G |
| 23 | DB | 1535 | A |
| 23 | DB | 1537 | G |
| 23 | DB | 1540 | G |
| 23 | DB | 1552 | A |
| 23 | DB | 1558 | C |
| 23 | DB | 1559 | U |
| 23 | DB | 1560 | G |
| 23 | DB | 1569 | A |
| 23 | DB | 1578 | U |
| 23 | DB | 1583 | A |
| 23 | DB | 1584 | U |
| 23 | DB | 1585 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DB | 1608 | A |
| 23 | DB | 1610 | A |
| 23 | DB | 1613 | G |
| 23 | DB | 1619 | G |
| 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 | 1714 | U |
| 23 | DB | 1715 | G |
| 23 | DB | 1723 | G |
| 23 | DB | 1729 | U |
| 23 | DB | 1730 | C |
| 23 | DB | 1733 | G |
| 23 | DB | 1738 | G |
| 23 | DB | 1756 | G |
| 23 | DB | 1758 | U |
| 23 | DB | 1764 | C |
| 23 | DB | 1772 | A |
| 23 | DB | 1773 | A |
| 23 | DB | 1800 | C |
| 23 | DB | 1816 | C |
| 23 | DB | 1829 | A |
| 23 | DB | 1848 | A |
| 23 | DB | 1857 | G |
| 23 | DB | 1870 | C |
| 23 | DB | 1906 | G |
| 23 | DB | 1913 | A |
| 23 | DB | 1914 | C |
| 23 | DB | 1915 | U |
| 23 | DB | 1916 | A |
| 23 | DB | 1926 | U |
| 23 | DB | 1929 | G |
| 23 | DB | 1930 | G |
| 23 | DB | 1938 | A |
| 23 | DB | 1939 | U |
| 23 | DB | 1940 | U |
| 23 | DB | 1955 | U |
| 23 | DB | 1966 | A |
| 23 | DB | 1967 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DB | 1970 | A |
| 23 | DB | 1971 | U |
| 23 | DB | 1972 | G |
| 23 | DB | 1991 | U |
| 23 | DB | 1993 | U |
| 23 | DB | 1996 | C |
| 23 | DB | 1997 | C |
| 23 | DB | 2022 | U |
| 23 | DB | 2023 | C |
| 23 | DB | 2031 | A |
| 23 | DB | 2043 | C |
| 23 | DB | 2055 | C |
| 23 | DB | 2056 | G |
| 23 | DB | 2060 | A |
| 23 | DB | 2061 | G |
| 23 | DB | 2062 | A |
| 23 | DB | 2069 | G |
| 23 | DB | 2093 | G |
| 23 | DB | 2095 | A |
| 23 | DB | 2096 | C |
| 23 | DB | 2100 | G |
| 23 | DB | 2101 | A |
| 23 | DB | 2102 | G |
| 23 | DB | 2106 | U |
| 23 | DB | 2107 | G |
| 23 | DB | 2108 | A |
| 23 | DB | 2109 | U |
| 23 | DB | 2110 | G |
| 23 | DB | 2144 | G |
| 23 | DB | 2145 | C |
| 23 | DB | 2147 | A |
| 23 | DB | 2150 | C |
| 23 | DB | 2155 | U |
| 23 | DB | 2156 | G |
| 23 | DB | 2157 | G |
| 23 | DB | 2181 | U |
| 23 | DB | 2188 | U |
| 23 | DB | 2193 | G |
| 23 | DB | 2198 | A |
| 23 | DB | 2199 | A |
| 23 | DB | 2203 | U |
| 23 | DB | 2204 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 2266 | A |
| 23 | DB | 2272 | U |
| 23 | DB | 2283 | C |
| 23 | DB | 2287 | A |
| 23 | DB | 2288 | A |
| 23 | DB | 2297 | A |
| 23 | DB | 2305 | U |
| 23 | DB | 2307 | G |
| 23 | DB | 2308 | G |
| 23 | DB | 2309 | A |
| 23 | DB | 2311 | A |
| 23 | DB | 2319 | G |
| 23 | DB | 2321 | U |
| 23 | DB | 2322 | A |
| 23 | DB | 2324 | U |
| 23 | DB | 2325 | G |
| 23 | DB | 2333 | A |
| 23 | DB | 2334 | U |
| 23 | DB | 2335 | A |
| 23 | DB | 2336 | A |
| 23 | DB | 2345 | G |
| 23 | DB | 2347 | C |
| 23 | DB | 2357 | G |
| 23 | DB | 2361 | G |
| 23 | DB | 2383 | G |
| 23 | DB | 2385 | C |
| 23 | DB | 2392 | A |
| 23 | DB | 2396 | G |
| 23 | DB | 2402 | U |
| 23 | DB | 2406 | A |
| 23 | DB | 2423 | U |
| 23 | DB | 2426 | A |
| 23 | DB | 2427 | C |
| 23 | DB | 2429 | G |
| 23 | DB | 2430 | A |
| 23 | DB | 2431 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DB | 2435 | A |
| 23 | DB | 2441 | U |
| 23 | DB | 2446 | G |
| 23 | DB | 2448 | A |
| 23 | DB | 2472 | G |
| 23 | DB | 2474 | U |
| 23 | DB | 2476 | A |
| 23 | DB | 2491 | U |
| 23 | DB | 2502 | G |
| 23 | DB | 2505 | G |
| 23 | DB | 2506 | U |
| 23 | DB | 2518 | A |
| 23 | DB | 2529 | G |
| 23 | DB | 2530 | A |
| 23 | DB | 2531 | A |
| 23 | DB | 2535 | G |
| 23 | DB | 2554 | U |
| 23 | DB | 2556 | C |
| 23 | DB | 2566 | A |
| 23 | DB | 2567 | G |
| 23 | DB | 2573 | C |
| 23 | DB | 2574 | G |
| 23 | DB | 2586 | U |
| 23 | DB | 2602 | A |
| 23 | DB | 2609 | U |
| 23 | DB | 2613 | U |
| 23 | DB | 2621 | G |
| 23 | DB | 2629 | U |
| 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 | 2726 | A |
| 23 | DB | 2739 | U |
| 23 | DB | 2744 | G |
| 23 | DB | 2748 | A |
| 23 | DB | 2757 | A |
| 23 | DB | 2760 | C |
| 23 | DB | 2765 | A |
| 23 | DB | 2778 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DB | 2790 | U |
| 23 | DB | 2791 | G |
| 23 | DB | 2792 | A |
| 23 | DB | 2798 | U |
| 23 | DB | 2799 | A |
| 23 | DB | 2800 | A |
| 23 | DB | 2801 | G |
| 23 | DB | 2808 | G |
| 23 | DB | 2809 | A |
| 23 | DB | 2820 | A |
| 23 | DB | 2821 | A |
| 23 | DB | 2823 | A |
| 23 | DB | 2832 | U |
| 23 | DB | 2834 | G |
| 23 | DB | 2836 | U |
| 23 | DB | 2861 | U |
| 23 | DB | 2867 | G |
| 23 | DB | 2872 | A |
| 23 | DB | 2873 | A |
| 23 | DB | 2883 | A |
| 23 | DB | 2886 | A |
| 23 | DB | 2903 | U |

All (92) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 51 | A |
| 1 | AA | 81 | A |
| 1 | AA | 84 | U |
| 1 | AA | 243 | A |
| 1 | AA | 279 | A |
| 1 | AA | 328 | C |
| 1 | AA | 366 | A |
| 1 | AA | 372 | C |
| 1 | AA | 412 | A |
| 1 | AA | 428 | G |
| 1 | AA | 429 | U |
| 1 | AA | 484 | G |
| 1 | AA | 576 | C |
| 1 | AA | 960 | U |
| 1 | AA | 975 | A |
| 1 | AA | 1030 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1049 | U |
| 1 | AA | 1065 | U |
| 1 | AA | 1201 | A |
| 1 | AA | 1213 | A |
| 1 | AA | 1226 | C |
| 1 | AA | 1285 | A |
| 1 | AA | 1302 | C |
| 1 | AA | 1362 | A |
| 1 | AA | 1397 | C |
| 1 | AA | 1451 | U |
| 1 | AA | 1492 | A |
| 23 | BB | 63 | A |
| 23 | BB | 162 | U |
| 23 | BB | 670 | A |
| 23 | BB | 858 | G |
| 23 | BB | 1133 | A |
| 23 | BB | 1210 | G |
| 23 | BB | 1419 | A |
| 23 | BB | 1509 | A |
| 23 | BB | 1912 | A |
| 23 | BB | 2213 | U |
| 23 | BB | 2282 | G |
| 23 | BB | 2286 | G |
| 23 | BB | 2425 | A |
| 23 | BB | 2430 | A |
| 23 | BB | 2756 | U |
| 23 | BB | 2808 | G |
| 23 | BB | 2873 | A |
| 1 | CA | 51 | A |
| 1 | CA | 239 | U |
| 1 | CA | 243 | A |
| 1 | CA | 266 | G |
| 1 | CA | 279 | A |
| 1 | CA | 328 | C |
| 1 | CA | 366 | A |
| 1 | CA | 372 | C |
| 1 | CA | 412 | A |
| 1 | CA | 428 | G |
| 1 | CA | 429 | U |
| 1 | CA | 484 | G |
| 1 | CA | 960 | U |
| 1 | CA | 975 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1030 | U |
| 1 | CA | 1049 | U |
| 1 | CA | 1065 | U |
| 1 | CA | 1201 | A |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1226 | C |
| 1 | CA | 1285 | A |
| 1 | CA | 1302 | C |
| 1 | CA | 1362 | A |
| 1 | CA | 1397 | C |
| 1 | CA | 1451 | U |
| 1 | CA | 1492 | A |
| 23 | DB | 63 | A |
| 23 | DB | 125 | A |
| 23 | DB | 162 | U |
| 23 | DB | 241 | A |
| 23 | DB | 544 | C |
| 23 | DB | 670 | A |
| 23 | DB | 858 | G |
| 23 | DB | 1133 | A |
| 23 | DB | 1210 | G |
| 23 | DB | 1419 | A |
| 23 | DB | 1509 | A |
| 23 | DB | 1914 | C |
| 23 | DB | 2180 | U |
| 23 | DB | 2213 | U |
| 23 | DB | 2282 | G |
| 23 | DB | 2286 | G |
| 23 | DB | 2425 | A |
| 23 | DB | 2430 | A |
| 23 | DB | 2756 | U |
| 23 | DB | 2808 | G |
| 23 | DB | 2873 | A |

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 347 ligands modelled in this entry, 345 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 54 | HYG | CA | 2062 | - | 35,39,39 | 1.38 | 6 (17%) | 43,60,60 | 1.45 | 5 (11%) |
| 54 | HYG | AA | 2059 | - | 35,39,39 | 1.36 | 6 (17%) | 43,60,60 | 1.45 | 5 (11%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 54 | HYG | CA | 2062 | - | - | 9/12/87/87 | 0/4/4/4 |
| 54 | HYG | AA | 2059 | - | - | 9/12/87/87 | 0/4/4/4 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54 | CA | 2062 | HYG | O28-C23 | 2.99 | 1.44 | 1.40 |
| 54 | AA | 2059 | HYG | O28-C23 | 2.97 | 1.44 | 1.40 |
| 54 | AA | 2059 | HYG | C27-C33 | 2.73 | 1.56 | 1.52 |
| 54 | CA | 2062 | HYG | C27-C33 | 2.72 | 1.56 | 1.52 |
| 54 | CA | 2062 | HYG | O22-C17 | -2.49 | 1.38 | 1.43 |
| 54 | CA | 2062 | HYG | C16-C15 | 2.19 | 1.57 | 1.53 |
| 54 | AA | 2059 | HYG | C16-C15 | 2.14 | 1.57 | 1.53 |
| 54 | CA | 2062 | HYG | C3-C4 | 2.12 | 1.56 | 1.53 |
| 54 | AA | 2059 | HYG | C3-C4 | 2.11 | 1.56 | 1.53 |
| 54 | AA | 2059 | HYG | C1-C6 | 2.09 | 1.57 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54 | CA | 2062 | HYG | C1-C6 | 2.08 | 1.57 | 1.52 |
| 54 | AA | 2059 | HYG | O22-C17 | -2.06 | 1.39 | 1.43 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | CA | 2062 | HYG | O22-C17-C16 | 4.52 | 122.21 | 111.22 |
| 54 | AA | 2059 | HYG | O22-C17-C16 | 4.46 | 122.08 | 111.22 |
| 54 | CA | 2062 | HYG | O8-C1-C2 | -4.38 | 101.78 | 109.81 |
| 54 | AA | 2059 | HYG | O8-C1-C2 | -4.36 | 101.81 | 109.81 |
| 54 | CA | 2062 | HYG | O35-C34-C33 | -3.56 | 103.94 | 111.43 |
| 54 | AA | 2059 | HYG | O35-C34-C33 | -3.55 | 103.97 | 111.43 |
| 54 | AA | 2059 | HYG | C26-C25-C24 | -2.24 | 108.22 | 111.30 |
| 54 | CA | 2062 | HYG | C26-C25-C24 | -2.21 | 108.26 | 111.30 |
| 54 | AA | 2059 | HYG | C23-O28-C27 | 2.03 | 115.86 | 112.00 |
| 54 | CA | 2062 | HYG | C23-O28-C27 | 2.02 | 115.84 | 112.00 |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 54 | CA | 2062 | HYG | C3-C4-N9-C10 |
| 54 | CA | 2062 | HYG | C5-C4-N9-C10 |
| 54 | CA | 2062 | HYG | N36-C33-C34-O35 |
| 54 | AA | 2059 | HYG | C5-C4-N9-C10 |
| 54 | AA | 2059 | HYG | N36-C33-C34-O35 |
| 54 | CA | 2062 | HYG | O14-C15-C19-O20 |
| 54 | CA | 2062 | HYG | C16-C15-C19-O20 |
| 54 | AA | 2059 | HYG | O14-C15-C19-O20 |
| 54 | AA | 2059 | HYG | C16-C15-C19-O20 |
| 54 | AA | 2059 | HYG | C3-C4-N9-C10 |
| 54 | CA | 2062 | HYG | C27-C33-C34-O35 |
| 54 | AA | 2059 | HYG | C27-C33-C34-O35 |
| 54 | AA | 2059 | HYG | C12-C13-O18-C6 |
| 54 | CA | 2062 | HYG | C12-C13-O18-C6 |
| 54 | CA | 2062 | HYG | O14-C13-O18-C6 |
| 54 | AA | 2059 | HYG | O14-C13-O18-C6 |
| 54 | CA | 2062 | HYG | C5-C6-O18-C13 |
| 54 | AA | 2059 | HYG | C5-C6-O18-C13 |

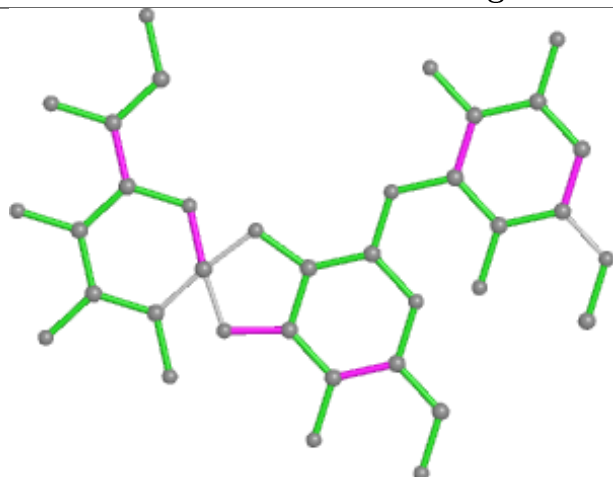
There are no ring outliers.

2 monomers are involved in 3 short contacts:

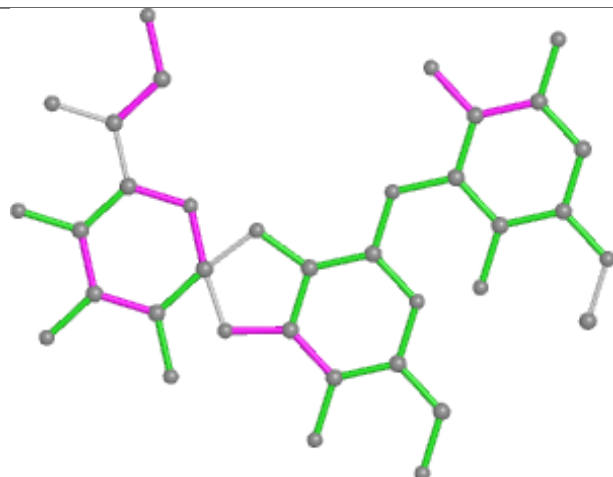
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 54 | CA | 2062 | HYG | 1 | 0 |
| 54 | AA | 2059 | HYG | 2 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

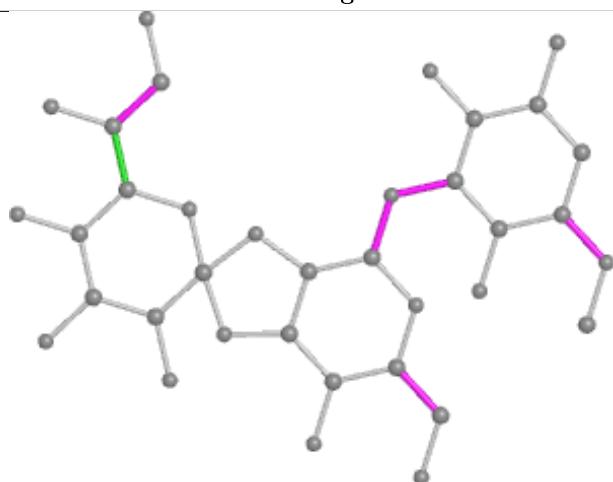
Ligand HYG CA 2062



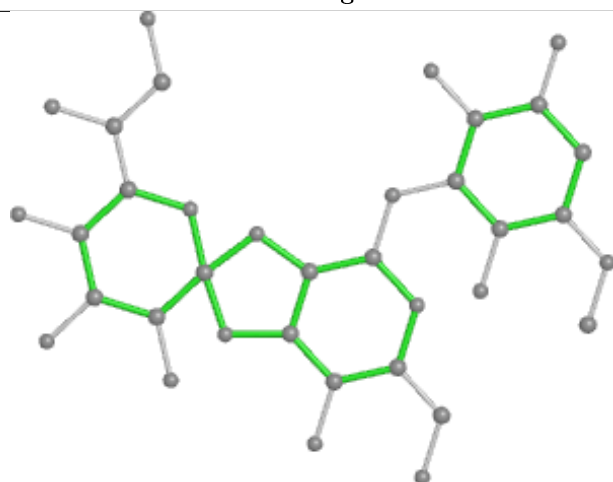
Bond lengths



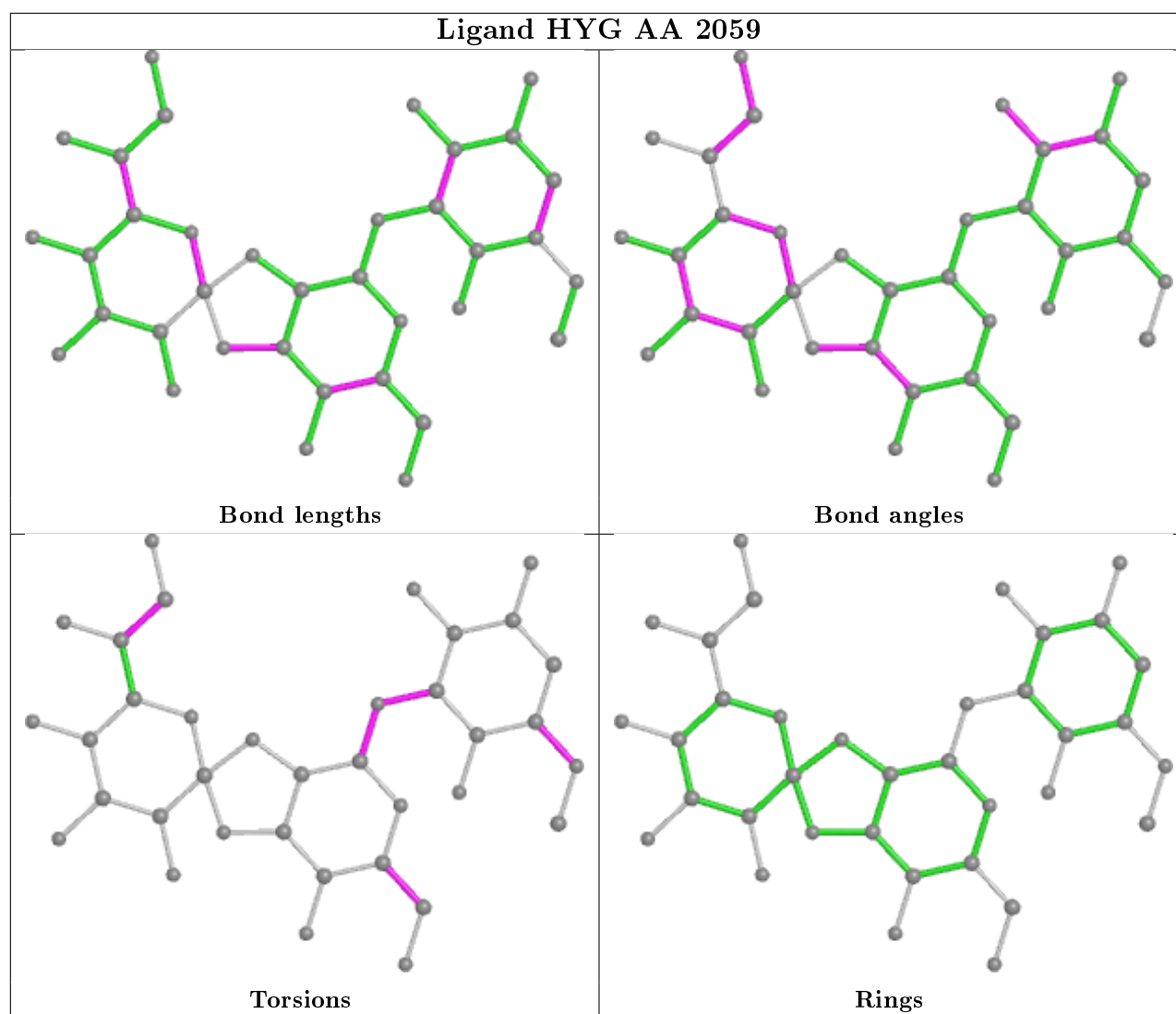
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1530/1542 (99%) | -0.72 | 7 (0%) 91 88 | 16, 85, 158, 180 | 0 |
| 1 | CA | 1530/1542 (99%) | -0.74 | 5 (0%) 94 91 | 8, 57, 142, 180 | 0 |
| 2 | AC | 206/232 (88%) | 0.84 | 30 (14%) 2 3 | 8, 89, 145, 180 | 0 |
| 2 | CC | 206/232 (88%) | 0.30 | 16 (7%) 13 13 | 15, 81, 138, 180 | 0 |
| 3 | AD | 205/205 (100%) | 0.63 | 25 (12%) 4 5 | 19, 97, 160, 180 | 0 |
| 3 | CD | 205/205 (100%) | -0.03 | 4 (1%) 65 60 | 5, 63, 135, 180 | 0 |
| 4 | AE | 150/166 (90%) | 0.16 | 5 (3%) 46 41 | 5, 76, 136, 167 | 0 |
| 4 | CE | 150/166 (90%) | 0.86 | 24 (16%) 1 2 | 5, 62, 135, 175 | 0 |
| 5 | AF | 100/135 (74%) | 1.19 | 27 (27%) 0 0 | 13, 81, 137, 180 | 0 |
| 5 | CF | 100/135 (74%) | 0.34 | 3 (3%) 50 44 | 14, 78, 126, 166 | 0 |
| 6 | AG | 150/178 (84%) | 0.38 | 22 (14%) 2 3 | 41, 110, 166, 180 | 0 |
| 6 | CG | 152/178 (85%) | 0.16 | 11 (7%) 15 15 | 27, 98, 156, 177 | 0 |
| 7 | AH | 129/129 (100%) | 0.24 | 10 (7%) 13 13 | 26, 91, 148, 180 | 0 |
| 7 | CH | 129/129 (100%) | 0.28 | 12 (9%) 8 9 | 5, 53, 117, 153 | 0 |
| 8 | AI | 127/129 (98%) | 0.85 | 27 (21%) 0 1 | 32, 103, 160, 180 | 0 |
| 8 | CI | 127/129 (98%) | 0.66 | 14 (11%) 5 6 | 32, 103, 162, 180 | 0 |
| 9 | AJ | 98/103 (95%) | 0.85 | 11 (11%) 5 6 | 34, 106, 162, 180 | 0 |
| 9 | CJ | 98/103 (95%) | 1.22 | 28 (28%) 0 0 | 42, 107, 156, 180 | 0 |
| 10 | AK | 117/128 (91%) | -0.06 | 2 (1%) 70 64 | 5, 71, 122, 174 | 0 |
| 10 | CK | 117/128 (91%) | 0.12 | 5 (4%) 35 31 | 5, 57, 112, 179 | 0 |
| 11 | AL | 123/123 (100%) | 0.51 | 16 (13%) 3 4 | 15, 82, 132, 153 | 0 |
| 11 | CL | 123/123 (100%) | -0.04 | 3 (2%) 59 53 | 5, 44, 109, 165 | 0 |
| 12 | AM | 114/117 (97%) | 0.68 | 16 (14%) 2 3 | 68, 130, 178, 180 | 0 |
| 12 | CM | 113/117 (96%) | 0.02 | 4 (3%) 44 39 | 32, 108, 156, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AN | 96/100 (96%) | 0.56 | 10 (10%) 6 7 | 32, 103, 161, 180 | 0 |
| 13 | CN | 96/100 (96%) | 0.18 | 6 (6%) 20 18 | 38, 99, 137, 171 | 0 |
| 14 | AO | 88/89 (98%) | 0.40 | 4 (4%) 33 29 | 35, 83, 132, 180 | 0 |
| 14 | CO | 88/89 (98%) | -0.03 | 2 (2%) 60 54 | 8, 54, 111, 165 | 0 |
| 15 | AP | 82/82 (100%) | 1.81 | 33 (40%) 0 0 | 43, 99, 163, 180 | 0 |
| 15 | CP | 80/82 (97%) | 0.07 | 4 (5%) 28 25 | 5, 51, 143, 164 | 0 |
| 16 | AQ | 80/83 (96%) | 1.10 | 18 (22%) 0 0 | 49, 106, 156, 177 | 0 |
| 16 | CQ | 81/83 (97%) | -0.09 | 0 100 100 | 5, 51, 121, 157 | 0 |
| 17 | AR | 55/74 (74%) | 0.29 | 3 (5%) 25 22 | 16, 78, 142, 152 | 0 |
| 17 | CR | 55/74 (74%) | 0.72 | 5 (9%) 9 9 | 13, 69, 132, 149 | 0 |
| 18 | AS | 79/91 (86%) | 1.07 | 22 (27%) 0 0 | 67, 128, 175, 180 | 0 |
| 18 | CS | 80/91 (87%) | -0.12 | 3 (3%) 40 36 | 49, 113, 171, 180 | 0 |
| 19 | AT | 85/86 (98%) | 0.02 | 3 (3%) 44 39 | 43, 100, 153, 175 | 0 |
| 19 | CT | 85/86 (98%) | -0.17 | 0 100 100 | 14, 58, 121, 177 | 0 |
| 20 | AB | 218/240 (90%) | 0.28 | 23 (10%) 6 7 | 30, 102, 152, 180 | 0 |
| 20 | CB | 218/240 (90%) | 1.40 | 71 (32%) 0 0 | 26, 106, 160, 180 | 0 |
| 21 | AU | 51/71 (71%) | 0.37 | 2 (3%) 39 35 | 26, 102, 172, 180 | 0 |
| 21 | CU | 51/71 (71%) | 0.77 | 8 (15%) 2 2 | 19, 85, 151, 180 | 0 |
| 22 | BA | 117/120 (97%) | -0.77 | 1 (0%) 84 79 | 43, 83, 131, 173 | 0 |
| 22 | DA | 117/120 (97%) | -0.82 | 1 (0%) 84 79 | 32, 75, 118, 180 | 0 |
| 23 | BB | 2841/2904 (97%) | -0.49 | 15 (0%) 91 88 | 6, 56, 146, 180 | 0 |
| 23 | DB | 2841/2904 (97%) | -0.53 | 7 (0%) 95 93 | 5, 40, 139, 180 | 0 |
| 24 | BV | 94/94 (100%) | 0.09 | 5 (5%) 26 24 | 11, 96, 146, 176 | 0 |
| 24 | DV | 94/94 (100%) | -0.10 | 3 (3%) 47 42 | 14, 86, 143, 180 | 0 |
| 25 | BC | 271/273 (99%) | 0.66 | 30 (11%) 5 6 | 7, 48, 104, 170 | 0 |
| 25 | DC | 271/273 (99%) | 0.47 | 23 (8%) 10 11 | 5, 28, 81, 120 | 0 |
| 26 | BD | 209/209 (100%) | 0.52 | 28 (13%) 3 4 | 5, 73, 138, 180 | 0 |
| 26 | DD | 209/209 (100%) | 0.43 | 21 (10%) 7 8 | 5, 42, 118, 180 | 0 |
| 27 | BE | 201/201 (100%) | 0.79 | 24 (11%) 4 5 | 5, 65, 142, 180 | 0 |
| 27 | DE | 201/201 (100%) | 0.35 | 12 (5%) 21 19 | 5, 67, 135, 180 | 0 |
| 28 | BF | 178/178 (100%) | 1.40 | 54 (30%) 0 0 | 50, 116, 175, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | DF | 178/178 (100%) | 1.08 | 34 (19%) 1 1 | 7, 101, 172, 180 | 0 |
| 29 | BG | 176/176 (100%) | 0.64 | 23 (13%) 3 4 | 23, 102, 155, 180 | 0 |
| 29 | DG | 176/176 (100%) | 0.19 | 11 (6%) 20 18 | 24, 90, 161, 180 | 0 |
| 30 | BH | 149/149 (100%) | 1.71 | 51 (34%) 0 0 | 14, 117, 177, 180 | 0 |
| 30 | DH | 149/149 (100%) | 0.52 | 13 (8%) 10 11 | 11, 100, 156, 180 | 0 |
| 31 | BJ | 142/142 (100%) | 0.35 | 8 (5%) 24 22 | 6, 80, 141, 171 | 0 |
| 31 | DJ | 142/142 (100%) | 0.31 | 8 (5%) 24 22 | 5, 60, 119, 165 | 0 |
| 32 | BK | 121/123 (98%) | 1.75 | 46 (38%) 0 0 | 5, 73, 135, 180 | 0 |
| 32 | DK | 121/123 (98%) | 0.56 | 11 (9%) 9 9 | 5, 35, 102, 145 | 0 |
| 33 | BL | 143/144 (99%) | 0.03 | 5 (3%) 44 39 | 10, 64, 128, 180 | 0 |
| 33 | DL | 143/144 (99%) | 0.54 | 18 (12%) 3 5 | 5, 54, 118, 162 | 0 |
| 34 | BM | 136/136 (100%) | 0.07 | 5 (3%) 41 37 | 8, 70, 129, 172 | 0 |
| 34 | DM | 136/136 (100%) | 0.75 | 19 (13%) 2 3 | 5, 51, 114, 168 | 0 |
| 35 | BN | 120/127 (94%) | 0.50 | 12 (10%) 7 8 | 7, 67, 132, 163 | 0 |
| 35 | DN | 120/127 (94%) | -0.09 | 1 (0%) 86 81 | 5, 42, 86, 145 | 0 |
| 36 | BO | 116/117 (99%) | 0.77 | 27 (23%) 0 0 | 27, 87, 135, 156 | 0 |
| 36 | DO | 116/117 (99%) | -0.04 | 1 (0%) 84 79 | 17, 78, 142, 180 | 0 |
| 37 | BP | 114/114 (100%) | 1.71 | 46 (40%) 0 0 | 20, 85, 149, 178 | 0 |
| 37 | DP | 114/114 (100%) | 0.14 | 4 (3%) 44 39 | 5, 48, 107, 159 | 0 |
| 38 | BQ | 117/117 (100%) | -0.18 | 4 (3%) 45 40 | 5, 63, 127, 180 | 0 |
| 38 | DQ | 117/117 (100%) | 0.41 | 5 (4%) 35 31 | 5, 48, 116, 150 | 0 |
| 39 | BR | 103/103 (100%) | -0.02 | 5 (4%) 29 26 | 16, 82, 145, 158 | 0 |
| 39 | DR | 103/103 (100%) | 0.54 | 9 (8%) 10 11 | 5, 73, 136, 180 | 0 |
| 40 | BS | 110/110 (100%) | 0.40 | 7 (6%) 19 18 | 5, 53, 116, 142 | 0 |
| 40 | DS | 110/110 (100%) | 0.98 | 21 (19%) 1 1 | 5, 42, 116, 146 | 0 |
| 41 | BT | 93/100 (93%) | 0.00 | 1 (1%) 80 75 | 6, 72, 139, 179 | 0 |
| 41 | DT | 93/100 (93%) | 0.79 | 16 (17%) 1 1 | 11, 64, 156, 180 | 0 |
| 42 | BU | 102/103 (99%) | 1.23 | 26 (25%) 0 0 | 5, 78, 144, 178 | 0 |
| 42 | DU | 102/103 (99%) | 0.08 | 2 (1%) 65 60 | 10, 90, 154, 180 | 0 |
| 43 | BW | 79/84 (94%) | 0.36 | 5 (6%) 20 18 | 10, 79, 157, 163 | 0 |
| 43 | DW | 79/84 (94%) | 0.16 | 4 (5%) 28 25 | 5, 75, 131, 174 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | BX | 63/63 (100%) | 0.88 | 13 (20%) 1 1 | 9, 74, 146, 179 | 0 |
| 44 | DX | 63/63 (100%) | 0.51 | 4 (6%) 20 18 | 17, 96, 147, 180 | 0 |
| 45 | BY | 58/58 (100%) | 0.32 | 4 (6%) 16 16 | 14, 78, 135, 170 | 0 |
| 45 | DY | 58/58 (100%) | -0.08 | 2 (3%) 45 40 | 10, 73, 129, 160 | 0 |
| 46 | BZ | 77/78 (98%) | 0.60 | 9 (11%) 4 5 | 5, 49, 121, 160 | 0 |
| 46 | DZ | 77/78 (98%) | -0.02 | 2 (2%) 56 49 | 5, 42, 107, 141 | 0 |
| 47 | B0 | 56/56 (100%) | 0.43 | 5 (8%) 9 10 | 5, 77, 144, 166 | 0 |
| 47 | D0 | 56/56 (100%) | 0.27 | 3 (5%) 25 23 | 8, 52, 128, 160 | 0 |
| 48 | B1 | 50/54 (92%) | 2.28 | 28 (56%) 0 0 | 51, 99, 149, 165 | 0 |
| 48 | D1 | 50/54 (92%) | 1.43 | 11 (22%) 0 0 | 43, 93, 138, 171 | 0 |
| 49 | B2 | 46/46 (100%) | 0.42 | 2 (4%) 35 31 | 7, 49, 103, 135 | 0 |
| 49 | D2 | 46/46 (100%) | 0.18 | 1 (2%) 62 56 | 5, 28, 99, 180 | 0 |
| 50 | B3 | 64/64 (100%) | 0.60 | 6 (9%) 8 9 | 16, 56, 110, 137 | 0 |
| 50 | D3 | 64/64 (100%) | 0.35 | 6 (9%) 8 9 | 5, 43, 112, 152 | 0 |
| 51 | B4 | 38/38 (100%) | 0.15 | 1 (2%) 56 49 | 33, 92, 143, 146 | 0 |
| 51 | D4 | 38/38 (100%) | -0.41 | 0 100 100 | 5, 68, 112, 150 | 0 |
| 52 | BI | 141/141 (100%) | 0.99 | 26 (18%) 1 1 | 67, 169, 180, 180 | 0 |
| 52 | DI | 141/141 (100%) | 0.82 | 23 (16%) 1 2 | 91, 160, 180, 180 | 0 |
| All | All | 20417/21050 (96%) | 0.03 | 1362 (6%) 17 16 | 5, 70, 153, 180 | 0 |

All (1362) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30 | BH | 84 | ALA | 9.6 |
| 15 | AP | 80 | LYS | 9.6 |
| 48 | D1 | 52 | LYS | 9.6 |
| 15 | AP | 81 | ALA | 9.4 |
| 30 | BH | 45 | GLU | 8.8 |
| 48 | B1 | 52 | LYS | 8.4 |
| 22 | DA | 88 | C | 7.7 |
| 30 | BH | 80 | ILE | 7.7 |
| 30 | DH | 149 | GLU | 7.2 |
| 48 | B1 | 51 | ALA | 7.2 |
| 30 | BH | 142 | VAL | 6.9 |
| 23 | BB | 139 | U | 6.8 |
| 52 | DI | 98 | GLY | 6.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 9 | CJ | 84 | VAL | 6.7 |
| 28 | BF | 131 | VAL | 6.5 |
| 37 | BP | 41 | ALA | 6.4 |
| 5 | AF | 5 | GLU | 6.3 |
| 17 | AR | 19 | GLU | 6.2 |
| 30 | BH | 130 | VAL | 6.2 |
| 1 | AA | 461 | A | 6.1 |
| 32 | BK | 84 | CYS | 6.1 |
| 15 | AP | 82 | ALA | 6.0 |
| 26 | BD | 186 | LEU | 6.0 |
| 6 | AG | 150 | PHE | 6.0 |
| 44 | DX | 63 | ALA | 6.0 |
| 30 | BH | 125 | THR | 5.9 |
| 1 | AA | 80 | A | 5.8 |
| 8 | CI | 129 | ARG | 5.8 |
| 25 | BC | 114 | GLN | 5.8 |
| 20 | CB | 50 | ASN | 5.8 |
| 9 | CJ | 34 | ALA | 5.7 |
| 7 | AH | 129 | ALA | 5.7 |
| 37 | BP | 71 | ARG | 5.7 |
| 32 | BK | 104 | THR | 5.6 |
| 27 | BE | 155 | GLU | 5.6 |
| 20 | CB | 220 | VAL | 5.5 |
| 4 | CE | 158 | LYS | 5.5 |
| 48 | B1 | 15 | GLY | 5.5 |
| 18 | AS | 30 | LEU | 5.5 |
| 30 | BH | 93 | SER | 5.5 |
| 52 | DI | 83 | ALA | 5.5 |
| 23 | BB | 546 | U | 5.5 |
| 48 | B1 | 10 | LEU | 5.4 |
| 18 | AS | 65 | MET | 5.4 |
| 30 | BH | 94 | ILE | 5.4 |
| 27 | BE | 188 | MET | 5.4 |
| 8 | CI | 127 | SER | 5.4 |
| 17 | CR | 19 | GLU | 5.4 |
| 9 | CJ | 36 | VAL | 5.4 |
| 37 | BP | 70 | GLU | 5.4 |
| 37 | BP | 42 | PHE | 5.4 |
| 48 | B1 | 16 | THR | 5.3 |
| 23 | BB | 2145 | C | 5.3 |
| 5 | AF | 66 | ALA | 5.3 |
| 20 | CB | 212 | TYR | 5.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | AF | 1 | MET | 5.3 |
| 28 | DF | 173 | ASP | 5.2 |
| 9 | CJ | 81 | GLU | 5.2 |
| 32 | BK | 121 | GLU | 5.1 |
| 23 | BB | 2147 | A | 5.1 |
| 48 | D1 | 27 | ARG | 5.1 |
| 43 | BW | 84 | GLU | 5.1 |
| 28 | DF | 30 | VAL | 5.1 |
| 20 | CB | 17 | HIS | 5.1 |
| 20 | CB | 68 | PHE | 5.1 |
| 8 | AI | 47 | VAL | 5.1 |
| 28 | BF | 116 | LEU | 5.0 |
| 37 | BP | 68 | GLY | 5.0 |
| 26 | DD | 1 | MET | 5.0 |
| 23 | BB | 140 | C | 5.0 |
| 27 | DE | 188 | MET | 5.0 |
| 32 | BK | 108 | ARG | 5.0 |
| 48 | B1 | 49 | LYS | 4.9 |
| 31 | DJ | 44 | TYR | 4.9 |
| 30 | DH | 130 | VAL | 4.9 |
| 44 | DX | 62 | GLY | 4.9 |
| 28 | DF | 44 | ALA | 4.9 |
| 48 | B1 | 14 | ALA | 4.9 |
| 27 | DE | 155 | GLU | 4.9 |
| 20 | CB | 49 | PHE | 4.9 |
| 52 | DI | 85 | ILE | 4.9 |
| 30 | BH | 128 | HIS | 4.8 |
| 37 | BP | 64 | SER | 4.8 |
| 14 | AO | 88 | ARG | 4.8 |
| 38 | DQ | 90 | ASP | 4.8 |
| 26 | BD | 111 | GLY | 4.8 |
| 28 | BF | 18 | GLU | 4.8 |
| 28 | DF | 27 | VAL | 4.8 |
| 20 | CB | 124 | THR | 4.7 |
| 30 | BH | 117 | LEU | 4.7 |
| 37 | BP | 62 | LYS | 4.7 |
| 6 | AG | 8 | GLN | 4.7 |
| 11 | CL | 123 | ALA | 4.7 |
| 2 | AC | 90 | VAL | 4.7 |
| 20 | CB | 52 | ALA | 4.7 |
| 28 | BF | 30 | VAL | 4.7 |
| 32 | BK | 71 | ARG | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 26 | BD | 27 | ILE | 4.7 |
| 9 | CJ | 35 | GLN | 4.6 |
| 1 | AA | 412 | A | 4.6 |
| 42 | BU | 93 | ARG | 4.6 |
| 9 | CJ | 80 | THR | 4.6 |
| 30 | BH | 85 | GLY | 4.6 |
| 3 | AD | 178 | GLU | 4.6 |
| 20 | CB | 160 | LEU | 4.6 |
| 5 | AF | 94 | HIS | 4.6 |
| 30 | BH | 133 | GLN | 4.6 |
| 6 | AG | 84 | TYR | 4.6 |
| 10 | CK | 13 | LYS | 4.6 |
| 30 | DH | 82 | SER | 4.6 |
| 1 | AA | 79 | G | 4.6 |
| 52 | DI | 97 | VAL | 4.5 |
| 30 | BH | 124 | THR | 4.5 |
| 2 | CC | 133 | MET | 4.5 |
| 52 | BI | 54 | ILE | 4.5 |
| 6 | AG | 80 | GLY | 4.5 |
| 32 | BK | 11 | ALA | 4.5 |
| 32 | BK | 110 | GLU | 4.5 |
| 41 | DT | 70 | HIS | 4.5 |
| 32 | BK | 103 | VAL | 4.5 |
| 46 | BZ | 60 | ASP | 4.5 |
| 10 | CK | 12 | ARG | 4.5 |
| 37 | BP | 65 | ASN | 4.5 |
| 30 | BH | 129 | GLU | 4.5 |
| 37 | BP | 27 | VAL | 4.5 |
| 52 | DI | 99 | LYS | 4.5 |
| 41 | DT | 93 | LEU | 4.5 |
| 23 | DB | 544 | C | 4.5 |
| 46 | BZ | 78 | TYR | 4.4 |
| 50 | D3 | 19 | GLY | 4.4 |
| 6 | AG | 78 | ARG | 4.4 |
| 20 | CB | 150 | ILE | 4.4 |
| 2 | AC | 93 | ILE | 4.4 |
| 47 | D0 | 56 | LYS | 4.4 |
| 30 | BH | 144 | VAL | 4.4 |
| 37 | BP | 61 | ARG | 4.4 |
| 26 | DD | 2 | ILE | 4.4 |
| 52 | BI | 14 | ALA | 4.4 |
| 2 | AC | 99 | GLN | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 37 | BP | 76 | HIS | 4.4 |
| 6 | AG | 85 | GLN | 4.4 |
| 27 | DE | 143 | LEU | 4.4 |
| 30 | BH | 131 | SER | 4.4 |
| 1 | AA | 86 | G | 4.4 |
| 46 | BZ | 71 | LEU | 4.3 |
| 6 | CG | 152 | HIS | 4.3 |
| 20 | CB | 69 | VAL | 4.3 |
| 52 | BI | 15 | GLY | 4.3 |
| 28 | BF | 29 | ARG | 4.3 |
| 52 | BI | 45 | THR | 4.3 |
| 32 | BK | 83 | ALA | 4.3 |
| 45 | BY | 1 | ALA | 4.3 |
| 9 | AJ | 8 | ILE | 4.3 |
| 37 | BP | 43 | GLU | 4.3 |
| 37 | BP | 69 | VAL | 4.3 |
| 8 | AI | 50 | PRO | 4.3 |
| 15 | AP | 19 | VAL | 4.3 |
| 18 | AS | 48 | ILE | 4.2 |
| 18 | AS | 73 | PHE | 4.2 |
| 20 | CB | 56 | LEU | 4.2 |
| 26 | BD | 187 | LEU | 4.2 |
| 16 | AQ | 78 | VAL | 4.2 |
| 36 | BO | 114 | GLY | 4.2 |
| 46 | DZ | 78 | TYR | 4.2 |
| 33 | DL | 2 | ARG | 4.2 |
| 9 | CJ | 25 | ILE | 4.2 |
| 20 | CB | 128 | LEU | 4.1 |
| 13 | AN | 65 | GLN | 4.1 |
| 9 | CJ | 102 | LEU | 4.1 |
| 20 | CB | 123 | GLY | 4.1 |
| 28 | BF | 118 | ALA | 4.1 |
| 11 | AL | 14 | LYS | 4.1 |
| 29 | BG | 42 | VAL | 4.1 |
| 20 | CB | 184 | ALA | 4.1 |
| 28 | BF | 28 | PRO | 4.1 |
| 11 | AL | 13 | ARG | 4.1 |
| 44 | BX | 10 | SER | 4.1 |
| 28 | BF | 35 | LEU | 4.1 |
| 37 | BP | 86 | LYS | 4.1 |
| 20 | CB | 67 | LEU | 4.1 |
| 28 | BF | 33 | ILE | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 27 | BE | 151 | GLY | 4.1 |
| 30 | DH | 12 | LEU | 4.0 |
| 52 | BI | 49 | GLU | 4.0 |
| 8 | AI | 49 | GLN | 4.0 |
| 26 | BD | 25 | THR | 4.0 |
| 23 | DB | 613 | A | 4.0 |
| 8 | AI | 29 | ILE | 4.0 |
| 34 | DM | 104 | GLU | 4.0 |
| 20 | AB | 66 | ILE | 4.0 |
| 42 | BU | 100 | GLU | 4.0 |
| 5 | AF | 8 | PHE | 4.0 |
| 23 | BB | 715 | A | 4.0 |
| 46 | BZ | 77 | LYS | 4.0 |
| 48 | D1 | 51 | ALA | 4.0 |
| 31 | DJ | 45 | THR | 4.0 |
| 8 | AI | 128 | LYS | 4.0 |
| 15 | CP | 52 | LEU | 4.0 |
| 30 | BH | 118 | PRO | 4.0 |
| 20 | AB | 192 | PRO | 3.9 |
| 32 | BK | 12 | ASP | 3.9 |
| 27 | BE | 190 | ALA | 3.9 |
| 26 | BD | 188 | LEU | 3.9 |
| 25 | BC | 34 | GLU | 3.9 |
| 26 | DD | 32 | ASN | 3.9 |
| 32 | BK | 77 | ILE | 3.9 |
| 4 | CE | 12 | GLU | 3.9 |
| 26 | BD | 28 | GLU | 3.9 |
| 28 | DF | 169 | LEU | 3.9 |
| 52 | BI | 18 | ASN | 3.9 |
| 25 | BC | 115 | ILE | 3.9 |
| 41 | DT | 3 | ARG | 3.9 |
| 27 | BE | 152 | GLU | 3.9 |
| 9 | CJ | 83 | THR | 3.9 |
| 23 | DB | 645 | C | 3.9 |
| 28 | BF | 161 | SER | 3.9 |
| 30 | DH | 81 | ALA | 3.9 |
| 6 | CG | 78 | ARG | 3.9 |
| 32 | BK | 122 | VAL | 3.9 |
| 15 | AP | 47 | GLU | 3.9 |
| 2 | AC | 41 | TYR | 3.9 |
| 18 | AS | 29 | PRO | 3.9 |
| 18 | AS | 68 | HIS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 8 | CI | 20 | ILE | 3.9 |
| 37 | BP | 58 | PHE | 3.9 |
| 4 | CE | 43 | GLY | 3.8 |
| 9 | CJ | 100 | ILE | 3.8 |
| 44 | BX | 62 | GLY | 3.8 |
| 32 | BK | 9 | ASN | 3.8 |
| 29 | BG | 167 | VAL | 3.8 |
| 3 | AD | 106 | PHE | 3.8 |
| 28 | BF | 178 | LYS | 3.8 |
| 8 | AI | 129 | ARG | 3.8 |
| 37 | BP | 67 | GLU | 3.8 |
| 10 | CK | 73 | VAL | 3.8 |
| 37 | BP | 44 | GLY | 3.8 |
| 7 | CH | 44 | PHE | 3.8 |
| 8 | CI | 126 | PHE | 3.8 |
| 52 | DI | 84 | GLY | 3.8 |
| 7 | CH | 98 | LEU | 3.8 |
| 3 | AD | 22 | SER | 3.8 |
| 26 | DD | 77 | ARG | 3.8 |
| 34 | DM | 103 | TYR | 3.8 |
| 28 | BF | 129 | MET | 3.8 |
| 44 | BX | 63 | ALA | 3.8 |
| 48 | B1 | 32 | LYS | 3.8 |
| 37 | BP | 26 | GLU | 3.8 |
| 28 | DF | 83 | PRO | 3.8 |
| 52 | BI | 47 | SER | 3.8 |
| 2 | AC | 133 | MET | 3.8 |
| 15 | AP | 38 | PHE | 3.8 |
| 16 | AQ | 79 | GLU | 3.8 |
| 28 | DF | 24 | VAL | 3.7 |
| 28 | DF | 124 | ARG | 3.7 |
| 20 | CB | 127 | LYS | 3.7 |
| 18 | AS | 64 | GLU | 3.7 |
| 37 | BP | 96 | LEU | 3.7 |
| 42 | BU | 84 | PHE | 3.7 |
| 37 | BP | 40 | GLN | 3.7 |
| 36 | BO | 92 | PHE | 3.7 |
| 12 | CM | 44 | ILE | 3.7 |
| 2 | AC | 75 | VAL | 3.7 |
| 20 | CB | 153 | MET | 3.7 |
| 34 | BM | 1 | MET | 3.7 |
| 28 | BF | 140 | ILE | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9 | CJ | 26 | VAL | 3.7 |
| 33 | DL | 92 | LEU | 3.7 |
| 31 | BJ | 54 | ILE | 3.7 |
| 4 | CE | 81 | GLN | 3.6 |
| 28 | DF | 157 | THR | 3.6 |
| 2 | AC | 156 | LEU | 3.6 |
| 8 | AI | 51 | LEU | 3.6 |
| 27 | DE | 169 | VAL | 3.6 |
| 37 | BP | 73 | PHE | 3.6 |
| 2 | AC | 45 | GLU | 3.6 |
| 8 | CI | 91 | GLU | 3.6 |
| 21 | CU | 23 | GLU | 3.6 |
| 26 | BD | 4 | LEU | 3.6 |
| 6 | AG | 7 | GLY | 3.6 |
| 7 | AH | 98 | LEU | 3.6 |
| 20 | CB | 91 | VAL | 3.6 |
| 49 | B2 | 13 | ASN | 3.6 |
| 20 | CB | 126 | ASP | 3.6 |
| 27 | BE | 144 | GLU | 3.6 |
| 8 | AI | 79 | ARG | 3.6 |
| 20 | CB | 185 | ILE | 3.6 |
| 20 | AB | 159 | ALA | 3.6 |
| 16 | AQ | 8 | GLN | 3.6 |
| 28 | BF | 157 | THR | 3.6 |
| 42 | BU | 52 | ASN | 3.6 |
| 10 | CK | 18 | GLY | 3.6 |
| 20 | CB | 38 | HIS | 3.6 |
| 32 | BK | 10 | VAL | 3.6 |
| 15 | AP | 4 | ILE | 3.6 |
| 20 | CB | 162 | VAL | 3.6 |
| 35 | BN | 82 | GLU | 3.6 |
| 28 | DF | 163 | GLU | 3.6 |
| 36 | BO | 26 | LEU | 3.6 |
| 20 | CB | 213 | LEU | 3.6 |
| 26 | DD | 74 | GLU | 3.6 |
| 48 | D1 | 26 | LYS | 3.5 |
| 36 | BO | 37 | ALA | 3.5 |
| 12 | AM | 55 | LEU | 3.5 |
| 28 | BF | 160 | LYS | 3.5 |
| 15 | AP | 6 | LEU | 3.5 |
| 30 | BH | 122 | LEU | 3.5 |
| 4 | AE | 158 | LYS | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | DB | 1175 | A | 3.5 |
| 28 | DF | 172 | PHE | 3.5 |
| 37 | BP | 47 | ILE | 3.5 |
| 26 | BD | 185 | ASN | 3.5 |
| 47 | B0 | 56 | LYS | 3.5 |
| 27 | BE | 189 | THR | 3.5 |
| 8 | CI | 96 | GLU | 3.5 |
| 28 | BF | 127 | TYR | 3.5 |
| 20 | CB | 161 | PHE | 3.5 |
| 16 | AQ | 80 | LYS | 3.5 |
| 25 | BC | 70 | LYS | 3.5 |
| 29 | BG | 25 | ILE | 3.5 |
| 3 | AD | 177 | MET | 3.5 |
| 4 | CE | 44 | ARG | 3.5 |
| 28 | BF | 34 | THR | 3.5 |
| 23 | DB | 846 | U | 3.5 |
| 30 | DH | 122 | LEU | 3.5 |
| 11 | CL | 13 | ARG | 3.5 |
| 20 | CB | 204 | ASP | 3.5 |
| 28 | DF | 82 | TYR | 3.5 |
| 8 | AI | 64 | ILE | 3.5 |
| 2 | AC | 167 | TYR | 3.5 |
| 9 | CJ | 85 | ASP | 3.5 |
| 20 | AB | 63 | LYS | 3.4 |
| 43 | BW | 6 | GLY | 3.4 |
| 15 | AP | 52 | LEU | 3.4 |
| 5 | AF | 4 | TYR | 3.4 |
| 25 | BC | 93 | VAL | 3.4 |
| 41 | BT | 3 | ARG | 3.4 |
| 20 | CB | 163 | ILE | 3.4 |
| 17 | AR | 22 | TYR | 3.4 |
| 26 | BD | 26 | VAL | 3.4 |
| 2 | AC | 205 | GLU | 3.4 |
| 27 | BE | 143 | LEU | 3.4 |
| 30 | BH | 55 | GLU | 3.4 |
| 30 | BH | 119 | ASN | 3.4 |
| 21 | CU | 3 | ILE | 3.4 |
| 25 | DC | 111 | ALA | 3.4 |
| 2 | AC | 100 | ILE | 3.4 |
| 29 | DG | 37 | ASN | 3.4 |
| 15 | AP | 36 | VAL | 3.4 |
| 30 | BH | 56 | ALA | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 42 | BU | 82 | VAL | 3.4 |
| 9 | CJ | 101 | SER | 3.4 |
| 9 | AJ | 27 | GLU | 3.4 |
| 46 | BZ | 76 | GLU | 3.4 |
| 41 | DT | 91 | GLN | 3.4 |
| 20 | AB | 161 | PHE | 3.4 |
| 42 | BU | 86 | PHE | 3.4 |
| 2 | CC | 167 | TYR | 3.4 |
| 8 | AI | 56 | MET | 3.4 |
| 37 | BP | 99 | LEU | 3.4 |
| 31 | DJ | 6 | ALA | 3.4 |
| 20 | CB | 51 | GLU | 3.4 |
| 52 | BI | 48 | ILE | 3.4 |
| 25 | DC | 79 | ARG | 3.4 |
| 20 | CB | 205 | ALA | 3.4 |
| 28 | DF | 10 | GLU | 3.4 |
| 20 | CB | 195 | VAL | 3.4 |
| 3 | AD | 108 | ALA | 3.4 |
| 28 | BF | 115 | GLY | 3.4 |
| 30 | BH | 98 | ASP | 3.4 |
| 31 | BJ | 63 | ALA | 3.4 |
| 30 | BH | 121 | VAL | 3.4 |
| 17 | CR | 31 | TYR | 3.4 |
| 44 | BX | 5 | GLU | 3.4 |
| 13 | AN | 91 | GLU | 3.4 |
| 15 | AP | 37 | GLY | 3.4 |
| 45 | BY | 58 | GLU | 3.4 |
| 16 | AQ | 82 | VAL | 3.4 |
| 52 | BI | 59 | THR | 3.3 |
| 31 | BJ | 64 | VAL | 3.3 |
| 42 | BU | 101 | THR | 3.3 |
| 14 | CO | 45 | HIS | 3.3 |
| 37 | BP | 25 | VAL | 3.3 |
| 4 | CE | 80 | LEU | 3.3 |
| 42 | BU | 3 | LYS | 3.3 |
| 8 | AI | 38 | PHE | 3.3 |
| 30 | BH | 46 | PHE | 3.3 |
| 43 | DW | 84 | GLU | 3.3 |
| 5 | AF | 9 | MET | 3.3 |
| 31 | BJ | 86 | GLN | 3.3 |
| 48 | B1 | 34 | GLU | 3.3 |
| 16 | AQ | 58 | VAL | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 52 | DI | 137 | LEU | 3.3 |
| 2 | AC | 42 | LEU | 3.3 |
| 2 | AC | 98 | ALA | 3.3 |
| 39 | DR | 95 | ASP | 3.3 |
| 44 | BX | 1 | MET | 3.3 |
| 27 | BE | 175 | ILE | 3.3 |
| 23 | BB | 613 | A | 3.3 |
| 11 | AL | 11 | ARG | 3.3 |
| 28 | DF | 75 | GLY | 3.3 |
| 32 | BK | 113 | MET | 3.3 |
| 8 | AI | 20 | ILE | 3.3 |
| 28 | DF | 174 | PHE | 3.3 |
| 14 | AO | 19 | ASN | 3.3 |
| 41 | DT | 92 | ASN | 3.3 |
| 36 | BO | 24 | THR | 3.3 |
| 12 | AM | 59 | VAL | 3.3 |
| 28 | BF | 174 | PHE | 3.3 |
| 9 | CJ | 29 | ALA | 3.3 |
| 40 | DS | 109 | ASP | 3.3 |
| 52 | BI | 141 | ASP | 3.3 |
| 5 | AF | 62 | MET | 3.3 |
| 34 | DM | 1 | MET | 3.3 |
| 8 | CI | 103 | VAL | 3.3 |
| 20 | CB | 40 | ILE | 3.3 |
| 26 | DD | 101 | PHE | 3.3 |
| 27 | DE | 148 | ILE | 3.3 |
| 30 | DH | 110 | VAL | 3.3 |
| 37 | BP | 85 | VAL | 3.3 |
| 16 | AQ | 43 | LEU | 3.2 |
| 33 | BL | 126 | ARG | 3.2 |
| 44 | BX | 39 | GLN | 3.2 |
| 4 | CE | 117 | ALA | 3.2 |
| 30 | BH | 88 | GLY | 3.2 |
| 6 | AG | 79 | VAL | 3.2 |
| 30 | BH | 145 | ASN | 3.2 |
| 52 | BI | 58 | ILE | 3.2 |
| 30 | BH | 59 | ALA | 3.2 |
| 27 | DE | 119 | ILE | 3.2 |
| 2 | CC | 198 | LYS | 3.2 |
| 32 | BK | 64 | ARG | 3.2 |
| 42 | BU | 94 | PHE | 3.2 |
| 29 | DG | 88 | LEU | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30 | BH | 90 | LEU | 3.2 |
| 27 | BE | 150 | THR | 3.2 |
| 4 | CE | 47 | PHE | 3.2 |
| 37 | BP | 66 | GLY | 3.2 |
| 32 | BK | 107 | LEU | 3.2 |
| 32 | BK | 120 | PRO | 3.2 |
| 52 | BI | 52 | LEU | 3.2 |
| 28 | DF | 171 | ALA | 3.2 |
| 9 | CJ | 74 | VAL | 3.2 |
| 26 | DD | 52 | THR | 3.2 |
| 29 | BG | 102 | ILE | 3.2 |
| 34 | DM | 33 | LEU | 3.2 |
| 28 | DF | 28 | PRO | 3.2 |
| 52 | BI | 19 | PRO | 3.2 |
| 1 | AA | 78 | A | 3.2 |
| 20 | CB | 194 | GLY | 3.2 |
| 52 | BI | 17 | ALA | 3.2 |
| 29 | DG | 160 | GLY | 3.2 |
| 15 | AP | 54 | LEU | 3.2 |
| 33 | DL | 108 | ALA | 3.2 |
| 2 | AC | 101 | ASN | 3.2 |
| 5 | AF | 35 | LYS | 3.2 |
| 7 | AH | 128 | VAL | 3.2 |
| 8 | AI | 27 | ILE | 3.2 |
| 36 | BO | 115 | LEU | 3.2 |
| 20 | CB | 216 | VAL | 3.2 |
| 15 | AP | 5 | ARG | 3.2 |
| 28 | BF | 151 | LEU | 3.2 |
| 27 | BE | 187 | VAL | 3.2 |
| 47 | B0 | 54 | ILE | 3.1 |
| 25 | DC | 78 | GLU | 3.1 |
| 34 | DM | 60 | GLN | 3.1 |
| 9 | CJ | 79 | PRO | 3.1 |
| 48 | B1 | 35 | LEU | 3.1 |
| 28 | BF | 119 | LYS | 3.1 |
| 20 | CB | 186 | VAL | 3.1 |
| 32 | BK | 78 | ARG | 3.1 |
| 29 | BG | 21 | GLN | 3.1 |
| 6 | AG | 143 | MET | 3.1 |
| 2 | AC | 46 | LEU | 3.1 |
| 26 | BD | 201 | LEU | 3.1 |
| 37 | BP | 59 | THR | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | CE | 144 | GLU | 3.1 |
| 5 | AF | 67 | PRO | 3.1 |
| 16 | AQ | 14 | ASP | 3.1 |
| 4 | CE | 71 | ILE | 3.1 |
| 25 | BC | 116 | GLN | 3.1 |
| 6 | AG | 86 | VAL | 3.1 |
| 27 | BE | 193 | VAL | 3.1 |
| 32 | BK | 82 | ASN | 3.1 |
| 18 | CS | 26 | ASP | 3.1 |
| 30 | BH | 86 | ASP | 3.1 |
| 25 | BC | 20 | ASN | 3.1 |
| 18 | AS | 40 | PHE | 3.1 |
| 43 | DW | 45 | HIS | 3.1 |
| 1 | CA | 1032 | G | 3.1 |
| 20 | CB | 66 | ILE | 3.1 |
| 27 | BE | 124 | PHE | 3.1 |
| 40 | DS | 68 | ASP | 3.1 |
| 29 | BG | 147 | LEU | 3.1 |
| 30 | BH | 141 | LYS | 3.1 |
| 38 | DQ | 4 | LYS | 3.1 |
| 7 | CH | 102 | VAL | 3.1 |
| 23 | BB | 645 | C | 3.1 |
| 33 | DL | 91 | ASP | 3.1 |
| 26 | DD | 48 | ILE | 3.1 |
| 37 | BP | 75 | THR | 3.1 |
| 6 | AG | 18 | GLY | 3.1 |
| 12 | CM | 55 | LEU | 3.1 |
| 3 | AD | 172 | VAL | 3.1 |
| 40 | DS | 3 | THR | 3.1 |
| 20 | CB | 206 | ILE | 3.1 |
| 35 | BN | 44 | LEU | 3.1 |
| 27 | DE | 124 | PHE | 3.1 |
| 28 | DF | 79 | ARG | 3.0 |
| 21 | CU | 10 | PRO | 3.0 |
| 13 | CN | 24 | ALA | 3.0 |
| 48 | B1 | 30 | PRO | 3.0 |
| 32 | BK | 105 | ARG | 3.0 |
| 5 | AF | 56 | LYS | 3.0 |
| 22 | BA | 88 | C | 3.0 |
| 2 | CC | 165 | GLU | 3.0 |
| 28 | DF | 33 | ILE | 3.0 |
| 26 | DD | 97 | SER | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 50 | B3 | 19 | GLY | 3.0 |
| 32 | BK | 102 | PRO | 3.0 |
| 4 | CE | 36 | THR | 3.0 |
| 34 | DM | 30 | SER | 3.0 |
| 41 | DT | 71 | GLY | 3.0 |
| 13 | AN | 34 | ASN | 3.0 |
| 28 | DF | 55 | ASP | 3.0 |
| 5 | AF | 88 | MET | 3.0 |
| 15 | AP | 3 | THR | 3.0 |
| 5 | AF | 39 | LEU | 3.0 |
| 20 | CB | 16 | GLY | 3.0 |
| 2 | AC | 92 | ASP | 3.0 |
| 5 | AF | 55 | HIS | 3.0 |
| 6 | CG | 74 | VAL | 3.0 |
| 20 | AB | 8 | MET | 3.0 |
| 32 | BK | 80 | ASP | 3.0 |
| 43 | BW | 14 | ASP | 3.0 |
| 47 | D0 | 54 | ILE | 3.0 |
| 25 | DC | 100 | ARG | 3.0 |
| 9 | AJ | 36 | VAL | 3.0 |
| 30 | BH | 147 | VAL | 3.0 |
| 2 | AC | 82 | ASP | 3.0 |
| 20 | CB | 45 | THR | 3.0 |
| 30 | BH | 27 | ARG | 3.0 |
| 37 | BP | 63 | ILE | 3.0 |
| 2 | CC | 46 | LEU | 3.0 |
| 9 | CJ | 33 | GLY | 3.0 |
| 32 | DK | 59 | LYS | 3.0 |
| 29 | DG | 161 | VAL | 2.9 |
| 48 | B1 | 13 | SER | 2.9 |
| 9 | CJ | 88 | MET | 2.9 |
| 2 | CC | 169 | GLU | 2.9 |
| 21 | CU | 35 | GLU | 2.9 |
| 52 | DI | 80 | LYS | 2.9 |
| 20 | CB | 183 | PHE | 2.9 |
| 27 | DE | 108 | ILE | 2.9 |
| 9 | CJ | 87 | LEU | 2.9 |
| 48 | B1 | 24 | LYS | 2.9 |
| 8 | AI | 48 | ARG | 2.9 |
| 32 | BK | 70 | ARG | 2.9 |
| 20 | AB | 183 | PHE | 2.9 |
| 40 | DS | 5 | ALA | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 29 | DG | 40 | VAL | 2.9 |
| 3 | AD | 157 | ALA | 2.9 |
| 5 | AF | 68 | GLN | 2.9 |
| 36 | BO | 90 | VAL | 2.9 |
| 37 | BP | 1 | SER | 2.9 |
| 39 | DR | 48 | LYS | 2.9 |
| 15 | AP | 39 | PHE | 2.9 |
| 25 | DC | 81 | GLU | 2.9 |
| 30 | DH | 1 | MET | 2.9 |
| 25 | BC | 171 | VAL | 2.9 |
| 52 | BI | 70 | THR | 2.9 |
| 20 | CB | 41 | ASN | 2.9 |
| 17 | CR | 36 | GLY | 2.9 |
| 34 | BM | 33 | LEU | 2.9 |
| 42 | BU | 33 | VAL | 2.9 |
| 25 | BC | 102 | TYR | 2.9 |
| 8 | AI | 78 | ILE | 2.9 |
| 28 | BF | 139 | GLU | 2.9 |
| 52 | DI | 86 | LYS | 2.9 |
| 3 | AD | 153 | ARG | 2.9 |
| 24 | BV | 74 | ALA | 2.9 |
| 52 | BI | 13 | ALA | 2.9 |
| 50 | B3 | 13 | PHE | 2.9 |
| 40 | DS | 1 | MET | 2.9 |
| 30 | BH | 91 | PHE | 2.9 |
| 6 | AG | 20 | GLU | 2.9 |
| 30 | BH | 115 | VAL | 2.9 |
| 15 | AP | 57 | ILE | 2.9 |
| 26 | BD | 15 | PHE | 2.9 |
| 12 | AM | 7 | ASN | 2.9 |
| 32 | DK | 82 | ASN | 2.9 |
| 20 | CB | 30 | ILE | 2.9 |
| 26 | DD | 96 | ILE | 2.9 |
| 40 | BS | 74 | ILE | 2.9 |
| 20 | AB | 68 | PHE | 2.9 |
| 20 | AB | 181 | PRO | 2.9 |
| 26 | BD | 20 | VAL | 2.9 |
| 40 | DS | 52 | GLU | 2.9 |
| 25 | DC | 20 | ASN | 2.9 |
| 28 | BF | 168 | LEU | 2.9 |
| 40 | DS | 69 | LEU | 2.9 |
| 33 | DL | 75 | ALA | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 42 | BU | 76 | THR | 2.8 |
| 11 | AL | 24 | GLU | 2.8 |
| 4 | AE | 147 | ASN | 2.8 |
| 25 | DC | 29 | PHE | 2.8 |
| 28 | BF | 72 | SER | 2.8 |
| 30 | BH | 82 | SER | 2.8 |
| 40 | BS | 75 | PHE | 2.8 |
| 9 | CJ | 75 | ASP | 2.8 |
| 20 | AB | 198 | VAL | 2.8 |
| 37 | BP | 60 | VAL | 2.8 |
| 30 | BH | 96 | THR | 2.8 |
| 13 | AN | 30 | ILE | 2.8 |
| 5 | AF | 34 | GLY | 2.8 |
| 20 | CB | 164 | ASP | 2.8 |
| 15 | AP | 48 | GLU | 2.8 |
| 32 | DK | 3 | GLN | 2.8 |
| 36 | BO | 81 | ARG | 2.8 |
| 26 | BD | 176 | ASP | 2.8 |
| 15 | AP | 22 | ALA | 2.8 |
| 26 | BD | 189 | VAL | 2.8 |
| 52 | DI | 136 | GLY | 2.8 |
| 5 | AF | 93 | LYS | 2.8 |
| 17 | CR | 35 | SER | 2.8 |
| 29 | DG | 114 | HIS | 2.8 |
| 37 | DP | 1 | SER | 2.8 |
| 16 | AQ | 20 | ILE | 2.8 |
| 32 | BK | 8 | LEU | 2.8 |
| 35 | BN | 87 | PHE | 2.8 |
| 30 | BH | 146 | VAL | 2.8 |
| 2 | AC | 107 | LYS | 2.8 |
| 35 | BN | 78 | LYS | 2.8 |
| 15 | AP | 21 | VAL | 2.8 |
| 32 | BK | 73 | ASP | 2.8 |
| 28 | DF | 167 | ALA | 2.8 |
| 18 | AS | 47 | THR | 2.8 |
| 21 | AU | 53 | LYS | 2.8 |
| 31 | DJ | 2 | LYS | 2.8 |
| 12 | CM | 47 | LEU | 2.8 |
| 28 | BF | 60 | SER | 2.8 |
| 29 | BG | 114 | HIS | 2.8 |
| 41 | DT | 5 | GLU | 2.8 |
| 42 | BU | 71 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 18 | AS | 60 | PHE | 2.8 |
| 20 | CB | 29 | PHE | 2.8 |
| 25 | DC | 109 | LEU | 2.8 |
| 30 | BH | 54 | LEU | 2.8 |
| 30 | BH | 132 | PHE | 2.8 |
| 36 | BO | 116 | GLN | 2.8 |
| 13 | CN | 19 | TYR | 2.8 |
| 15 | AP | 60 | TRP | 2.8 |
| 33 | DL | 141 | LYS | 2.8 |
| 3 | AD | 173 | ASP | 2.8 |
| 20 | CB | 125 | PHE | 2.8 |
| 25 | DC | 80 | LEU | 2.8 |
| 20 | CB | 129 | THR | 2.8 |
| 28 | BF | 156 | THR | 2.8 |
| 33 | DL | 57 | LEU | 2.8 |
| 4 | AE | 85 | LYS | 2.8 |
| 5 | AF | 61 | LEU | 2.8 |
| 6 | AG | 22 | LEU | 2.8 |
| 37 | BP | 31 | VAL | 2.8 |
| 36 | BO | 88 | LYS | 2.8 |
| 40 | BS | 94 | ASP | 2.8 |
| 5 | AF | 63 | ASN | 2.8 |
| 8 | AI | 54 | VAL | 2.7 |
| 20 | CB | 130 | LYS | 2.7 |
| 3 | AD | 174 | ALA | 2.7 |
| 4 | CE | 10 | LEU | 2.7 |
| 7 | CH | 73 | SER | 2.7 |
| 27 | BE | 11 | ALA | 2.7 |
| 5 | AF | 10 | VAL | 2.7 |
| 2 | AC | 157 | GLY | 2.7 |
| 6 | CG | 70 | PRO | 2.7 |
| 3 | AD | 145 | ARG | 2.7 |
| 32 | DK | 83 | ALA | 2.7 |
| 25 | BC | 103 | ILE | 2.7 |
| 20 | CB | 158 | ASP | 2.7 |
| 36 | BO | 80 | GLU | 2.7 |
| 19 | AT | 35 | TYR | 2.7 |
| 41 | DT | 72 | GLN | 2.7 |
| 40 | DS | 62 | ASP | 2.7 |
| 28 | BF | 106 | ALA | 2.7 |
| 42 | BU | 92 | VAL | 2.7 |
| 48 | B1 | 11 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 52 | BI | 26 | ALA | 2.7 |
| 25 | DC | 101 | ARG | 2.7 |
| 50 | B3 | 22 | LYS | 2.7 |
| 20 | CB | 14 | HIS | 2.7 |
| 28 | DF | 1 | ALA | 2.7 |
| 21 | CU | 34 | ARG | 2.7 |
| 33 | DL | 123 | ARG | 2.7 |
| 52 | DI | 52 | LEU | 2.7 |
| 14 | AO | 43 | ALA | 2.7 |
| 16 | AQ | 60 | ILE | 2.7 |
| 9 | CJ | 90 | LEU | 2.7 |
| 48 | D1 | 6 | GLU | 2.7 |
| 16 | AQ | 11 | VAL | 2.7 |
| 2 | AC | 102 | ILE | 2.7 |
| 7 | CH | 129 | ALA | 2.7 |
| 20 | AB | 64 | GLY | 2.7 |
| 26 | DD | 3 | GLY | 2.7 |
| 32 | BK | 101 | GLY | 2.7 |
| 16 | AQ | 52 | CYS | 2.7 |
| 40 | DS | 104 | THR | 2.7 |
| 3 | CD | 171 | GLU | 2.7 |
| 25 | DC | 22 | GLU | 2.7 |
| 36 | BO | 106 | LEU | 2.7 |
| 41 | DT | 11 | LEU | 2.7 |
| 39 | DR | 98 | ILE | 2.7 |
| 25 | BC | 125 | PRO | 2.7 |
| 15 | AP | 18 | GLN | 2.7 |
| 15 | CP | 47 | GLU | 2.7 |
| 31 | BJ | 122 | LEU | 2.7 |
| 5 | AF | 38 | ARG | 2.7 |
| 13 | AN | 45 | LEU | 2.7 |
| 20 | CB | 200 | PRO | 2.7 |
| 37 | DP | 111 | GLU | 2.7 |
| 17 | AR | 28 | LEU | 2.7 |
| 9 | AJ | 96 | VAL | 2.7 |
| 40 | DS | 30 | SER | 2.7 |
| 28 | BF | 153 | ILE | 2.7 |
| 48 | D1 | 4 | ILE | 2.7 |
| 28 | BF | 99 | PHE | 2.7 |
| 29 | BG | 169 | ARG | 2.6 |
| 26 | DD | 30 | GLU | 2.6 |
| 6 | CG | 84 | TYR | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | AC | 76 | ILE | 2.6 |
| 39 | DR | 67 | GLY | 2.6 |
| 48 | B1 | 47 | ILE | 2.6 |
| 3 | AD | 3 | TYR | 2.6 |
| 3 | AD | 146 | GLU | 2.6 |
| 15 | AP | 71 | VAL | 2.6 |
| 24 | DV | 72 | VAL | 2.6 |
| 9 | AJ | 24 | GLU | 2.6 |
| 30 | BH | 87 | GLU | 2.6 |
| 20 | CB | 64 | GLY | 2.6 |
| 20 | CB | 90 | PHE | 2.6 |
| 32 | BK | 60 | ALA | 2.6 |
| 40 | DS | 105 | VAL | 2.6 |
| 30 | BH | 120 | GLY | 2.6 |
| 10 | AK | 73 | VAL | 2.6 |
| 25 | DC | 110 | LYS | 2.6 |
| 43 | BW | 45 | HIS | 2.6 |
| 18 | AS | 42 | ASN | 2.6 |
| 18 | AS | 61 | VAL | 2.6 |
| 48 | B1 | 37 | LYS | 2.6 |
| 16 | AQ | 9 | GLY | 2.6 |
| 20 | CB | 157 | PRO | 2.6 |
| 20 | CB | 159 | ALA | 2.6 |
| 29 | BG | 7 | PRO | 2.6 |
| 28 | DF | 77 | LYS | 2.6 |
| 37 | BP | 84 | SER | 2.6 |
| 52 | DI | 89 | SER | 2.6 |
| 26 | DD | 4 | LEU | 2.6 |
| 28 | BF | 90 | LEU | 2.6 |
| 52 | DI | 114 | ALA | 2.6 |
| 8 | AI | 127 | SER | 2.6 |
| 15 | AP | 34 | GLU | 2.6 |
| 30 | BH | 60 | GLU | 2.6 |
| 31 | DJ | 1 | MET | 2.6 |
| 38 | DQ | 73 | ILE | 2.6 |
| 3 | AD | 142 | VAL | 2.6 |
| 25 | BC | 1 | ALA | 2.6 |
| 25 | DC | 1 | ALA | 2.6 |
| 52 | DI | 82 | ALA | 2.6 |
| 3 | AD | 23 | GLY | 2.6 |
| 13 | AN | 24 | ALA | 2.6 |
| 48 | B1 | 18 | HIS | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | CE | 149 | PRO | 2.6 |
| 37 | BP | 33 | GLU | 2.6 |
| 46 | BZ | 72 | ARG | 2.6 |
| 2 | AC | 54 | ILE | 2.6 |
| 48 | B1 | 20 | TYR | 2.6 |
| 50 | D3 | 13 | PHE | 2.6 |
| 28 | DF | 168 | LEU | 2.6 |
| 32 | BK | 75 | SER | 2.6 |
| 41 | DT | 16 | VAL | 2.6 |
| 9 | AJ | 91 | ASP | 2.6 |
| 42 | BU | 102 | ILE | 2.6 |
| 6 | AG | 140 | VAL | 2.6 |
| 12 | AM | 73 | SER | 2.6 |
| 12 | AM | 82 | LEU | 2.6 |
| 15 | AP | 2 | VAL | 2.6 |
| 34 | BM | 93 | VAL | 2.6 |
| 35 | BN | 24 | MET | 2.6 |
| 30 | DH | 140 | ALA | 2.6 |
| 23 | BB | 1095 | A | 2.6 |
| 36 | BO | 117 | PHE | 2.6 |
| 8 | AI | 99 | LYS | 2.6 |
| 30 | BH | 79 | THR | 2.6 |
| 49 | B2 | 31 | LEU | 2.6 |
| 32 | BK | 69 | VAL | 2.6 |
| 9 | CJ | 30 | LYS | 2.5 |
| 20 | AB | 100 | LEU | 2.5 |
| 45 | DY | 58 | GLU | 2.5 |
| 20 | CB | 198 | VAL | 2.5 |
| 37 | BP | 107 | ALA | 2.5 |
| 13 | AN | 20 | PHE | 2.5 |
| 52 | DI | 47 | SER | 2.5 |
| 8 | AI | 66 | VAL | 2.5 |
| 19 | AT | 27 | MET | 2.5 |
| 28 | BF | 62 | GLN | 2.5 |
| 36 | BO | 93 | ASP | 2.5 |
| 11 | AL | 60 | PHE | 2.5 |
| 28 | BF | 113 | PHE | 2.5 |
| 40 | DS | 103 | ILE | 2.5 |
| 29 | BG | 160 | GLY | 2.5 |
| 26 | BD | 110 | THR | 2.5 |
| 28 | BF | 89 | THR | 2.5 |
| 45 | BY | 55 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | CI | 84 | ARG | 2.5 |
| 28 | BF | 124 | ARG | 2.5 |
| 42 | BU | 75 | ALA | 2.5 |
| 52 | DI | 95 | ASP | 2.5 |
| 9 | CJ | 76 | ILE | 2.5 |
| 25 | DC | 102 | TYR | 2.5 |
| 26 | BD | 29 | VAL | 2.5 |
| 11 | AL | 12 | ALA | 2.5 |
| 12 | AM | 72 | ILE | 2.5 |
| 37 | BP | 109 | ILE | 2.5 |
| 33 | BL | 6 | LEU | 2.5 |
| 24 | BV | 57 | TYR | 2.5 |
| 15 | AP | 67 | ILE | 2.5 |
| 7 | CH | 126 | CYS | 2.5 |
| 9 | CJ | 37 | ARG | 2.5 |
| 29 | DG | 41 | GLU | 2.5 |
| 33 | BL | 144 | GLU | 2.5 |
| 28 | BF | 103 | ILE | 2.5 |
| 26 | DD | 46 | ARG | 2.5 |
| 44 | BX | 37 | LEU | 2.5 |
| 16 | AQ | 75 | VAL | 2.5 |
| 39 | DR | 96 | VAL | 2.5 |
| 48 | B1 | 12 | SER | 2.5 |
| 12 | AM | 28 | ARG | 2.5 |
| 34 | DM | 59 | ARG | 2.5 |
| 8 | AI | 19 | PHE | 2.5 |
| 52 | DI | 81 | LYS | 2.5 |
| 17 | CR | 71 | ASP | 2.5 |
| 28 | BF | 56 | LEU | 2.5 |
| 48 | B1 | 17 | GLY | 2.5 |
| 36 | BO | 28 | VAL | 2.5 |
| 52 | BI | 21 | PRO | 2.5 |
| 4 | CE | 85 | LYS | 2.5 |
| 27 | BE | 23 | PHE | 2.5 |
| 6 | CG | 79 | VAL | 2.5 |
| 12 | AM | 4 | ALA | 2.5 |
| 28 | DF | 15 | LEU | 2.5 |
| 1 | CA | 1031 | C | 2.5 |
| 23 | BB | 1583 | A | 2.5 |
| 26 | DD | 35 | THR | 2.5 |
| 29 | BG | 168 | VAL | 2.5 |
| 4 | CE | 13 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | DD | 55 | LYS | 2.5 |
| 26 | BD | 101 | PHE | 2.5 |
| 3 | AD | 4 | LEU | 2.5 |
| 7 | AH | 99 | GLY | 2.5 |
| 12 | AM | 76 | ILE | 2.5 |
| 18 | AS | 39 | ILE | 2.5 |
| 20 | AB | 180 | ILE | 2.5 |
| 20 | CB | 217 | ALA | 2.5 |
| 25 | BC | 76 | VAL | 2.5 |
| 30 | BH | 111 | ALA | 2.5 |
| 33 | DL | 77 | ILE | 2.5 |
| 40 | DS | 107 | VAL | 2.5 |
| 48 | B1 | 48 | TYR | 2.5 |
| 9 | CJ | 89 | ARG | 2.5 |
| 27 | BE | 148 | ILE | 2.5 |
| 38 | BQ | 90 | ASP | 2.5 |
| 42 | BU | 49 | PRO | 2.5 |
| 46 | BZ | 6 | GLN | 2.5 |
| 8 | AI | 45 | MET | 2.5 |
| 28 | DF | 78 | ILE | 2.5 |
| 48 | D1 | 3 | GLY | 2.5 |
| 40 | DS | 75 | PHE | 2.5 |
| 27 | BE | 64 | GLY | 2.4 |
| 37 | BP | 46 | VAL | 2.4 |
| 28 | BF | 176 | PHE | 2.4 |
| 3 | AD | 24 | VAL | 2.4 |
| 29 | BG | 101 | VAL | 2.4 |
| 37 | DP | 114 | ASN | 2.4 |
| 1 | CA | 1534 | A | 2.4 |
| 3 | AD | 94 | GLU | 2.4 |
| 16 | AQ | 33 | TYR | 2.4 |
| 36 | BO | 99 | TYR | 2.4 |
| 39 | DR | 12 | HIS | 2.4 |
| 15 | AP | 35 | ARG | 2.4 |
| 37 | BP | 102 | ARG | 2.4 |
| 50 | B3 | 14 | LYS | 2.4 |
| 7 | AH | 13 | ILE | 2.4 |
| 8 | AI | 65 | THR | 2.4 |
| 43 | BW | 62 | ALA | 2.4 |
| 50 | D3 | 20 | GLY | 2.4 |
| 15 | AP | 51 | ARG | 2.4 |
| 40 | BS | 73 | LYS | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 26 | DD | 75 | ALA | 2.4 |
| 37 | BP | 48 | ALA | 2.4 |
| 9 | CJ | 66 | GLU | 2.4 |
| 2 | AC | 63 | ILE | 2.4 |
| 27 | DE | 181 | ILE | 2.4 |
| 34 | DM | 29 | GLY | 2.4 |
| 36 | DO | 2 | ASP | 2.4 |
| 35 | DN | 83 | LEU | 2.4 |
| 20 | CB | 82 | ALA | 2.4 |
| 29 | DG | 147 | LEU | 2.4 |
| 32 | DK | 17 | ARG | 2.4 |
| 28 | DF | 43 | ILE | 2.4 |
| 14 | AO | 42 | PHE | 2.4 |
| 21 | CU | 36 | PHE | 2.4 |
| 7 | CH | 127 | TYR | 2.4 |
| 8 | CI | 54 | VAL | 2.4 |
| 15 | AP | 66 | THR | 2.4 |
| 28 | BF | 117 | SER | 2.4 |
| 20 | CB | 15 | PHE | 2.4 |
| 29 | BG | 20 | GLY | 2.4 |
| 18 | AS | 18 | VAL | 2.4 |
| 18 | CS | 15 | LEU | 2.4 |
| 20 | CB | 131 | LYS | 2.4 |
| 26 | BD | 179 | ARG | 2.4 |
| 31 | DJ | 64 | VAL | 2.4 |
| 25 | BC | 22 | GLU | 2.4 |
| 42 | BU | 59 | GLU | 2.4 |
| 12 | AM | 87 | GLY | 2.4 |
| 18 | AS | 43 | MET | 2.4 |
| 32 | BK | 34 | GLY | 2.4 |
| 2 | CC | 130 | ARG | 2.4 |
| 15 | AP | 28 | ARG | 2.4 |
| 5 | AF | 7 | VAL | 2.4 |
| 29 | DG | 42 | VAL | 2.4 |
| 52 | BI | 60 | VAL | 2.4 |
| 5 | AF | 6 | ILE | 2.4 |
| 29 | DG | 113 | ASP | 2.4 |
| 48 | B1 | 33 | LEU | 2.4 |
| 4 | AE | 149 | PRO | 2.4 |
| 38 | DQ | 70 | GLN | 2.4 |
| 13 | CN | 29 | ILE | 2.4 |
| 20 | AB | 158 | ASP | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | BF | 112 | ASP | 2.4 |
| 31 | BJ | 123 | LYS | 2.4 |
| 52 | BI | 16 | MET | 2.4 |
| 34 | DM | 132 | THR | 2.4 |
| 35 | BN | 83 | LEU | 2.4 |
| 37 | BP | 24 | THR | 2.4 |
| 41 | DT | 69 | ARG | 2.4 |
| 8 | AI | 46 | VAL | 2.4 |
| 30 | DH | 18 | GLN | 2.4 |
| 5 | AF | 65 | GLU | 2.4 |
| 40 | DS | 4 | ILE | 2.4 |
| 5 | CF | 88 | MET | 2.4 |
| 20 | AB | 179 | GLY | 2.4 |
| 30 | BH | 116 | ARG | 2.4 |
| 47 | B0 | 1 | ALA | 2.4 |
| 2 | AC | 14 | VAL | 2.4 |
| 4 | CE | 115 | GLU | 2.4 |
| 52 | BI | 68 | PHE | 2.4 |
| 52 | DI | 96 | LYS | 2.4 |
| 23 | DB | 100 | U | 2.4 |
| 48 | B1 | 21 | THR | 2.4 |
| 29 | DG | 117 | PRO | 2.4 |
| 32 | DK | 39 | ILE | 2.4 |
| 52 | BI | 25 | PRO | 2.4 |
| 29 | BG | 9 | VAL | 2.4 |
| 6 | CG | 105 | GLU | 2.3 |
| 12 | AM | 38 | ILE | 2.3 |
| 28 | DF | 84 | ILE | 2.3 |
| 33 | DL | 144 | GLU | 2.3 |
| 7 | AH | 71 | VAL | 2.3 |
| 29 | BG | 161 | VAL | 2.3 |
| 36 | BO | 27 | VAL | 2.3 |
| 1 | CA | 1033 | G | 2.3 |
| 7 | AH | 44 | PHE | 2.3 |
| 8 | AI | 83 | THR | 2.3 |
| 20 | AB | 193 | ASP | 2.3 |
| 29 | BG | 33 | THR | 2.3 |
| 33 | DL | 135 | ILE | 2.3 |
| 37 | BP | 23 | ASP | 2.3 |
| 40 | BS | 78 | GLU | 2.3 |
| 25 | DC | 21 | PRO | 2.3 |
| 26 | DD | 76 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 28 | BF | 65 | LEU | 2.3 |
| 30 | DH | 27 | ARG | 2.3 |
| 3 | AD | 154 | VAL | 2.3 |
| 28 | BF | 64 | PRO | 2.3 |
| 28 | BF | 130 | GLY | 2.3 |
| 27 | BE | 119 | ILE | 2.3 |
| 20 | CB | 219 | THR | 2.3 |
| 25 | BC | 113 | ASP | 2.3 |
| 28 | BF | 134 | GLN | 2.3 |
| 41 | DT | 53 | VAL | 2.3 |
| 28 | BF | 172 | PHE | 2.3 |
| 41 | DT | 12 | ARG | 2.3 |
| 12 | AM | 47 | LEU | 2.3 |
| 20 | AB | 160 | LEU | 2.3 |
| 25 | BC | 78 | GLU | 2.3 |
| 8 | CI | 83 | THR | 2.3 |
| 41 | DT | 73 | ARG | 2.3 |
| 45 | BY | 33 | HIS | 2.3 |
| 2 | AC | 65 | VAL | 2.3 |
| 28 | BF | 102 | LEU | 2.3 |
| 32 | DK | 9 | ASN | 2.3 |
| 44 | BX | 14 | LEU | 2.3 |
| 3 | AD | 51 | GLY | 2.3 |
| 12 | AM | 36 | ALA | 2.3 |
| 6 | AG | 14 | ASP | 2.3 |
| 4 | CE | 140 | ILE | 2.3 |
| 7 | AH | 74 | ILE | 2.3 |
| 26 | BD | 8 | LYS | 2.3 |
| 29 | BG | 171 | LYS | 2.3 |
| 6 | AG | 76 | SER | 2.3 |
| 3 | CD | 24 | VAL | 2.3 |
| 26 | BD | 30 | GLU | 2.3 |
| 52 | DI | 49 | GLU | 2.3 |
| 48 | D1 | 15 | GLY | 2.3 |
| 6 | CG | 85 | GLN | 2.3 |
| 2 | AC | 89 | VAL | 2.3 |
| 20 | AB | 87 | ASP | 2.3 |
| 25 | DC | 59 | GLN | 2.3 |
| 7 | CH | 71 | VAL | 2.3 |
| 12 | CM | 42 | VAL | 2.3 |
| 48 | D1 | 16 | THR | 2.3 |
| 6 | AG | 11 | ILE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 7 | AH | 100 | ILE | 2.3 |
| 34 | DM | 102 | LEU | 2.3 |
| 34 | DM | 133 | LYS | 2.3 |
| 2 | CC | 180 | ASP | 2.3 |
| 8 | AI | 102 | PHE | 2.3 |
| 52 | BI | 41 | PHE | 2.3 |
| 5 | AF | 42 | TRP | 2.3 |
| 29 | BG | 45 | ALA | 2.3 |
| 24 | BV | 63 | ILE | 2.3 |
| 25 | BC | 94 | LEU | 2.3 |
| 29 | BG | 19 | ASN | 2.3 |
| 2 | CC | 106 | ARG | 2.3 |
| 4 | CE | 118 | GLY | 2.3 |
| 25 | BC | 101 | ARG | 2.3 |
| 52 | BI | 3 | LYS | 2.3 |
| 30 | DH | 19 | VAL | 2.3 |
| 25 | BC | 37 | SER | 2.3 |
| 20 | CB | 35 | ASN | 2.3 |
| 29 | BG | 37 | ASN | 2.3 |
| 4 | CE | 143 | LEU | 2.3 |
| 28 | DF | 155 | ILE | 2.3 |
| 39 | DR | 101 | ILE | 2.3 |
| 5 | AF | 96 | VAL | 2.3 |
| 14 | CO | 39 | GLN | 2.3 |
| 28 | DF | 29 | ARG | 2.3 |
| 35 | BN | 1 | MET | 2.3 |
| 36 | BO | 79 | ALA | 2.3 |
| 6 | AG | 83 | THR | 2.3 |
| 8 | AI | 18 | VAL | 2.3 |
| 28 | BF | 173 | ASP | 2.3 |
| 6 | AG | 4 | ARG | 2.2 |
| 25 | BC | 100 | ARG | 2.2 |
| 15 | CP | 80 | LYS | 2.2 |
| 40 | DS | 48 | LYS | 2.2 |
| 50 | D3 | 64 | ALA | 2.2 |
| 52 | DI | 44 | LYS | 2.2 |
| 27 | BE | 14 | VAL | 2.2 |
| 33 | BL | 125 | LEU | 2.2 |
| 34 | DM | 64 | TRP | 2.2 |
| 24 | BV | 56 | PHE | 2.2 |
| 32 | BK | 106 | GLU | 2.2 |
| 6 | AG | 19 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9 | AJ | 76 | ILE | 2.2 |
| 42 | BU | 11 | ILE | 2.2 |
| 5 | CF | 4 | TYR | 2.2 |
| 9 | CJ | 49 | PHE | 2.2 |
| 13 | CN | 23 | ARG | 2.2 |
| 20 | AB | 212 | TYR | 2.2 |
| 48 | B1 | 6 | GLU | 2.2 |
| 48 | B1 | 50 | GLU | 2.2 |
| 40 | DS | 12 | SER | 2.2 |
| 6 | CG | 4 | ARG | 2.2 |
| 13 | CN | 42 | ASN | 2.2 |
| 35 | BN | 94 | TYR | 2.2 |
| 26 | DD | 93 | GLY | 2.2 |
| 27 | BE | 7 | ASP | 2.2 |
| 34 | DM | 37 | GLY | 2.2 |
| 36 | BO | 89 | ASP | 2.2 |
| 43 | DW | 6 | GLY | 2.2 |
| 4 | CE | 146 | MET | 2.2 |
| 34 | DM | 41 | LEU | 2.2 |
| 5 | CF | 87 | SER | 2.2 |
| 12 | AM | 62 | PHE | 2.2 |
| 41 | DT | 51 | PHE | 2.2 |
| 33 | DL | 86 | GLU | 2.2 |
| 44 | BX | 13 | GLU | 2.2 |
| 12 | AM | 80 | MET | 2.2 |
| 27 | BE | 154 | ASP | 2.2 |
| 42 | DU | 69 | VAL | 2.2 |
| 51 | B4 | 7 | VAL | 2.2 |
| 25 | DC | 198 | GLU | 2.2 |
| 30 | BH | 114 | GLU | 2.2 |
| 20 | CB | 33 | ALA | 2.2 |
| 20 | CB | 48 | MET | 2.2 |
| 32 | BK | 13 | ASN | 2.2 |
| 37 | BP | 45 | VAL | 2.2 |
| 34 | BM | 103 | TYR | 2.2 |
| 6 | AG | 6 | ILE | 2.2 |
| 26 | BD | 163 | GLY | 2.2 |
| 13 | CN | 16 | ALA | 2.2 |
| 25 | BC | 181 | ARG | 2.2 |
| 15 | CP | 15 | PRO | 2.2 |
| 27 | BE | 116 | ASP | 2.2 |
| 41 | DT | 14 | PRO | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | BD | 5 | VAL | 2.2 |
| 18 | AS | 28 | LYS | 2.2 |
| 25 | BC | 75 | ALA | 2.2 |
| 42 | BU | 91 | LYS | 2.2 |
| 50 | B3 | 21 | PHE | 2.2 |
| 18 | AS | 26 | ASP | 2.2 |
| 23 | BB | 1731 | G | 2.2 |
| 8 | CI | 94 | ARG | 2.2 |
| 20 | CB | 39 | ILE | 2.2 |
| 32 | BK | 24 | VAL | 2.2 |
| 38 | DQ | 86 | SER | 2.2 |
| 52 | BI | 34 | ILE | 2.2 |
| 31 | BJ | 87 | ALA | 2.2 |
| 48 | B1 | 9 | LYS | 2.2 |
| 52 | DI | 132 | ALA | 2.2 |
| 29 | BG | 116 | LEU | 2.2 |
| 34 | BM | 129 | THR | 2.2 |
| 7 | CH | 124 | ILE | 2.2 |
| 18 | AS | 59 | VAL | 2.2 |
| 44 | BX | 17 | GLU | 2.2 |
| 20 | AB | 75 | ALA | 2.2 |
| 31 | DJ | 4 | PHE | 2.2 |
| 46 | DZ | 77 | LYS | 2.2 |
| 11 | AL | 86 | VAL | 2.2 |
| 13 | AN | 93 | PRO | 2.2 |
| 2 | CC | 107 | LYS | 2.2 |
| 2 | CC | 203 | LYS | 2.2 |
| 7 | CH | 122 | GLY | 2.2 |
| 25 | DC | 90 | ILE | 2.2 |
| 48 | B1 | 22 | THR | 2.2 |
| 36 | BO | 77 | ALA | 2.2 |
| 36 | BO | 95 | SER | 2.2 |
| 36 | BO | 107 | ALA | 2.2 |
| 2 | CC | 199 | VAL | 2.2 |
| 25 | DC | 94 | LEU | 2.2 |
| 20 | CB | 59 | ILE | 2.2 |
| 15 | AP | 55 | ASP | 2.2 |
| 25 | BC | 36 | ASN | 2.2 |
| 29 | BG | 148 | ARG | 2.2 |
| 33 | DL | 124 | GLY | 2.2 |
| 37 | DP | 23 | ASP | 2.2 |
| 2 | CC | 186 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 31 | DJ | 20 | ALA | 2.2 |
| 40 | DS | 108 | SER | 2.2 |
| 8 | CI | 128 | LYS | 2.2 |
| 13 | AN | 40 | ARG | 2.2 |
| 25 | DC | 33 | LEU | 2.2 |
| 28 | BF | 114 | ARG | 2.2 |
| 30 | BH | 102 | ALA | 2.2 |
| 34 | DM | 136 | MET | 2.2 |
| 35 | BN | 25 | ALA | 2.2 |
| 1 | CA | 461 | A | 2.2 |
| 16 | AQ | 42 | LYS | 2.2 |
| 20 | CB | 147 | LEU | 2.2 |
| 20 | AB | 194 | GLY | 2.2 |
| 20 | AB | 199 | ILE | 2.2 |
| 34 | DM | 32 | GLY | 2.2 |
| 11 | CL | 122 | LYS | 2.2 |
| 37 | BP | 28 | LYS | 2.2 |
| 30 | DH | 80 | ILE | 2.2 |
| 8 | AI | 101 | GLY | 2.1 |
| 52 | BI | 53 | PRO | 2.1 |
| 25 | DC | 19 | VAL | 2.1 |
| 25 | DC | 62 | ARG | 2.1 |
| 32 | BK | 14 | SER | 2.1 |
| 33 | DL | 90 | VAL | 2.1 |
| 39 | DR | 24 | LYS | 2.1 |
| 2 | AC | 67 | ILE | 2.1 |
| 28 | BF | 96 | TRP | 2.1 |
| 30 | BH | 143 | ILE | 2.1 |
| 32 | DK | 38 | ILE | 2.1 |
| 12 | AM | 1 | ALA | 2.1 |
| 2 | AC | 88 | LYS | 2.1 |
| 4 | CE | 114 | LEU | 2.1 |
| 9 | AJ | 74 | VAL | 2.1 |
| 11 | AL | 15 | VAL | 2.1 |
| 19 | AT | 19 | HIS | 2.1 |
| 26 | DD | 203 | VAL | 2.1 |
| 28 | DF | 160 | LYS | 2.1 |
| 2 | CC | 181 | ILE | 2.1 |
| 4 | CE | 31 | SER | 2.1 |
| 26 | DD | 183 | GLU | 2.1 |
| 7 | CH | 9 | MET | 2.1 |
| 36 | BO | 113 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | DL | 125 | LEU | 2.1 |
| 10 | CK | 58 | THR | 2.1 |
| 11 | AL | 61 | GLU | 2.1 |
| 18 | AS | 63 | ASP | 2.1 |
| 28 | BF | 120 | SER | 2.1 |
| 34 | DM | 126 | ILE | 2.1 |
| 47 | B0 | 42 | ILE | 2.1 |
| 23 | BB | 1537 | G | 2.1 |
| 30 | BH | 92 | GLY | 2.1 |
| 21 | CU | 24 | LYS | 2.1 |
| 32 | DK | 18 | ARG | 2.1 |
| 37 | BP | 80 | VAL | 2.1 |
| 32 | BK | 39 | ILE | 2.1 |
| 48 | B1 | 8 | ILE | 2.1 |
| 8 | CI | 58 | GLU | 2.1 |
| 28 | BF | 71 | LYS | 2.1 |
| 30 | BH | 81 | ALA | 2.1 |
| 32 | BK | 59 | LYS | 2.1 |
| 37 | BP | 57 | ALA | 2.1 |
| 27 | DE | 175 | ILE | 2.1 |
| 40 | BS | 103 | ILE | 2.1 |
| 48 | D1 | 8 | ILE | 2.1 |
| 39 | BR | 46 | GLU | 2.1 |
| 42 | BU | 9 | GLU | 2.1 |
| 20 | CB | 76 | SER | 2.1 |
| 27 | BE | 65 | THR | 2.1 |
| 29 | BG | 24 | THR | 2.1 |
| 11 | AL | 92 | VAL | 2.1 |
| 42 | BU | 12 | VAL | 2.1 |
| 7 | AH | 127 | TYR | 2.1 |
| 15 | AP | 33 | ILE | 2.1 |
| 24 | DV | 91 | PHE | 2.1 |
| 31 | BJ | 119 | PHE | 2.1 |
| 11 | AL | 17 | LYS | 2.1 |
| 13 | AN | 90 | GLY | 2.1 |
| 30 | BH | 126 | GLY | 2.1 |
| 44 | BX | 60 | LYS | 2.1 |
| 2 | AC | 152 | VAL | 2.1 |
| 3 | AD | 35 | GLN | 2.1 |
| 6 | CG | 104 | VAL | 2.1 |
| 16 | AQ | 7 | LEU | 2.1 |
| 35 | BN | 17 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | CE | 147 | ASN | 2.1 |
| 9 | AJ | 100 | ILE | 2.1 |
| 28 | DF | 127 | TYR | 2.1 |
| 8 | CI | 93 | LEU | 2.1 |
| 9 | AJ | 62 | ARG | 2.1 |
| 26 | BD | 3 | GLY | 2.1 |
| 15 | AP | 20 | VAL | 2.1 |
| 20 | CB | 26 | MET | 2.1 |
| 23 | DB | 2799 | A | 2.1 |
| 34 | DM | 31 | PHE | 2.1 |
| 39 | BR | 77 | PHE | 2.1 |
| 1 | AA | 87 | C | 2.1 |
| 11 | AL | 29 | LYS | 2.1 |
| 28 | DF | 164 | GLU | 2.1 |
| 39 | BR | 73 | LYS | 2.1 |
| 11 | AL | 85 | ARG | 2.1 |
| 42 | BU | 83 | GLY | 2.1 |
| 44 | DX | 17 | GLU | 2.1 |
| 47 | D0 | 26 | SER | 2.1 |
| 3 | CD | 54 | LEU | 2.1 |
| 18 | AS | 66 | VAL | 2.1 |
| 32 | BK | 3 | GLN | 2.1 |
| 36 | BO | 36 | TYR | 2.1 |
| 6 | AG | 87 | PRO | 2.1 |
| 15 | AP | 23 | ASP | 2.1 |
| 28 | BF | 141 | ASP | 2.1 |
| 2 | CC | 156 | LEU | 2.1 |
| 20 | CB | 214 | GLY | 2.1 |
| 25 | DC | 93 | VAL | 2.1 |
| 32 | BK | 52 | VAL | 2.1 |
| 52 | DI | 138 | VAL | 2.1 |
| 26 | BD | 209 | ALA | 2.1 |
| 32 | BK | 7 | MET | 2.1 |
| 32 | DK | 60 | ALA | 2.1 |
| 7 | CH | 125 | ILE | 2.1 |
| 43 | DW | 43 | LYS | 2.1 |
| 44 | DX | 36 | GLN | 2.1 |
| 28 | BF | 162 | ASP | 2.1 |
| 35 | BN | 120 | GLU | 2.1 |
| 39 | BR | 95 | ASP | 2.1 |
| 40 | BS | 104 | THR | 2.1 |
| 44 | BX | 7 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 25 | BC | 92 | LEU | 2.1 |
| 2 | CC | 70 | ALA | 2.1 |
| 5 | AF | 90 | MET | 2.1 |
| 32 | DK | 33 | ALA | 2.1 |
| 16 | AQ | 24 | ILE | 2.1 |
| 21 | AU | 3 | ILE | 2.1 |
| 28 | BF | 21 | TYR | 2.1 |
| 37 | BP | 98 | TYR | 2.1 |
| 40 | DS | 70 | LYS | 2.1 |
| 4 | AE | 92 | ARG | 2.1 |
| 11 | AL | 18 | SER | 2.1 |
| 18 | AS | 58 | PRO | 2.1 |
| 32 | BK | 76 | VAL | 2.1 |
| 3 | AD | 176 | LYS | 2.1 |
| 36 | BO | 87 | ILE | 2.1 |
| 39 | DR | 73 | LYS | 2.1 |
| 24 | DV | 56 | PHE | 2.1 |
| 25 | BC | 126 | GLY | 2.1 |
| 34 | DM | 108 | VAL | 2.1 |
| 42 | BU | 51 | LEU | 2.1 |
| 9 | AJ | 34 | ALA | 2.1 |
| 33 | DL | 101 | ILE | 2.1 |
| 20 | AB | 195 | VAL | 2.1 |
| 32 | BK | 85 | VAL | 2.1 |
| 3 | AD | 175 | GLY | 2.1 |
| 38 | BQ | 17 | LEU | 2.1 |
| 44 | BX | 57 | LEU | 2.1 |
| 46 | BZ | 49 | LEU | 2.1 |
| 42 | BU | 90 | LYS | 2.0 |
| 18 | AS | 38 | THR | 2.0 |
| 40 | DS | 32 | ALA | 2.0 |
| 45 | DY | 1 | ALA | 2.0 |
| 11 | AL | 19 | ASN | 2.0 |
| 11 | AL | 58 | ASN | 2.0 |
| 38 | BQ | 108 | LEU | 2.0 |
| 3 | AD | 57 | LYS | 2.0 |
| 32 | BK | 112 | PHE | 2.0 |
| 50 | B3 | 20 | GLY | 2.0 |
| 33 | BL | 77 | ILE | 2.0 |
| 47 | B0 | 55 | ALA | 2.0 |
| 9 | CJ | 65 | TYR | 2.0 |
| 20 | CB | 210 | THR | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | CE | 35 | LEU | 2.0 |
| 20 | CB | 32 | GLY | 2.0 |
| 33 | DL | 107 | PHE | 2.0 |
| 42 | BU | 89 | GLY | 2.0 |
| 25 | BC | 172 | THR | 2.0 |
| 24 | BV | 91 | PHE | 2.0 |
| 26 | BD | 118 | PHE | 2.0 |
| 3 | CD | 195 | ASN | 2.0 |
| 35 | BN | 52 | ILE | 2.0 |
| 40 | DS | 74 | ILE | 2.0 |
| 42 | DU | 49 | PRO | 2.0 |
| 52 | DI | 116 | MET | 2.0 |
| 28 | DF | 12 | VAL | 2.0 |
| 36 | BO | 29 | HIS | 2.0 |
| 32 | BK | 100 | PHE | 2.0 |
| 32 | BK | 111 | LYS | 2.0 |
| 21 | CU | 12 | ASP | 2.0 |
| 50 | D3 | 53 | ASP | 2.0 |
| 23 | BB | 1730 | C | 2.0 |
| 28 | BF | 155 | ILE | 2.0 |
| 46 | BZ | 74 | ARG | 2.0 |
| 10 | AK | 88 | PRO | 2.0 |
| 20 | CB | 197 | PHE | 2.0 |
| 27 | DE | 180 | LEU | 2.0 |
| 38 | BQ | 13 | HIS | 2.0 |
| 23 | BB | 654 | A | 2.0 |
| 23 | BB | 1067 | A | 2.0 |
| 25 | BC | 132 | ARG | 2.0 |
| 36 | BO | 25 | ARG | 2.0 |
| 49 | D2 | 29 | GLN | 2.0 |
| 25 | BC | 61 | TYR | 2.0 |
| 33 | DL | 58 | TYR | 2.0 |
| 18 | CS | 40 | PHE | 2.0 |
| 48 | D1 | 33 | LEU | 2.0 |
| 3 | AD | 159 | GLU | 2.0 |
| 25 | BC | 167 | ASP | 2.0 |
| 26 | BD | 200 | ASP | 2.0 |
| 2 | AC | 203 | LYS | 2.0 |
| 6 | CG | 153 | TYR | 2.0 |
| 25 | BC | 110 | LYS | 2.0 |
| 26 | BD | 109 | VAL | 2.0 |
| 27 | BE | 153 | LEU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 32 | BK | 63 | VAL | 2.0 |
| 50 | D3 | 9 | ALA | 2.0 |
| 39 | BR | 35 | PHE | 2.0 |
| 27 | DE | 122 | GLU | 2.0 |
| 42 | BU | 36 | GLU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | BB | 3042 | 1/1 | 0.13 | 0.10 | 168,168,168,168 | 0 |
| 53 | MG | AA | 2023 | 1/1 | 0.54 | 0.36 | 66,66,66,66 | 1 |
| 53 | MG | AA | 2037 | 1/1 | 0.58 | 0.33 | 138,138,138,138 | 0 |
| 53 | MG | AA | 2057 | 1/1 | 0.62 | 0.17 | 141,141,141,141 | 0 |
| 53 | MG | CA | 2011 | 1/1 | 0.65 | 0.28 | 132,132,132,132 | 0 |
| 53 | MG | CA | 2015 | 1/1 | 0.68 | 0.10 | 149,149,149,149 | 0 |
| 53 | MG | AA | 2014 | 1/1 | 0.68 | 0.22 | 112,112,112,112 | 0 |
| 53 | MG | CA | 2027 | 1/1 | 0.69 | 0.13 | 50,50,50,50 | 1 |
| 53 | MG | DB | 3060 | 1/1 | 0.71 | 0.20 | 112,112,112,112 | 0 |
| 53 | MG | BB | 3100 | 1/1 | 0.72 | 0.20 | 129,129,129,129 | 0 |
| 53 | MG | AN | 201 | 1/1 | 0.72 | 0.12 | 69,69,69,69 | 0 |
| 53 | MG | AA | 2031 | 1/1 | 0.74 | 0.09 | 58,58,58,58 | 0 |
| 53 | MG | AA | 2047 | 1/1 | 0.74 | 0.04 | 100,100,100,100 | 0 |
| 53 | MG | AA | 2008 | 1/1 | 0.76 | 0.08 | 125,125,125,125 | 0 |
| 53 | MG | AA | 2019 | 1/1 | 0.78 | 0.06 | 107,107,107,107 | 0 |
| 53 | MG | CA | 2059 | 1/1 | 0.78 | 0.12 | 94,94,94,94 | 0 |
| 53 | MG | AA | 2033 | 1/1 | 0.79 | 0.11 | 99,99,99,99 | 0 |
| 53 | MG | CA | 2021 | 1/1 | 0.79 | 0.36 | 125,125,125,125 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | AA | 2056 | 1/1 | 0.79 | 0.12 | 124,124,124,124 | 0 |
| 53 | MG | CA | 2023 | 1/1 | 0.79 | 0.20 | 137,137,137,137 | 0 |
| 53 | MG | DB | 3066 | 1/1 | 0.80 | 0.08 | 146,146,146,146 | 0 |
| 53 | MG | DB | 3059 | 1/1 | 0.80 | 0.12 | 180,180,180,180 | 0 |
| 53 | MG | CA | 2057 | 1/1 | 0.80 | 0.09 | 99,99,99,99 | 0 |
| 53 | MG | AE | 201 | 1/1 | 0.80 | 0.07 | 144,144,144,144 | 0 |
| 53 | MG | AA | 2012 | 1/1 | 0.81 | 0.09 | 84,84,84,84 | 0 |
| 53 | MG | CA | 2060 | 1/1 | 0.81 | 0.05 | 80,80,80,80 | 0 |
| 53 | MG | AA | 2018 | 1/1 | 0.81 | 0.09 | 131,131,131,131 | 0 |
| 53 | MG | BB | 3080 | 1/1 | 0.81 | 0.18 | 39,39,39,39 | 0 |
| 53 | MG | BB | 3010 | 1/1 | 0.82 | 0.10 | 44,44,44,44 | 0 |
| 53 | MG | AA | 2005 | 1/1 | 0.82 | 0.08 | 69,69,69,69 | 0 |
| 53 | MG | CA | 2026 | 1/1 | 0.83 | 0.20 | 26,26,26,26 | 1 |
| 53 | MG | AA | 2055 | 1/1 | 0.83 | 0.20 | 102,102,102,102 | 0 |
| 53 | MG | CA | 2008 | 1/1 | 0.83 | 0.09 | 93,93,93,93 | 0 |
| 53 | MG | AA | 2035 | 1/1 | 0.83 | 0.34 | 137,137,137,137 | 0 |
| 53 | MG | CA | 2038 | 1/1 | 0.83 | 0.12 | 128,128,128,128 | 0 |
| 53 | MG | BB | 3099 | 1/1 | 0.85 | 0.17 | 40,40,40,40 | 0 |
| 53 | MG | BB | 3081 | 1/1 | 0.86 | 0.22 | 46,46,46,46 | 0 |
| 53 | MG | CE | 201 | 1/1 | 0.86 | 0.15 | 127,127,127,127 | 0 |
| 53 | MG | BB | 3037 | 1/1 | 0.86 | 0.11 | 23,23,23,23 | 0 |
| 53 | MG | AA | 2050 | 1/1 | 0.87 | 0.14 | 105,105,105,105 | 0 |
| 53 | MG | DB | 3045 | 1/1 | 0.87 | 0.06 | 57,57,57,57 | 0 |
| 53 | MG | AA | 2013 | 1/1 | 0.87 | 0.12 | 122,122,122,122 | 0 |
| 53 | MG | DB | 3095 | 1/1 | 0.87 | 0.15 | 89,89,89,89 | 0 |
| 53 | MG | CA | 2042 | 1/1 | 0.87 | 0.08 | 58,58,58,58 | 0 |
| 53 | MG | AA | 2024 | 1/1 | 0.87 | 0.08 | 5,5,5,5 | 1 |
| 53 | MG | BB | 3097 | 1/1 | 0.88 | 0.18 | 114,114,114,114 | 0 |
| 53 | MG | AA | 2044 | 1/1 | 0.88 | 0.12 | 112,112,112,112 | 0 |
| 53 | MG | BB | 3077 | 1/1 | 0.88 | 0.09 | 36,36,36,36 | 0 |
| 53 | MG | DB | 3013 | 1/1 | 0.88 | 0.17 | 51,51,51,51 | 0 |
| 53 | MG | DB | 3090 | 1/1 | 0.88 | 0.08 | 37,37,37,37 | 0 |
| 53 | MG | AA | 2026 | 1/1 | 0.89 | 0.08 | 65,65,65,65 | 0 |
| 53 | MG | BB | 3017 | 1/1 | 0.90 | 0.14 | 34,34,34,34 | 0 |
| 54 | HYG | AA | 2059 | 36/36 | 0.90 | 0.24 | 52,52,52,52 | 0 |
| 53 | MG | DB | 3023 | 1/1 | 0.90 | 0.08 | 32,32,32,32 | 0 |
| 53 | MG | CA | 2052 | 1/1 | 0.90 | 0.09 | 73,73,73,73 | 0 |
| 53 | MG | DB | 3029 | 1/1 | 0.90 | 0.16 | 88,88,88,88 | 0 |
| 53 | MG | CA | 2035 | 1/1 | 0.90 | 0.08 | 89,89,89,89 | 0 |
| 53 | MG | BB | 3071 | 1/1 | 0.90 | 0.09 | 26,26,26,26 | 0 |
| 53 | MG | CA | 2029 | 1/1 | 0.90 | 0.05 | 23,23,23,23 | 1 |
| 53 | MG | CA | 2014 | 1/1 | 0.90 | 0.07 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | BB | 3052 | 1/1 | 0.90 | 0.08 | 38,38,38,38 | 0 |
| 53 | MG | AA | 2030 | 1/1 | 0.90 | 0.09 | 99,99,99,99 | 0 |
| 53 | MG | CA | 2054 | 1/1 | 0.90 | 0.08 | 104,104,104,104 | 0 |
| 53 | MG | DB | 3036 | 1/1 | 0.91 | 0.09 | 30,30,30,30 | 0 |
| 53 | MG | AA | 2049 | 1/1 | 0.91 | 0.06 | 75,75,75,75 | 0 |
| 54 | HYG | CA | 2062 | 36/36 | 0.91 | 0.22 | 45,45,45,45 | 0 |
| 53 | MG | AA | 2017 | 1/1 | 0.91 | 0.12 | 87,87,87,87 | 0 |
| 53 | MG | CA | 2007 | 1/1 | 0.91 | 0.04 | 46,46,46,46 | 0 |
| 53 | MG | AA | 2051 | 1/1 | 0.91 | 0.10 | 41,41,41,41 | 0 |
| 53 | MG | AA | 2052 | 1/1 | 0.91 | 0.07 | 78,78,78,78 | 0 |
| 53 | MG | BB | 3014 | 1/1 | 0.91 | 0.05 | 50,50,50,50 | 0 |
| 53 | MG | BB | 3104 | 1/1 | 0.91 | 0.18 | 36,36,36,36 | 0 |
| 53 | MG | DB | 3092 | 1/1 | 0.91 | 0.13 | 66,66,66,66 | 0 |
| 53 | MG | DB | 3050 | 1/1 | 0.92 | 0.08 | 90,90,90,90 | 0 |
| 53 | MG | BB | 3048 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 53 | MG | BB | 3051 | 1/1 | 0.92 | 0.14 | 35,35,35,35 | 0 |
| 53 | MG | AA | 2045 | 1/1 | 0.92 | 0.64 | 92,92,92,92 | 0 |
| 53 | MG | AA | 2021 | 1/1 | 0.92 | 0.31 | 5,5,5,5 | 1 |
| 53 | MG | AA | 2004 | 1/1 | 0.92 | 0.14 | 56,56,56,56 | 0 |
| 53 | MG | CA | 2028 | 1/1 | 0.93 | 0.07 | 75,75,75,75 | 0 |
| 53 | MG | BB | 3032 | 1/1 | 0.93 | 0.10 | 56,56,56,56 | 0 |
| 53 | MG | BB | 3049 | 1/1 | 0.93 | 0.10 | 10,10,10,10 | 0 |
| 53 | MG | AA | 2046 | 1/1 | 0.93 | 0.07 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3024 | 1/1 | 0.93 | 0.11 | 15,15,15,15 | 0 |
| 53 | MG | BB | 3093 | 1/1 | 0.93 | 0.24 | 71,71,71,71 | 0 |
| 53 | MG | DB | 3044 | 1/1 | 0.93 | 0.11 | 24,24,24,24 | 0 |
| 53 | MG | BB | 3053 | 1/1 | 0.93 | 0.06 | 28,28,28,28 | 0 |
| 53 | MG | AA | 2001 | 1/1 | 0.93 | 0.07 | 35,35,35,35 | 0 |
| 53 | MG | DB | 3058 | 1/1 | 0.93 | 0.33 | 151,151,151,151 | 0 |
| 53 | MG | CA | 2037 | 1/1 | 0.93 | 0.08 | 94,94,94,94 | 0 |
| 53 | MG | AA | 2016 | 1/1 | 0.93 | 0.09 | 89,89,89,89 | 0 |
| 53 | MG | BB | 3033 | 1/1 | 0.93 | 0.33 | 125,125,125,125 | 0 |
| 53 | MG | BB | 3046 | 1/1 | 0.93 | 0.11 | 22,22,22,22 | 0 |
| 53 | MG | AA | 2015 | 1/1 | 0.93 | 0.06 | 24,24,24,24 | 0 |
| 53 | MG | AA | 2054 | 1/1 | 0.93 | 0.08 | 110,110,110,110 | 0 |
| 53 | MG | BB | 3085 | 1/1 | 0.93 | 0.17 | 103,103,103,103 | 0 |
| 53 | MG | BB | 3031 | 1/1 | 0.93 | 0.14 | 41,41,41,41 | 0 |
| 53 | MG | AA | 2032 | 1/1 | 0.93 | 0.08 | 62,62,62,62 | 0 |
| 53 | MG | BB | 3054 | 1/1 | 0.93 | 0.06 | 77,77,77,77 | 0 |
| 53 | MG | BB | 3020 | 1/1 | 0.94 | 0.10 | 26,26,26,26 | 0 |
| 53 | MG | CA | 2058 | 1/1 | 0.94 | 0.11 | 106,106,106,106 | 0 |
| 53 | MG | BB | 3055 | 1/1 | 0.94 | 0.15 | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | CA | 2033 | 1/1 | 0.94 | 0.15 | 56,56,56,56 | 0 |
| 53 | MG | DB | 3015 | 1/1 | 0.94 | 0.07 | 33,33,33,33 | 0 |
| 53 | MG | BB | 3039 | 1/1 | 0.94 | 0.18 | 7,7,7,7 | 0 |
| 53 | MG | CA | 2010 | 1/1 | 0.94 | 0.08 | 33,33,33,33 | 0 |
| 53 | MG | CA | 2024 | 1/1 | 0.94 | 0.06 | 29,29,29,29 | 0 |
| 53 | MG | BB | 3057 | 1/1 | 0.94 | 0.19 | 28,28,28,28 | 0 |
| 53 | MG | DB | 3052 | 1/1 | 0.94 | 0.12 | 100,100,100,100 | 0 |
| 53 | MG | BB | 3027 | 1/1 | 0.94 | 0.08 | 33,33,33,33 | 0 |
| 53 | MG | CA | 2036 | 1/1 | 0.94 | 0.17 | 101,101,101,101 | 0 |
| 53 | MG | AA | 2002 | 1/1 | 0.94 | 0.06 | 99,99,99,99 | 0 |
| 53 | MG | CA | 2019 | 1/1 | 0.94 | 0.10 | 73,73,73,73 | 0 |
| 53 | MG | BB | 3001 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 53 | MG | DB | 3097 | 1/1 | 0.95 | 0.14 | 38,38,38,38 | 0 |
| 53 | MG | DB | 3046 | 1/1 | 0.95 | 0.09 | 24,24,24,24 | 0 |
| 53 | MG | CA | 2049 | 1/1 | 0.95 | 0.06 | 74,74,74,74 | 0 |
| 53 | MG | AA | 2025 | 1/1 | 0.95 | 0.17 | 58,58,58,58 | 0 |
| 53 | MG | CA | 2016 | 1/1 | 0.95 | 0.04 | 53,53,53,53 | 0 |
| 53 | MG | DB | 3035 | 1/1 | 0.95 | 0.06 | 55,55,55,55 | 0 |
| 53 | MG | AA | 2022 | 1/1 | 0.95 | 0.07 | 82,82,82,82 | 0 |
| 53 | MG | BB | 3083 | 1/1 | 0.95 | 0.22 | 12,12,12,12 | 0 |
| 53 | MG | DB | 3041 | 1/1 | 0.95 | 0.11 | 29,29,29,29 | 0 |
| 53 | MG | DB | 3072 | 1/1 | 0.95 | 0.12 | 18,18,18,18 | 0 |
| 53 | MG | CA | 2009 | 1/1 | 0.95 | 0.06 | 67,67,67,67 | 0 |
| 53 | MG | DB | 3005 | 1/1 | 0.95 | 0.12 | 10,10,10,10 | 0 |
| 53 | MG | BB | 3063 | 1/1 | 0.95 | 0.09 | 11,11,11,11 | 0 |
| 53 | MG | DB | 3074 | 1/1 | 0.95 | 0.09 | 12,12,12,12 | 0 |
| 53 | MG | BB | 3102 | 1/1 | 0.95 | 0.12 | 20,20,20,20 | 0 |
| 53 | MG | CA | 2047 | 1/1 | 0.95 | 0.06 | 121,121,121,121 | 0 |
| 53 | MG | AA | 2029 | 1/1 | 0.95 | 0.06 | 39,39,39,39 | 0 |
| 53 | MG | BB | 3088 | 1/1 | 0.95 | 0.06 | 28,28,28,28 | 0 |
| 53 | MG | BB | 3045 | 1/1 | 0.95 | 0.10 | 31,31,31,31 | 0 |
| 53 | MG | DB | 3073 | 1/1 | 0.95 | 0.10 | 14,14,14,14 | 0 |
| 53 | MG | BB | 3008 | 1/1 | 0.95 | 0.10 | 89,89,89,89 | 0 |
| 53 | MG | BB | 3047 | 1/1 | 0.95 | 0.06 | 75,75,75,75 | 0 |
| 53 | MG | AA | 2028 | 1/1 | 0.95 | 0.17 | 100,100,100,100 | 0 |
| 53 | MG | AA | 2007 | 1/1 | 0.95 | 0.06 | 31,31,31,31 | 0 |
| 53 | MG | CA | 2043 | 1/1 | 0.95 | 0.04 | 19,19,19,19 | 0 |
| 53 | MG | DB | 3110 | 1/1 | 0.95 | 0.14 | 21,21,21,21 | 0 |
| 53 | MG | DB | 3080 | 1/1 | 0.95 | 0.10 | 10,10,10,10 | 0 |
| 53 | MG | BB | 3061 | 1/1 | 0.95 | 0.04 | 48,48,48,48 | 0 |
| 53 | MG | BB | 3064 | 1/1 | 0.95 | 0.08 | 35,35,35,35 | 0 |
| 53 | MG | BB | 3036 | 1/1 | 0.95 | 0.11 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | AA | 2006 | 1/1 | 0.95 | 0.03 | 60,60,60,60 | 0 |
| 53 | MG | DB | 3003 | 1/1 | 0.96 | 0.19 | 63,63,63,63 | 0 |
| 53 | MG | BB | 3016 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 53 | MG | CA | 2048 | 1/1 | 0.96 | 0.11 | 58,58,58,58 | 0 |
| 53 | MG | CA | 2040 | 1/1 | 0.96 | 0.09 | 48,48,48,48 | 0 |
| 53 | MG | BB | 3068 | 1/1 | 0.96 | 0.12 | 53,53,53,53 | 0 |
| 53 | MG | DB | 3108 | 1/1 | 0.96 | 0.09 | 37,37,37,37 | 0 |
| 53 | MG | AA | 2042 | 1/1 | 0.96 | 0.09 | 69,69,69,69 | 0 |
| 53 | MG | AA | 2039 | 1/1 | 0.96 | 0.12 | 64,64,64,64 | 0 |
| 53 | MG | CA | 2044 | 1/1 | 0.96 | 0.07 | 59,59,59,59 | 0 |
| 53 | MG | AA | 2048 | 1/1 | 0.96 | 0.03 | 99,99,99,99 | 0 |
| 53 | MG | AA | 2009 | 1/1 | 0.96 | 0.10 | 7,7,7,7 | 0 |
| 53 | MG | DB | 3026 | 1/1 | 0.96 | 0.08 | 34,34,34,34 | 0 |
| 53 | MG | DB | 3071 | 1/1 | 0.96 | 0.06 | 16,16,16,16 | 0 |
| 53 | MG | DB | 3032 | 1/1 | 0.96 | 0.09 | 63,63,63,63 | 0 |
| 53 | MG | BB | 3078 | 1/1 | 0.96 | 0.15 | 70,70,70,70 | 0 |
| 53 | MG | DB | 3057 | 1/1 | 0.96 | 0.06 | 71,71,71,71 | 0 |
| 53 | MG | BB | 3098 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 53 | MG | BB | 3038 | 1/1 | 0.96 | 0.03 | 71,71,71,71 | 0 |
| 53 | MG | DB | 3021 | 1/1 | 0.96 | 0.23 | 11,11,11,11 | 0 |
| 53 | MG | DB | 3111 | 1/1 | 0.96 | 0.09 | 38,38,38,38 | 0 |
| 53 | MG | BB | 3034 | 1/1 | 0.96 | 0.10 | 35,35,35,35 | 0 |
| 53 | MG | CA | 2020 | 1/1 | 0.96 | 0.21 | 73,73,73,73 | 0 |
| 53 | MG | DB | 3047 | 1/1 | 0.96 | 0.17 | 14,14,14,14 | 0 |
| 53 | MG | BB | 3087 | 1/1 | 0.96 | 0.16 | 57,57,57,57 | 0 |
| 53 | MG | AA | 2041 | 1/1 | 0.96 | 0.07 | 83,83,83,83 | 0 |
| 53 | MG | DB | 3011 | 1/1 | 0.96 | 0.16 | 17,17,17,17 | 0 |
| 53 | MG | BB | 3003 | 1/1 | 0.96 | 0.07 | 32,32,32,32 | 0 |
| 53 | MG | CA | 2025 | 1/1 | 0.96 | 0.12 | 50,50,50,50 | 0 |
| 53 | MG | BB | 3021 | 1/1 | 0.96 | 0.08 | 30,30,30,30 | 0 |
| 53 | MG | DB | 3093 | 1/1 | 0.96 | 0.22 | 11,11,11,11 | 0 |
| 53 | MG | BB | 3056 | 1/1 | 0.96 | 0.08 | 26,26,26,26 | 0 |
| 53 | MG | DB | 3034 | 1/1 | 0.96 | 0.16 | 52,52,52,52 | 0 |
| 53 | MG | CA | 2041 | 1/1 | 0.96 | 0.05 | 46,46,46,46 | 0 |
| 53 | MG | DB | 3054 | 1/1 | 0.96 | 0.04 | 19,19,19,19 | 0 |
| 53 | MG | BB | 3109 | 1/1 | 0.96 | 0.09 | 54,54,54,54 | 0 |
| 53 | MG | AA | 2038 | 1/1 | 0.96 | 0.11 | 71,71,71,71 | 0 |
| 53 | MG | AA | 2058 | 1/1 | 0.96 | 0.14 | 86,86,86,86 | 0 |
| 53 | MG | BB | 3082 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 53 | MG | AA | 2011 | 1/1 | 0.97 | 0.07 | 85,85,85,85 | 0 |
| 53 | MG | DB | 3025 | 1/1 | 0.97 | 0.15 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3075 | 1/1 | 0.97 | 0.21 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | CA | 2005 | 1/1 | 0.97 | 0.09 | 24,24,24,24 | 0 |
| 53 | MG | AA | 2040 | 1/1 | 0.97 | 0.10 | 83,83,83,83 | 0 |
| 53 | MG | DB | 3070 | 1/1 | 0.97 | 0.08 | 45,45,45,45 | 0 |
| 53 | MG | CA | 2034 | 1/1 | 0.97 | 0.11 | 6,6,6,6 | 0 |
| 53 | MG | BB | 3029 | 1/1 | 0.97 | 0.07 | 14,14,14,14 | 0 |
| 53 | MG | DB | 3103 | 1/1 | 0.97 | 0.13 | 27,27,27,27 | 0 |
| 53 | MG | DB | 3105 | 1/1 | 0.97 | 0.14 | 23,23,23,23 | 0 |
| 53 | MG | BB | 3062 | 1/1 | 0.97 | 0.17 | 14,14,14,14 | 0 |
| 53 | MG | CA | 2004 | 1/1 | 0.97 | 0.09 | 8,8,8,8 | 0 |
| 53 | MG | BB | 3069 | 1/1 | 0.97 | 0.11 | 17,17,17,17 | 0 |
| 53 | MG | DB | 3086 | 1/1 | 0.97 | 0.15 | 11,11,11,11 | 0 |
| 53 | MG | DB | 3033 | 1/1 | 0.97 | 0.08 | 9,9,9,9 | 0 |
| 53 | MG | BB | 3043 | 1/1 | 0.97 | 0.05 | 104,104,104,104 | 0 |
| 53 | MG | AA | 2034 | 1/1 | 0.97 | 0.06 | 68,68,68,68 | 0 |
| 53 | MG | BB | 3009 | 1/1 | 0.97 | 0.04 | 46,46,46,46 | 0 |
| 53 | MG | BB | 3035 | 1/1 | 0.97 | 0.07 | 15,15,15,15 | 0 |
| 53 | MG | DB | 3109 | 1/1 | 0.97 | 0.10 | 9,9,9,9 | 0 |
| 53 | MG | DB | 3102 | 1/1 | 0.97 | 0.09 | 12,12,12,12 | 0 |
| 53 | MG | DB | 3082 | 1/1 | 0.97 | 0.10 | 30,30,30,30 | 0 |
| 53 | MG | BB | 3058 | 1/1 | 0.97 | 0.10 | 22,22,22,22 | 0 |
| 53 | MG | DB | 3100 | 1/1 | 0.97 | 0.16 | 13,13,13,13 | 0 |
| 53 | MG | DB | 3088 | 1/1 | 0.97 | 0.14 | 25,25,25,25 | 0 |
| 53 | MG | DB | 3022 | 1/1 | 0.97 | 0.08 | 25,25,25,25 | 0 |
| 53 | MG | BB | 3026 | 1/1 | 0.97 | 0.08 | 39,39,39,39 | 0 |
| 53 | MG | AA | 2043 | 1/1 | 0.97 | 0.08 | 96,96,96,96 | 0 |
| 53 | MG | BB | 3090 | 1/1 | 0.97 | 0.12 | 112,112,112,112 | 0 |
| 55 | ZN | B4 | 101 | 1/1 | 0.97 | 0.04 | 80,80,80,80 | 0 |
| 53 | MG | DB | 3087 | 1/1 | 0.97 | 0.15 | 53,53,53,53 | 0 |
| 53 | MG | CA | 2061 | 1/1 | 0.97 | 0.08 | 23,23,23,23 | 0 |
| 53 | MG | BB | 3023 | 1/1 | 0.97 | 0.14 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3055 | 1/1 | 0.97 | 0.11 | 26,26,26,26 | 0 |
| 53 | MG | AA | 2010 | 1/1 | 0.97 | 0.04 | 60,60,60,60 | 0 |
| 53 | MG | DB | 3094 | 1/1 | 0.97 | 0.03 | 29,29,29,29 | 0 |
| 53 | MG | DB | 3078 | 1/1 | 0.97 | 0.08 | 27,27,27,27 | 0 |
| 53 | MG | CA | 2046 | 1/1 | 0.97 | 0.09 | 57,57,57,57 | 0 |
| 53 | MG | BB | 3013 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 53 | MG | BB | 3005 | 1/1 | 0.97 | 0.19 | 5,5,5,5 | 0 |
| 53 | MG | AA | 2036 | 1/1 | 0.97 | 0.04 | 31,31,31,31 | 0 |
| 53 | MG | BB | 3004 | 1/1 | 0.97 | 0.06 | 32,32,32,32 | 0 |
| 53 | MG | DB | 3010 | 1/1 | 0.97 | 0.08 | 8,8,8,8 | 0 |
| 53 | MG | BB | 3065 | 1/1 | 0.97 | 0.06 | 29,29,29,29 | 0 |
| 53 | MG | DB | 3009 | 1/1 | 0.97 | 0.07 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | DB | 3038 | 1/1 | 0.97 | 0.12 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3007 | 1/1 | 0.97 | 0.14 | 18,18,18,18 | 0 |
| 53 | MG | DB | 3061 | 1/1 | 0.97 | 0.09 | 69,69,69,69 | 0 |
| 53 | MG | CA | 2022 | 1/1 | 0.97 | 0.10 | 63,63,63,63 | 0 |
| 53 | MG | DB | 3028 | 1/1 | 0.97 | 0.06 | 24,24,24,24 | 0 |
| 53 | MG | BB | 3060 | 1/1 | 0.97 | 0.13 | 19,19,19,19 | 0 |
| 53 | MG | BB | 3074 | 1/1 | 0.97 | 0.07 | 28,28,28,28 | 0 |
| 53 | MG | DB | 3039 | 1/1 | 0.97 | 0.04 | 22,22,22,22 | 0 |
| 53 | MG | BB | 3096 | 1/1 | 0.97 | 0.11 | 34,34,34,34 | 0 |
| 53 | MG | DB | 3030 | 1/1 | 0.97 | 0.17 | 6,6,6,6 | 0 |
| 53 | MG | BB | 3066 | 1/1 | 0.97 | 0.12 | 23,23,23,23 | 0 |
| 53 | MG | BB | 3091 | 1/1 | 0.97 | 0.09 | 16,16,16,16 | 0 |
| 53 | MG | AA | 2027 | 1/1 | 0.97 | 0.09 | 36,36,36,36 | 0 |
| 53 | MG | DB | 3056 | 1/1 | 0.97 | 0.09 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3040 | 1/1 | 0.98 | 0.18 | 26,26,26,26 | 0 |
| 53 | MG | BB | 3079 | 1/1 | 0.98 | 0.04 | 19,19,19,19 | 0 |
| 53 | MG | DB | 3063 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 53 | MG | CA | 2056 | 1/1 | 0.98 | 0.05 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3089 | 1/1 | 0.98 | 0.17 | 7,7,7,7 | 0 |
| 53 | MG | BB | 3028 | 1/1 | 0.98 | 0.20 | 86,86,86,86 | 0 |
| 53 | MG | DB | 3043 | 1/1 | 0.98 | 0.11 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3105 | 1/1 | 0.98 | 0.08 | 20,20,20,20 | 0 |
| 53 | MG | BB | 3101 | 1/1 | 0.98 | 0.09 | 24,24,24,24 | 0 |
| 53 | MG | BB | 3025 | 1/1 | 0.98 | 0.13 | 30,30,30,30 | 0 |
| 53 | MG | DB | 3049 | 1/1 | 0.98 | 0.09 | 36,36,36,36 | 0 |
| 53 | MG | DB | 3031 | 1/1 | 0.98 | 0.18 | 8,8,8,8 | 0 |
| 53 | MG | BB | 3086 | 1/1 | 0.98 | 0.26 | 42,42,42,42 | 0 |
| 53 | MG | DB | 3069 | 1/1 | 0.98 | 0.18 | 11,11,11,11 | 0 |
| 55 | ZN | D4 | 101 | 1/1 | 0.98 | 0.06 | 46,46,46,46 | 0 |
| 53 | MG | CA | 2013 | 1/1 | 0.98 | 0.08 | 73,73,73,73 | 0 |
| 53 | MG | DB | 3040 | 1/1 | 0.98 | 0.16 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3104 | 1/1 | 0.98 | 0.08 | 33,33,33,33 | 0 |
| 53 | MG | DB | 3042 | 1/1 | 0.98 | 0.10 | 6,6,6,6 | 0 |
| 53 | MG | CA | 2032 | 1/1 | 0.98 | 0.17 | 33,33,33,33 | 0 |
| 53 | MG | BB | 3012 | 1/1 | 0.98 | 0.09 | 32,32,32,32 | 0 |
| 53 | MG | CA | 2051 | 1/1 | 0.98 | 0.05 | 39,39,39,39 | 0 |
| 53 | MG | BB | 3044 | 1/1 | 0.98 | 0.15 | 53,53,53,53 | 0 |
| 53 | MG | BB | 3006 | 1/1 | 0.98 | 0.07 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3002 | 1/1 | 0.98 | 0.07 | 12,12,12,12 | 0 |
| 53 | MG | DB | 3008 | 1/1 | 0.98 | 0.18 | 6,6,6,6 | 0 |
| 53 | MG | BB | 3108 | 1/1 | 0.98 | 0.10 | 47,47,47,47 | 0 |
| 53 | MG | DB | 3004 | 1/1 | 0.98 | 0.11 | 6,6,6,6 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | DB | 3065 | 1/1 | 0.98 | 0.05 | 37,37,37,37 | 0 |
| 53 | MG | DB | 3017 | 1/1 | 0.98 | 0.10 | 13,13,13,13 | 0 |
| 53 | MG | DB | 3075 | 1/1 | 0.98 | 0.10 | 57,57,57,57 | 0 |
| 53 | MG | BB | 3103 | 1/1 | 0.98 | 0.08 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2017 | 1/1 | 0.98 | 0.11 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3095 | 1/1 | 0.98 | 0.07 | 33,33,33,33 | 0 |
| 53 | MG | BB | 3073 | 1/1 | 0.98 | 0.09 | 39,39,39,39 | 0 |
| 53 | MG | BB | 3094 | 1/1 | 0.98 | 0.07 | 28,28,28,28 | 0 |
| 53 | MG | AA | 2053 | 1/1 | 0.98 | 0.07 | 79,79,79,79 | 0 |
| 53 | MG | DB | 3051 | 1/1 | 0.98 | 0.19 | 23,23,23,23 | 0 |
| 53 | MG | DB | 3107 | 1/1 | 0.98 | 0.07 | 10,10,10,10 | 0 |
| 53 | MG | CA | 2045 | 1/1 | 0.98 | 0.16 | 48,48,48,48 | 0 |
| 53 | MG | BB | 3059 | 1/1 | 0.98 | 0.12 | 26,26,26,26 | 0 |
| 53 | MG | CA | 2055 | 1/1 | 0.98 | 0.07 | 11,11,11,11 | 0 |
| 53 | MG | DB | 3064 | 1/1 | 0.98 | 0.05 | 20,20,20,20 | 0 |
| 53 | MG | BB | 3089 | 1/1 | 0.98 | 0.15 | 56,56,56,56 | 0 |
| 53 | MG | DB | 3106 | 1/1 | 0.98 | 0.13 | 23,23,23,23 | 0 |
| 53 | MG | DB | 3024 | 1/1 | 0.98 | 0.13 | 63,63,63,63 | 0 |
| 53 | MG | CA | 2006 | 1/1 | 0.98 | 0.05 | 95,95,95,95 | 0 |
| 53 | MG | CA | 2039 | 1/1 | 0.98 | 0.12 | 16,16,16,16 | 0 |
| 53 | MG | BB | 3011 | 1/1 | 0.98 | 0.19 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3079 | 1/1 | 0.98 | 0.14 | 28,28,28,28 | 0 |
| 53 | MG | DB | 3062 | 1/1 | 0.98 | 0.04 | 77,77,77,77 | 0 |
| 53 | MG | DB | 3027 | 1/1 | 0.98 | 0.15 | 6,6,6,6 | 0 |
| 53 | MG | CA | 2001 | 1/1 | 0.98 | 0.05 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3006 | 1/1 | 0.98 | 0.10 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3083 | 1/1 | 0.98 | 0.16 | 85,85,85,85 | 0 |
| 53 | MG | AA | 2020 | 1/1 | 0.98 | 0.07 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3016 | 1/1 | 0.98 | 0.05 | 15,15,15,15 | 0 |
| 53 | MG | DB | 3048 | 1/1 | 0.98 | 0.12 | 28,28,28,28 | 0 |
| 53 | MG | DB | 3037 | 1/1 | 0.98 | 0.16 | 28,28,28,28 | 0 |
| 53 | MG | BB | 3072 | 1/1 | 0.98 | 0.12 | 17,17,17,17 | 0 |
| 53 | MG | DB | 3068 | 1/1 | 0.98 | 0.10 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3077 | 1/1 | 0.98 | 0.21 | 54,54,54,54 | 0 |
| 53 | MG | DB | 3099 | 1/1 | 0.98 | 0.19 | 7,7,7,7 | 0 |
| 53 | MG | BB | 3022 | 1/1 | 0.98 | 0.26 | 34,34,34,34 | 0 |
| 53 | MG | CA | 2030 | 1/1 | 0.98 | 0.12 | 7,7,7,7 | 0 |
| 53 | MG | DB | 3096 | 1/1 | 0.98 | 0.12 | 6,6,6,6 | 0 |
| 53 | MG | BB | 3067 | 1/1 | 0.98 | 0.09 | 44,44,44,44 | 0 |
| 53 | MG | BB | 3084 | 1/1 | 0.98 | 0.16 | 24,24,24,24 | 0 |
| 53 | MG | BB | 3019 | 1/1 | 0.98 | 0.05 | 22,22,22,22 | 0 |
| 53 | MG | DB | 3067 | 1/1 | 0.98 | 0.07 | 5,5,5,5 | 0 |

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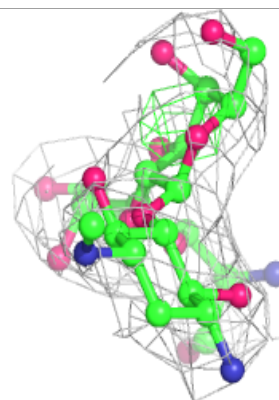
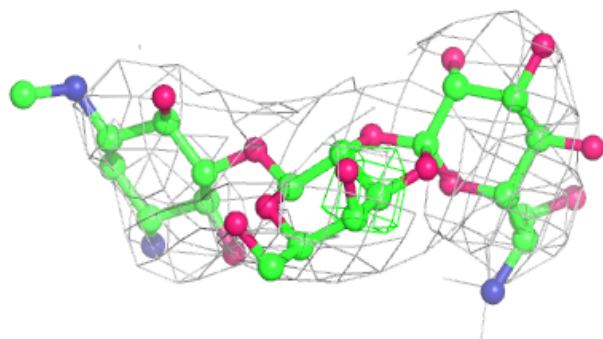
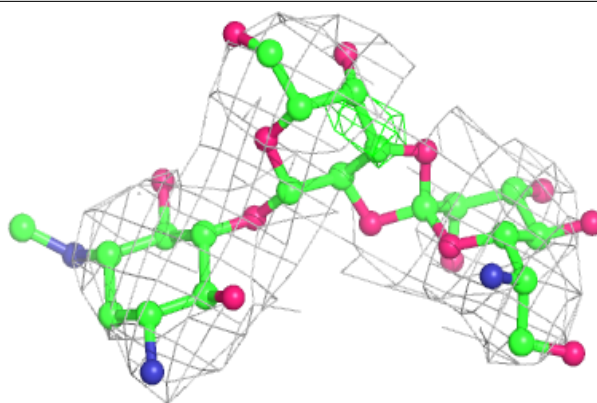
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | DB | 3084 | 1/1 | 0.98 | 0.17 | 5,5,5,5 | 0 |
| 53 | MG | AA | 2003 | 1/1 | 0.99 | 0.17 | 39,39,39,39 | 0 |
| 53 | MG | CA | 2018 | 1/1 | 0.99 | 0.03 | 6,6,6,6 | 0 |
| 53 | MG | DB | 3076 | 1/1 | 0.99 | 0.10 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3020 | 1/1 | 0.99 | 0.15 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2050 | 1/1 | 0.99 | 0.11 | 8,8,8,8 | 0 |
| 53 | MG | BB | 3092 | 1/1 | 0.99 | 0.06 | 54,54,54,54 | 0 |
| 53 | MG | DB | 3098 | 1/1 | 0.99 | 0.22 | 44,44,44,44 | 0 |
| 53 | MG | BB | 3070 | 1/1 | 0.99 | 0.14 | 37,37,37,37 | 0 |
| 53 | MG | DB | 3081 | 1/1 | 0.99 | 0.13 | 18,18,18,18 | 0 |
| 53 | MG | BB | 3050 | 1/1 | 0.99 | 0.12 | 28,28,28,28 | 0 |
| 53 | MG | BB | 3110 | 1/1 | 0.99 | 0.15 | 23,23,23,23 | 0 |
| 53 | MG | BB | 3015 | 1/1 | 0.99 | 0.09 | 13,13,13,13 | 0 |
| 53 | MG | DB | 3014 | 1/1 | 0.99 | 0.05 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2031 | 1/1 | 0.99 | 0.06 | 28,28,28,28 | 0 |
| 53 | MG | CA | 2053 | 1/1 | 0.99 | 0.06 | 30,30,30,30 | 0 |
| 53 | MG | DB | 3053 | 1/1 | 0.99 | 0.07 | 35,35,35,35 | 0 |
| 53 | MG | BB | 3076 | 1/1 | 0.99 | 0.05 | 38,38,38,38 | 0 |
| 53 | MG | CA | 2003 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |
| 53 | MG | BB | 3106 | 1/1 | 0.99 | 0.12 | 62,62,62,62 | 0 |
| 53 | MG | DB | 3001 | 1/1 | 0.99 | 0.10 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3041 | 1/1 | 0.99 | 0.08 | 7,7,7,7 | 0 |
| 53 | MG | DB | 3085 | 1/1 | 0.99 | 0.12 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3002 | 1/1 | 0.99 | 0.07 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3107 | 1/1 | 0.99 | 0.11 | 6,6,6,6 | 0 |
| 53 | MG | DB | 3091 | 1/1 | 0.99 | 0.18 | 13,13,13,13 | 0 |
| 53 | MG | DB | 3012 | 1/1 | 0.99 | 0.20 | 9,9,9,9 | 0 |
| 53 | MG | BB | 3030 | 1/1 | 0.99 | 0.03 | 35,35,35,35 | 0 |
| 53 | MG | CA | 2012 | 1/1 | 0.99 | 0.08 | 93,93,93,93 | 0 |
| 53 | MG | DB | 3019 | 1/1 | 0.99 | 0.09 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3018 | 1/1 | 0.99 | 0.07 | 22,22,22,22 | 0 |
| 53 | MG | BB | 3007 | 1/1 | 0.99 | 0.14 | 82,82,82,82 | 0 |
| 53 | MG | DB | 3101 | 1/1 | 0.99 | 0.20 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3018 | 1/1 | 0.99 | 0.14 | 32,32,32,32 | 0 |
| 53 | MG | CA | 2002 | 1/1 | 1.00 | 0.11 | 5,5,5,5 | 0 |

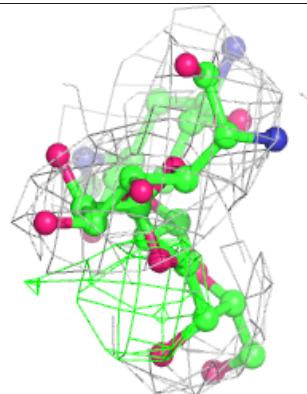
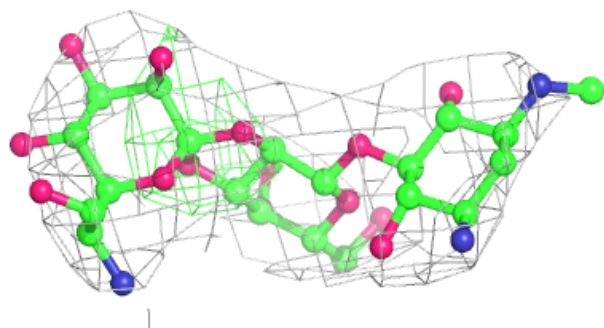
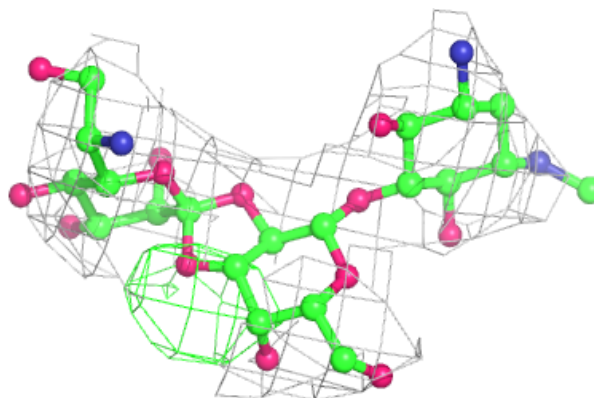
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HYG AA 2059:

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

**Electron density around HYG CA 2062:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.