



Full wwPDB X-ray Structure Validation Report

Jun 16, 2014 – 08:55 PM BST

PDB ID : 4V8B
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-06
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

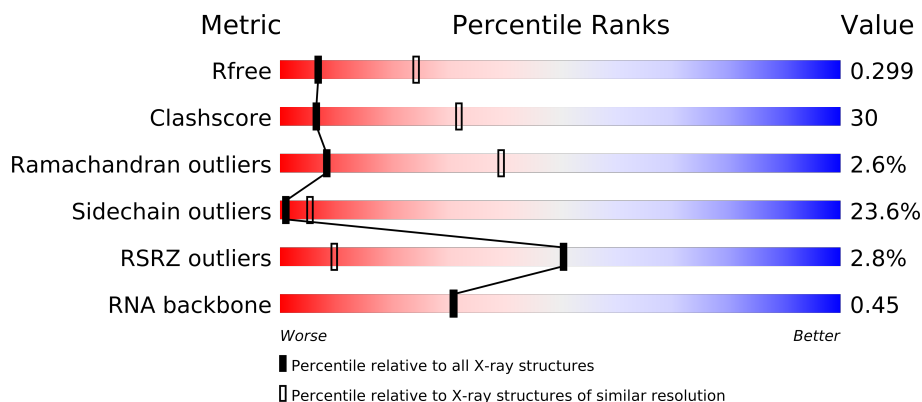
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1216 (3.00-3.00) |
| Clashscore | 79885 | 1594 (3.00-3.00) |
| Ramachandran outliers | 78287 | 1537 (3.00-3.00) |
| Sidechain outliers | 78261 | 1540 (3.00-3.00) |
| RSRZ outliers | 66119 | 1217 (3.00-3.00) |
| RNA backbone | 1838 | 1070 (3.50-2.50) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AA | 1506 | |
| 1 | CA | 1506 | |
| 2 | AE | 256 | |
| 2 | CE | 256 | |
| 3 | AF | 239 | |
| 3 | CF | 239 | |
| 4 | AG | 208 | |
| 4 | CG | 208 | |
| 5 | AH | 162 | |
| 5 | CH | 162 | |
| 6 | AI | 101 | |
| 6 | CI | 101 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 7 | AJ | 156 | |
| 7 | CJ | 156 | |
| 8 | AK | 138 | |
| 8 | CK | 138 | |
| 9 | AL | 128 | |
| 9 | CL | 128 | |
| 10 | AM | 105 | |
| 10 | CM | 105 | |
| 11 | AN | 129 | |
| 11 | CN | 129 | |
| 12 | AO | 132 | |
| 12 | CO | 132 | |
| 13 | AP | 126 | |
| 13 | CP | 126 | |
| 14 | AQ | 61 | |
| 14 | CQ | 61 | |
| 15 | AR | 89 | |
| 15 | CR | 89 | |
| 16 | AS | 88 | |
| 16 | CS | 88 | |
| 17 | AT | 105 | |
| 17 | CT | 105 | |
| 18 | AU | 88 | |
| 18 | CU | 88 | |
| 19 | AV | 93 | |
| 19 | CV | 93 | |
| 20 | AW | 106 | |
| 20 | CW | 106 | |
| 21 | AX | 27 | |
| 21 | CX | 27 | |
| 22 | AB | 87 | |
| 22 | CB | 87 | |
| 23 | AC | 77 | |
| 23 | AD | 77 | |
| 23 | CC | 77 | |
| 23 | CD | 77 | |
| 24 | A1 | 10 | |
| 24 | C1 | 10 | |
| 25 | BA | 2912 | |
| 25 | DA | 2912 | |
| 26 | BB | 122 | |
| 26 | DB | 122 | |

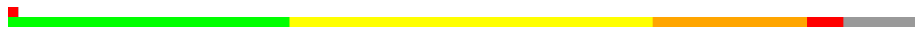
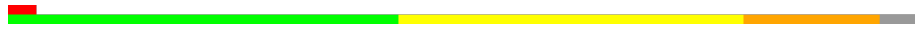


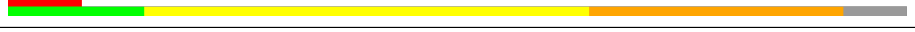
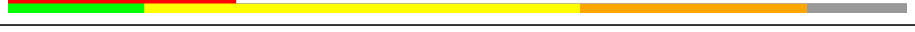
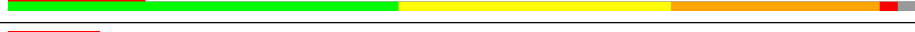



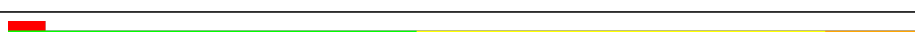
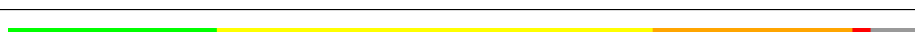
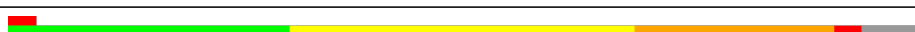
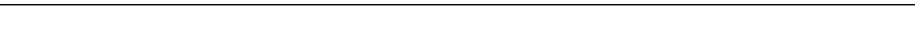
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27 | BD | 276 | |
| 27 | DD | 276 | |
| 28 | BE | 206 | |
| 28 | DE | 206 | |
| 29 | BF | 210 | |
| 29 | DF | 210 | |
| 30 | BG | 182 | |
| 30 | DG | 182 | |
| 31 | BH | 180 | |
| 31 | DH | 180 | |
| 32 | BK | 148 | |
| 32 | DK | 148 | |
| 33 | BM | 140 | |
| 33 | DM | 140 | |
| 34 | BN | 122 | |
| 34 | DN | 122 | |
| 35 | BO | 150 | |
| 35 | DO | 150 | |
| 36 | BP | 141 | |
| 36 | DP | 141 | |
| 37 | B0 | 118 | |
| 37 | D0 | 118 | |
| 38 | BQ | 112 | |
| 38 | DQ | 112 | |
| 39 | BR | 146 | |
| 39 | DR | 146 | |
| 40 | B1 | 118 | |
| 40 | D1 | 118 | |
| 41 | B2 | 101 | |
| 41 | D2 | 101 | |
| 42 | BS | 113 | |
| 42 | DS | 113 | |
| 43 | BT | 96 | |
| 43 | DT | 96 | |
| 44 | BU | 110 | |
| 44 | DU | 110 | |
| 45 | BV | 206 | |
| 45 | DV | 206 | |
| 46 | B3 | 85 | |
| 46 | D3 | 85 | |
| 47 | BZ | 98 | |
| 47 | DZ | 98 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 48 | BW | 72 |  |
| 48 | DW | 72 |  |
| 49 | BX | 60 |  |
| 49 | DX | 60 |  |
| 50 | B4 | 71 |  |
| 50 | D4 | 71 |  |
| 51 | B5 | 60 |  |
| 51 | D5 | 60 |  |
| 52 | B6 | 54 |  |
| 52 | D6 | 54 |  |
| 53 | B7 | 49 |  |
| 53 | D7 | 49 |  |
| 54 | B8 | 65 |  |
| 54 | D8 | 65 |  |

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299552 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1506 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32369 | 14408 | 5997 | 10459 | 1505 | | | |
| 1 | CA | 1506 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32372 | 14408 | 5997 | 10461 | 1506 | | | |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AE | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |
| 2 | CE | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AF | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | CF | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1016 | 314 | 281 | 1 | | | |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AH | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 5 | CH | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9 | AL | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | | |
| 9 | CL | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | | |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AM | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | CM | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AO | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |
| 12 | CO | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AP | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 928 | 574 | 191 | 161 | 2 | | | |
| 13 | CP | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 577 | 192 | 162 | 2 | | | |

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

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AR | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | CR | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |
| 16 | CS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AT | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | CT | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | AU | 72 | Total | C | N | O | 0 | 0 | 0 |
| | | | 591 | 376 | 117 | 98 | | | |
| 18 | CU | 72 | Total | C | N | O | 0 | 0 | 0 |
| | | | 591 | 376 | 117 | 98 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AV | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 624 | 398 | 115 | 109 | 2 | | | |
| 19 | CV | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 624 | 398 | 115 | 109 | 2 | | | |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AX | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | CX | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called TRNA-LEU.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | AB | 87 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1861 | 829 | 333 | 612 | 87 | | | |
| 22 | CB | 87 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1861 | 829 | 333 | 612 | 87 | | | |

- Molecule 23 is a RNA chain called TRNA-FMET.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23 | AC | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1643 | 732 | 298 | 536 | 77 | | | |
| 23 | AD | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1643 | 732 | 298 | 536 | 77 | | | |
| 23 | CC | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1643 | 732 | 298 | 536 | 77 | | | |
| 23 | CD | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1643 | 732 | 298 | 536 | 77 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|---------------|
| AC | 18 | C | U | CONFLICT | GB AP012306.1 |
| AD | 18 | C | U | CONFLICT | GB AP012306.1 |
| CC | 18 | C | U | CONFLICT | GB AP012306.1 |
| CD | 18 | C | U | CONFLICT | GB AP012306.1 |

- Molecule 24 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| 24 | A1 | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 205 | 92 | 26 | 77 | 10 | | | |
| 24 | C1 | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 205 | 92 | 26 | 77 | 10 | | | |

- Molecule 25 is a RNA chain called RNA (2912-MER).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25 | BA | 2912 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62707 | 27911 | 11722 | 20163 | 2911 | | | |
| 25 | DA | 2907 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62607 | 27866 | 11712 | 20123 | 2906 | | | |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|---------------|
| BA | 161 | U | - | EXPRESSION TAG | GB AP008226.1 |
| BA | 654A | A | G | CONFLICT | GB AP008226.1 |
| BA | 654E | C | G | CONFLICT | GB AP008226.1 |
| BA | 654P | G | C | CONFLICT | GB AP008226.1 |
| BA | 654T | A | C | CONFLICT | GB AP008226.1 |
| BA | 1058 | U | G | CONFLICT | GB AP008226.1 |
| BA | 1080 | A | C | CONFLICT | GB AP008226.1 |
| DA | 168 | U | - | INSERTION | GB AP008226.1 |
| DA | 654A | A | G | CONFLICT | GB AP008226.1 |
| DA | 654E | C | G | CONFLICT | GB AP008226.1 |
| DA | 654P | G | C | CONFLICT | GB AP008226.1 |
| DA | 654T | A | C | CONFLICT | GB AP008226.1 |
| DA | 1058 | U | G | CONFLICT | GB AP008226.1 |
| DA | 1080 | A | C | CONFLICT | GB AP008226.1 |

- Molecule 26 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | BB | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |
| 26 | DB | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | BD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |
| 27 | DD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |
| 28 | DE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | BF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |
| 29 | DF | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1627 | 1037 | 304 | 283 | 3 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 30 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | BH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |
| 31 | DH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BK | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |
| 32 | DK | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BM | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | DM | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BN | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 34 | DN | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BO | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |
| 35 | DO | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | BP | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 36 | DP | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | B0 | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 37 | D0 | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | | |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 38 | BQ | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |
| 38 | DQ | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BR | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 39 | DR | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | B1 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |
| 40 | D1 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | B2 | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 41 | D2 | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BS | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |
| 42 | DS | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43 | BT | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |
| 43 | DT | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BU | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |
| 44 | DU | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BV | 175 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1397 | 892 | 251 | 251 | 3 | | | |
| 45 | DV | 179 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1428 | 911 | 255 | 259 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | B3 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 607 | 376 | 128 | 102 | 1 | | | |
| 46 | D3 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 613 | 379 | 129 | 104 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | BZ | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |
| 47 | DZ | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | BW | 66 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 558 | 346 | 113 | 98 | 1 | | | |
| 48 | DW | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49 | BX | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49 | DX | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B4 | 66 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 533 | 335 | 96 | 97 | 5 | | | |
| 50 | D4 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 515 | 326 | 93 | 91 | 5 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 51 | D5 | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 454 | 285 | 89 | 75 | 5 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B6 | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 389 | 241 | 79 | 65 | 4 | | | |
| 52 | D6 | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 389 | 241 | 79 | 65 | 4 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | B7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |
| 53 | D7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54 | B8 | 61 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 488 | 312 | 99 | 75 | 2 | | | |
| 54 | D8 | 61 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 488 | 312 | 99 | 75 | 2 | | | |

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 55 | BA | 623 | Total 623 | Mg 623 | 0 | 0 |
| 55 | CA | 207 | Total 207 | Mg 207 | 0 | 0 |
| 55 | AB | 5 | Total 5 | Mg 5 | 0 | 0 |
| 55 | B8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | BE | 5 | Total 5 | Mg 5 | 0 | 0 |
| 55 | DU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | B1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | AN | 2 | Total 2 | Mg 2 | 0 | 0 |
| 55 | CN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | B5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | BB | 17 | Total 17 | Mg 17 | 0 | 0 |
| 55 | D3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | BF | 3 | Total 3 | Mg 3 | 0 | 0 |
| 55 | DR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | B2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | AA | 242 | Total 242 | Mg 242 | 0 | 0 |
| 55 | CG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 55 | BU | 2 | Total 2 | Mg 2 | 0 | 0 |
| 55 | A1 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 55 | AD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | CC | 8 | Total 8 | Mg 8 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 55 | DE | 3 | Total 3 | Mg 3 | 0 | 0 |
| 55 | B3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | DA | 526 | Total 526 | Mg 526 | 0 | 0 |
| 55 | B7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | AG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | BO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 55 | AQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | D1 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 55 | AH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | DP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | AC | 9 | Total 9 | Mg 9 | 0 | 0 |
| 55 | CB | 3 | Total 3 | Mg 3 | 0 | 0 |
| 55 | D5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | BD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | B0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | CS | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | DB | 14 | Total 14 | Mg 14 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 56 | AG | 1 | Total 1 | Zn 1 | 0 | 0 |
| 56 | AQ | 1 | Total 1 | Zn 1 | 0 | 0 |

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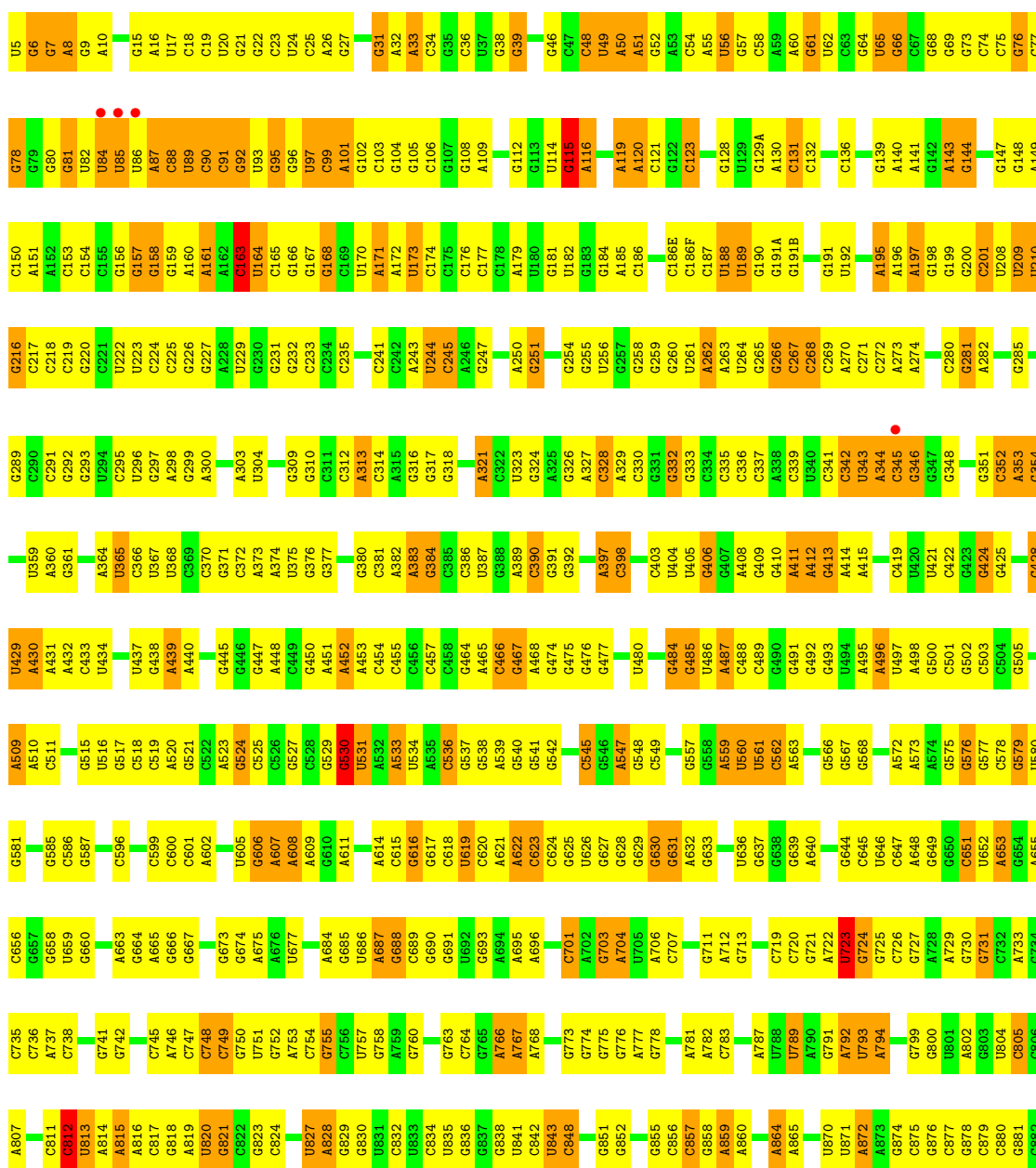
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 56 | CQ | 1 | Total 1 | Zn 1 | 0 | 0 |
| 56 | CG | 1 | Total 1 | Zn 1 | 0 | 0 |

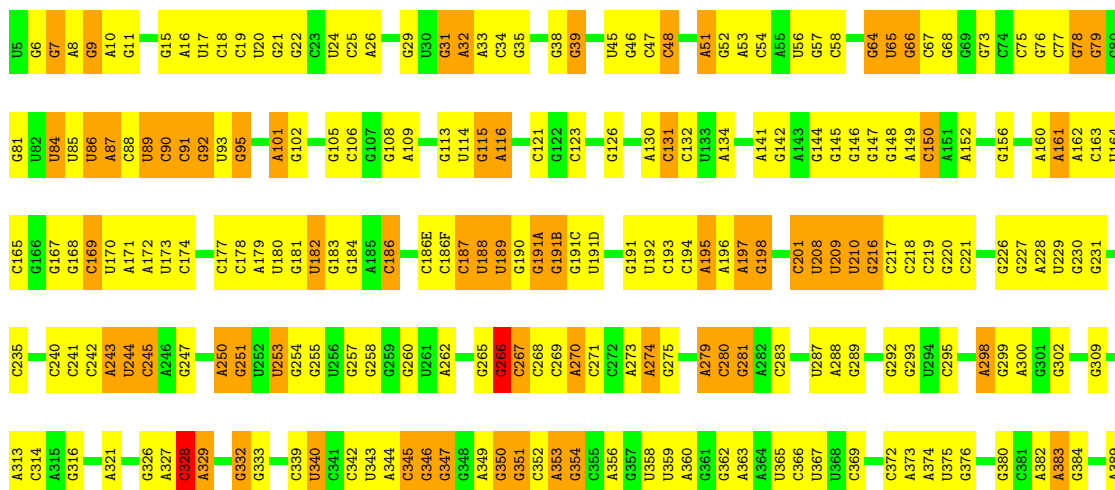
3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA

Chain AA:



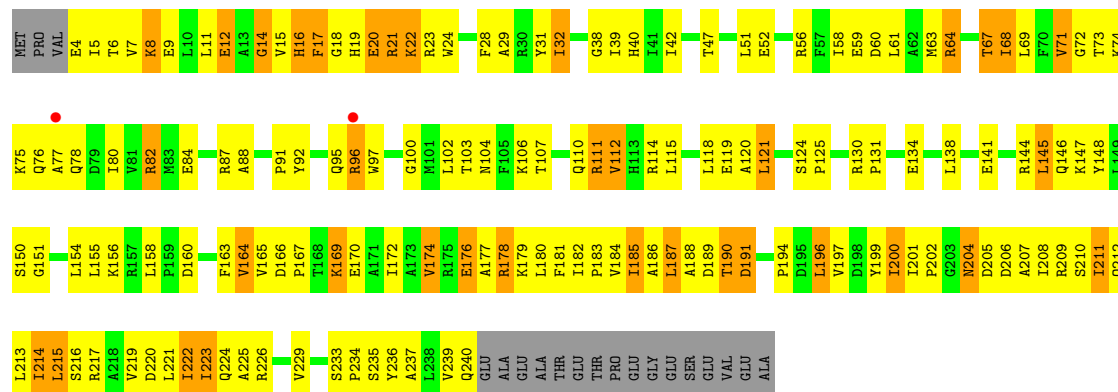


| | | | | | | | | | | | | |
|-------|--------|-------|-------|-------|-------|--------|------|------|------|------|------|------|
| G1416 | A1350 | G1287 | C1223 | G1160 | G1034 | A978 | G917 | G755 | G682 | G541 | G467 | C390 |
| G1417 | U1351 | A1288 | G1224 | C1161 | A1035 | C979 | A918 | C756 | G683 | G542 | A468 | G391 |
| G1418 | C1352 | A1289 | A1225 | C1162 | G1036 | C980 | A919 | U757 | A684 | C543 | G474 | G392 |
| G1419 | G1353 | C1290 | C1226 | C1163 | C1037 | C981 | U920 | G758 | G685 | C544 | G475 | A393 |
| | C1354 | A1291 | A1227 | C1164 | C1038 | C982 | U921 | | U686 | C545 | G476 | G394 |
| G1423 | G1355 | U1292 | C1228 | C1165 | G1039 | A983 | G836 | G763 | A687 | C546 | G477 | C395 |
| C1424 | G1356 | C1293 | | G1166 | C1040 | C984 | G938 | C764 | G688 | A547 | A478 | G396 |
| | A1357 | G1294 | G1231 | | A1041 | C985 | U941 | C765 | C689 | G548 | | A397 |
| C1429 | C1358 | G1295 | U1232 | A1170 | G1042 | A986 | G926 | A766 | C690 | A621 | G481 | C398 |
| C1430 | | C1296 | G1233 | G1171 | C1043 | C987 | G927 | | G691 | G550 | A482 | |
| | G1361 | C1297 | C1234 | C1172 | G1044 | G988 | G928 | G769 | U692 | C624 | A483 | U404 |
| A1434 | C1362 | A1298 | U1235 | G1173 | A1110 | C989 | G929 | G773 | A693 | G625 | G484 | U405 |
| A1435 | C1362A | A1299 | G1174 | G1174 | G1045 | C990 | C849 | G774 | A694 | U626 | G485 | G406 |
| U1436 | A1363 | G1300 | C1237 | G1175 | U991 | U992 | C931 | | A695 | G627 | U486 | G407 |
| C1437 | G1364 | U1301 | A1239 | A1176 | G1047 | C993 | G932 | G775 | A696 | G628 | A487 | A409 |
| C1438 | G1365 | C1303 | G1177 | G1177 | G1048 | C994 | G933 | G776 | | G629 | C488 | G409 |
| C1439 | C1366 | G1304 | G1178 | U1178 | | A994 | C934 | A777 | G700 | G630 | C489 | G410 |
| | C1367 | G1305 | A1179 | A1179 | G1052 | C995 | A935 | G778 | G701 | A559 | | A411 |
| G1442 | G1368 | A1306 | G1241 | A1180 | C1054 | A996 | C936 | C779 | A702 | U560 | A495 | A412 |
| A1446 | C1369 | | G1181 | G1181 | A1055 | U997 | A937 | A780 | G703 | U561 | A496 | G413 |
| G1447 | G1370 | | G1182 | G1182 | U1056 | G998 | A938 | | A704 | C562 | U497 | A414 |
| C1448 | U1371 | G1309 | | A1183 | U1057 | C998A | A939 | G783 | U705 | A563 | A498 | |
| C1449 | G1372 | G1310 | U1247 | G1184 | G1058 | U999 | G940 | C784 | A706 | C564 | G500 | U420 |
| U1450 | G1373 | G1311 | A1248 | G1185 | C1059 | G1000 | G941 | C785 | C707 | G565 | G501 | U421 |
| A1451 | A1374 | G1312 | C1249 | G1186 | G1060 | G1001 | G942 | G786 | | U566 | G502 | C422 |
| A1452 | A1375 | U1313 | A1250 | G1187 | G1061 | G1002 | U943 | A787 | G710 | G567 | C503 | G423 |
| C1452 | U1376 | C1314 | A1251 | A1189 | U1062 | G1003 | G944 | U788 | G711 | G568 | C504 | G424 |
| G1453 | A1377 | C1315 | G1252 | G1189 | C1063 | A1004 | G945 | | A712 | C569 | G505 | G425 |
| G1454 | C1378 | G1316 | G1253 | G1190 | G1064 | A1005 | A946 | G791 | G713 | C570 | G506 | U426 |
| | G1379 | C1317 | C1254 | A1191 | U1065 | G1006 | G947 | A792 | U646 | U571 | | U427 |
| | U1380 | A1318 | G1255 | G1192 | C1066 | C1007 | G948 | U793 | G647 | A572 | A509 | G428 |
| C1465 | U1381 | A1319 | A1256 | G1193 | A1067 | C1008 | A949 | A794 | A648 | A573 | A510 | U429 |
| C1466 | C1382 | C1320 | U1257 | G1194 | G1068 | G1009 | U950 | C795 | G649 | C511 | A430 | |
| A1468 | | C1321 | C1258 | C1195 | G1069 | G1010 | U951 | C796 | G650 | U512 | U431 | A432 |
| G1469 | G1386 | C1322 | C1259 | U1196 | C1071 | | G952 | C797 | C651 | G575 | C513 | A433 |
| | G1387 | G1323 | C1260 | G1197 | G1072 | A1013 | G953 | G798 | U652 | G577 | G514 | C433 |
| | C1388 | A1324 | A1261 | G1198 | U1073 | A1014 | G954 | G799 | A653 | C578 | G515 | U434 |
| | | C1325 | C1262 | U1199 | U1074 | A1015 | U955 | G800 | G654 | G579 | U516 | C435 |
| C1477 | | C1326 | C1263 | C1200 | G1075 | A1016 | U956 | U801 | A655 | U580 | G517 | C436 |
| C1478 | U1391 | G1327 | | A1201 | C1076 | G1017 | U957 | A802 | G656 | G581 | C518 | U437 |
| C1479 | G1392 | C1328 | G1266 | G1202 | C1140 | C1018 | A958 | G803 | | U582 | C519 | G438 |
| U1481 | A1393 | A1267 | C1267 | C1203 | C1141 | C1019 | A959 | U804 | G660 | A583 | A520 | A439 |
| G1482 | C1394 | U1330 | A1268 | A1204 | G1142 | U1020 | U960 | C805 | G661 | G584 | G521 | A440 |
| A1483 | C1395 | G1331 | A1269 | U1205 | G1143 | G1021 | U961 | | G662 | G585 | C522 | |
| | A1396 | A1332 | C1270 | G1206 | G1144 | G1022 | C962 | C810 | A663 | C586 | | C444 |
| G1486 | C1397 | | G1271 | C1207 | C1145 | G1023 | G963 | C811 | G671 | C587 | C526 | G445 |
| G1487 | A1398 | G1333 | G1272 | C1208 | A1146 | G1024 | A964 | C812 | U740 | G588 | G527 | G446 |
| G1488 | C1399 | C1334 | G1273 | C1209 | C1147 | U1025 | A965 | U813 | G741 | C589 | C528 | G447 |
| G1489 | C1400 | | G1274 | | U1148 | G1026 | G966 | A814 | G742 | | G529 | A448 |
| C1490 | G1401 | G1337 | A1275 | U1212 | U1085 | C1027 | C967 | A815 | | G593 | G530 | C449 |
| A1491 | C1402 | A1338 | G1276 | A1213 | U1086 | C1028 | A968 | A816 | C745 | | U531 | G450 |
| A1492 | C1403 | A1339 | C1277 | G1215 | | C1028A | A969 | C817 | A746 | C600 | A532 | A451 |
| | C1404 | | U1278 | G1216 | U1089 | C1028B | C970 | G818 | C747 | C601 | A533 | A452 |
| G1494 | G1405 | C1342 | A1279 | C1217 | U1090 | G1029 | G971 | A819 | G748 | U534 | A453 | |
| U1495 | U1406 | G1343 | G1280 | C1218 | A1092 | C1030 | G972 | U820 | C749 | G604 | A535 | |
| C1496 | | C1344 | U1281 | G1155 | A1093 | G1031 | G973 | G821 | G750 | U605 | C536 | C457 |
| G1497 | C1411 | U1345 | U1282 | G1156 | G1094 | A1032 | A974 | | U751 | G606 | G537 | C458 |
| U1498 | C1412 | A1346 | C1282 | A1157 | U1095 | G1032A | A975 | U827 | U752 | A607 | G538 | G464 |
| A1499 | U1413 | C1347 | | C1158 | C1096 | G1032B | A976 | A828 | A753 | A608 | A539 | A465 |
| | | A1285 | A1286 | U1159 | C1097 | G1033 | A977 | G829 | C754 | A609 | G540 | C466 |



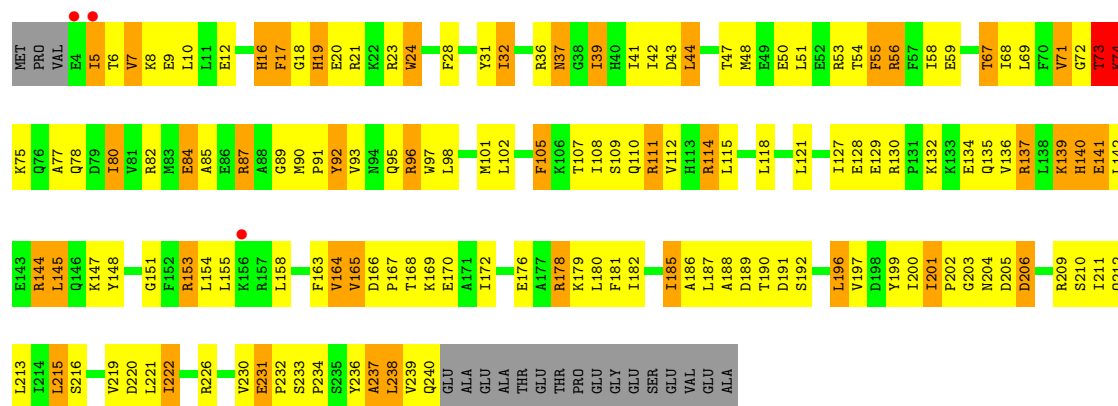
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AE:



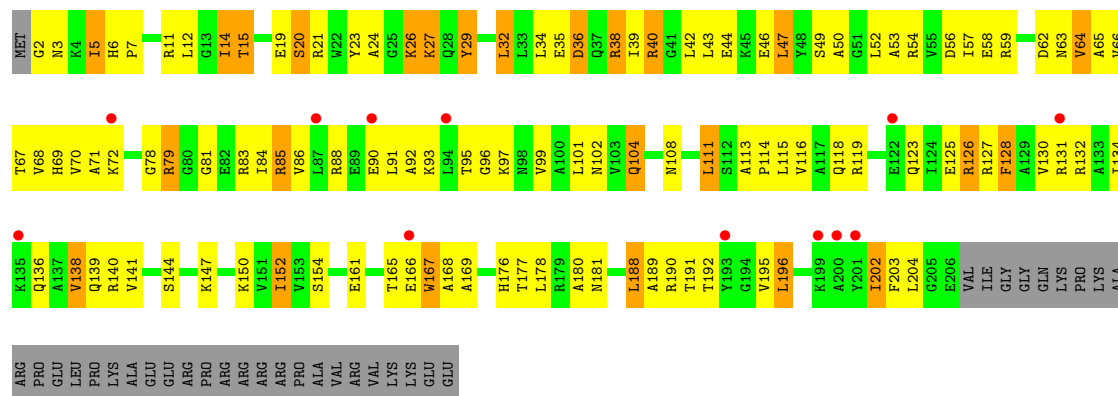
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

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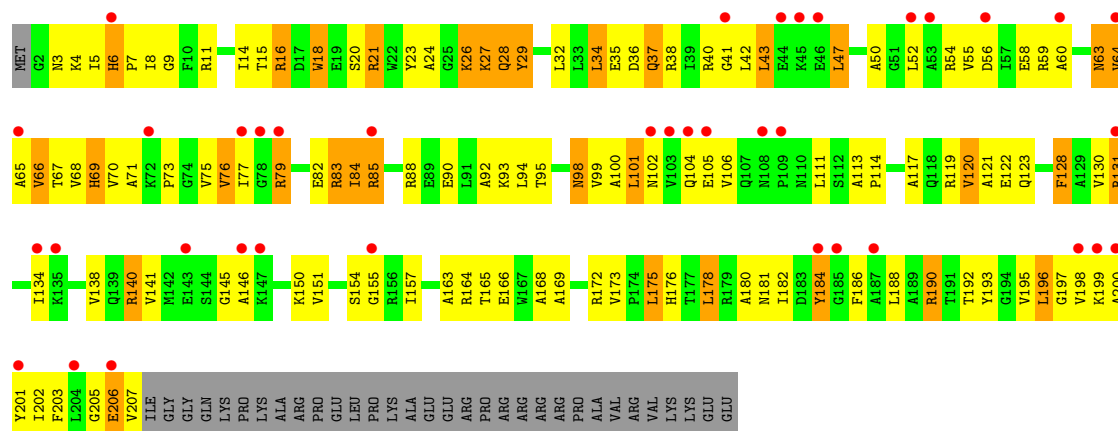
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AF:



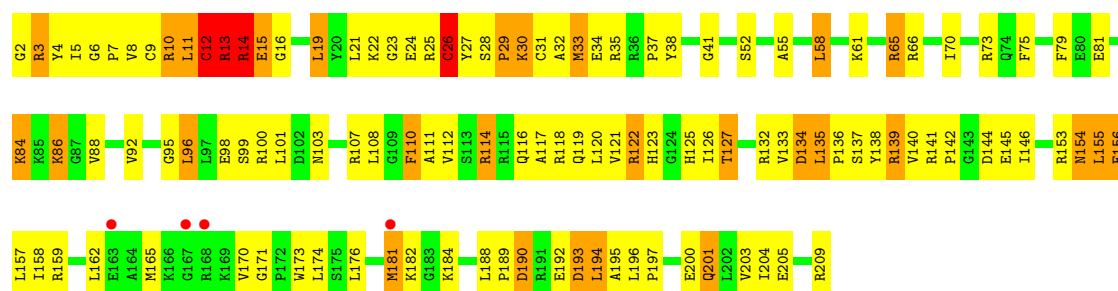
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CF:



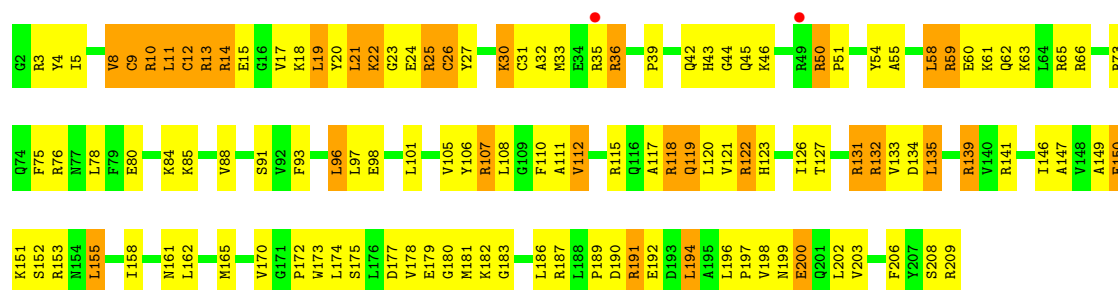
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG:



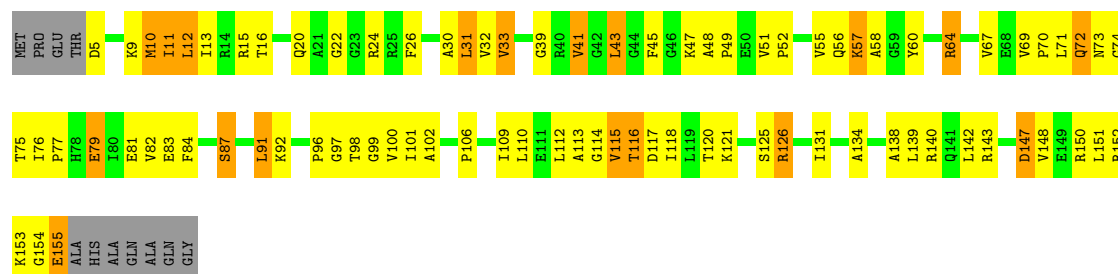
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG:



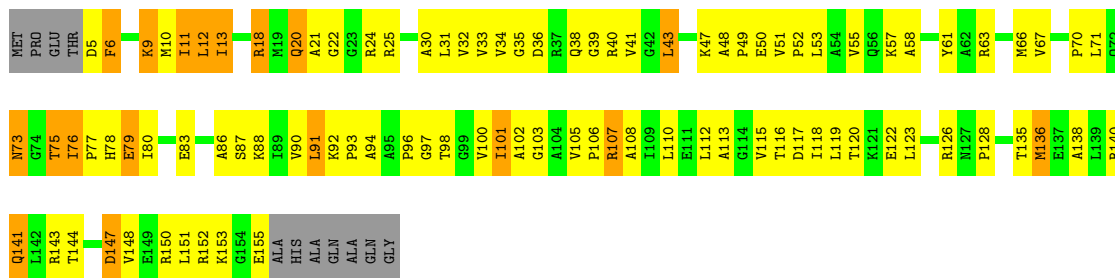
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH:



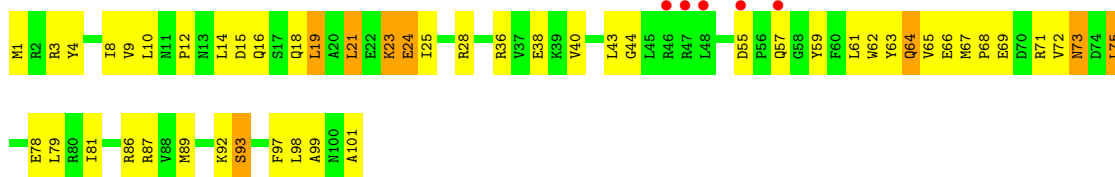
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH:



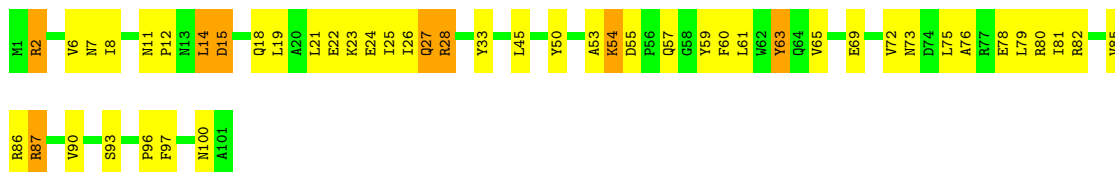
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI:



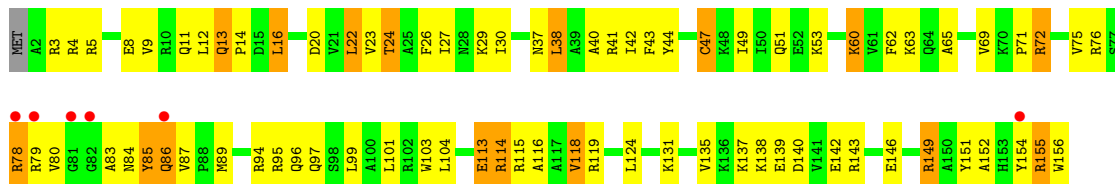
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AJ:



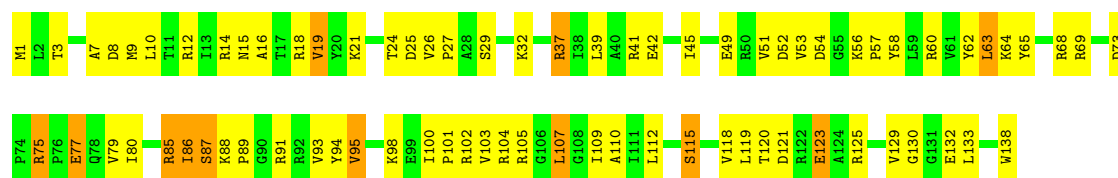
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



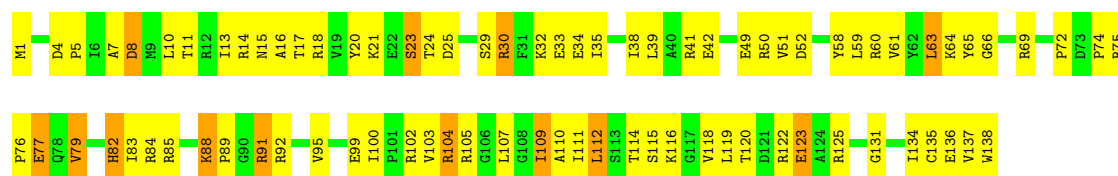
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK:



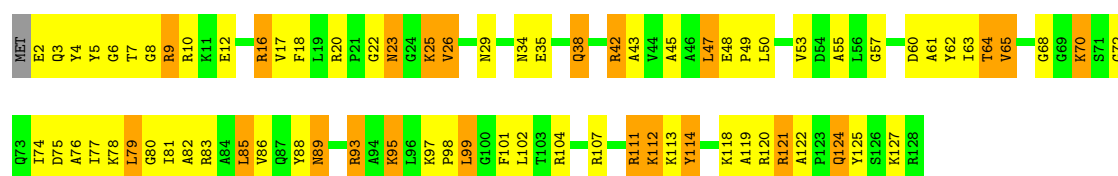
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK:



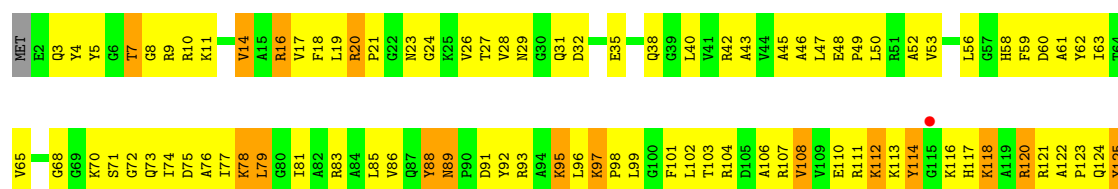
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL:



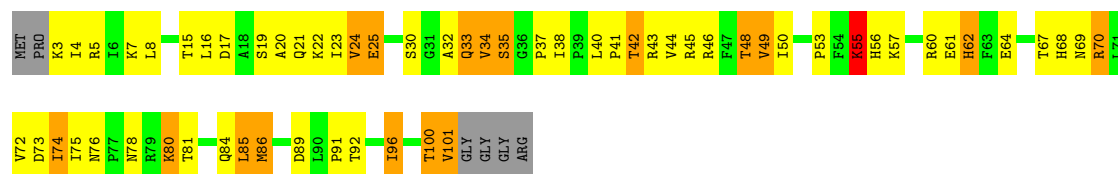
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

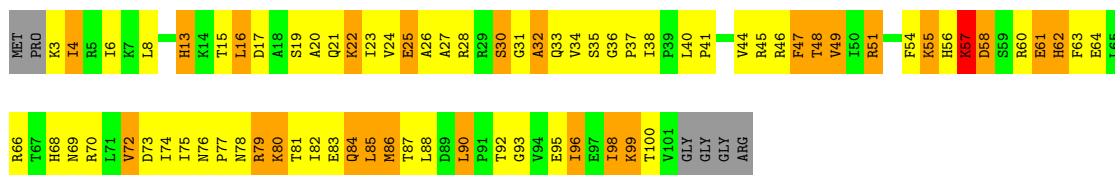
Chain AM:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

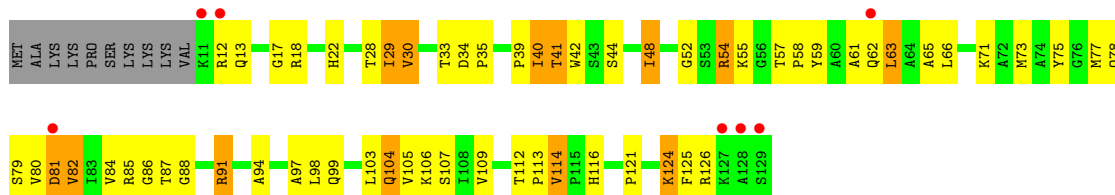
Chain CM:





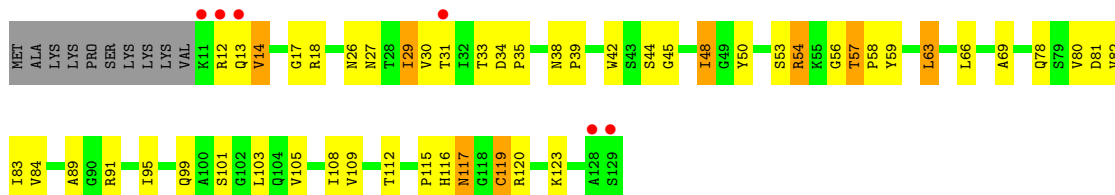
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AN:



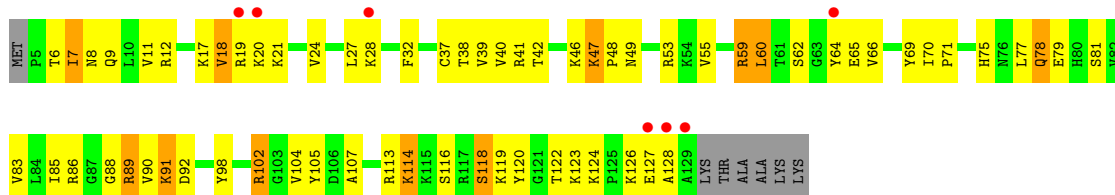
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CN:



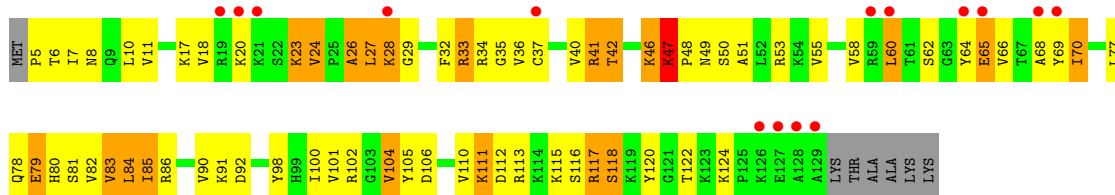
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AO:



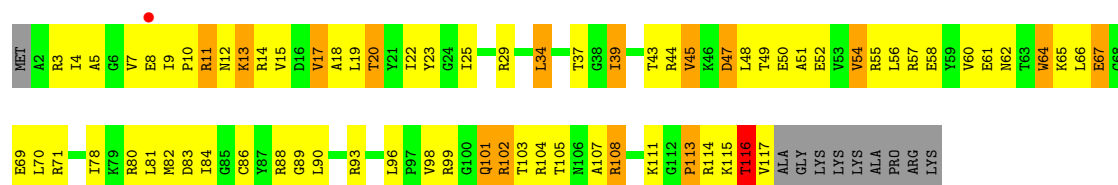
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CO:



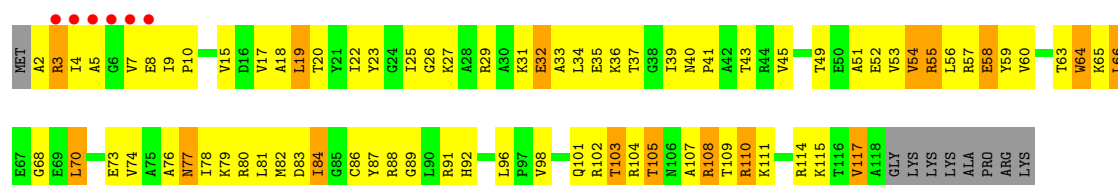
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AP:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP:



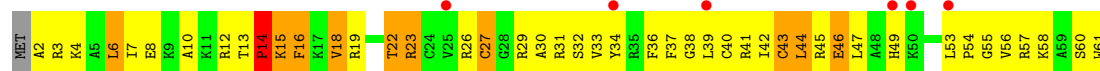
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:



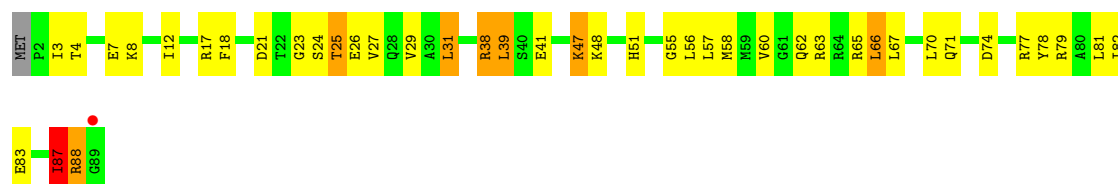
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



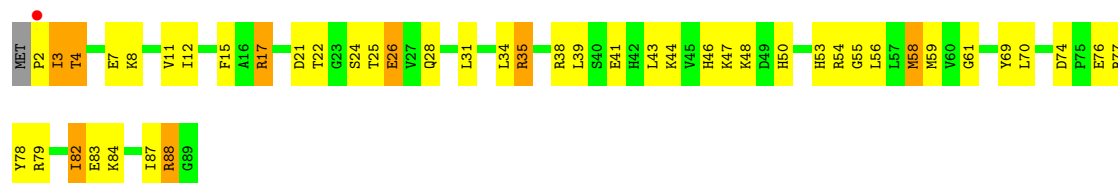
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:



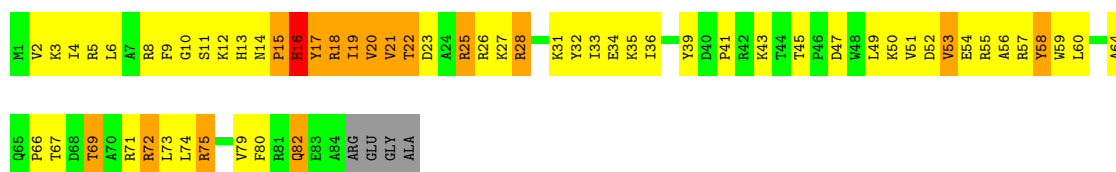
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR:



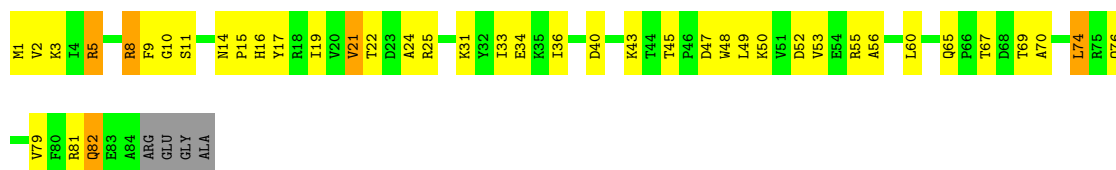
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS:



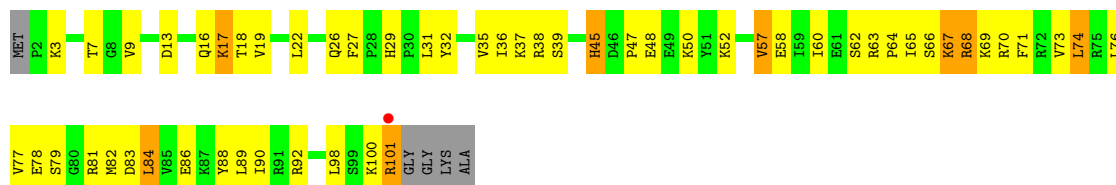
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:



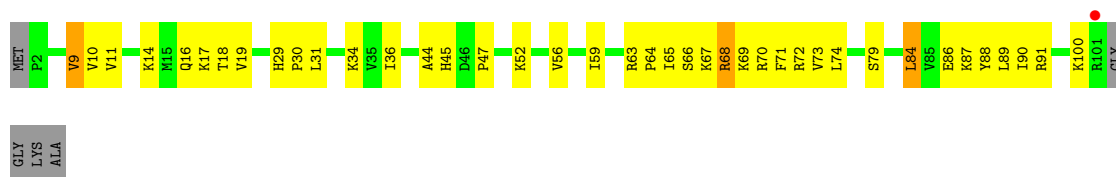
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:



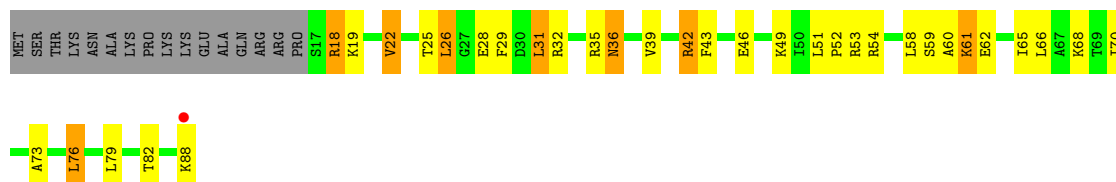
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

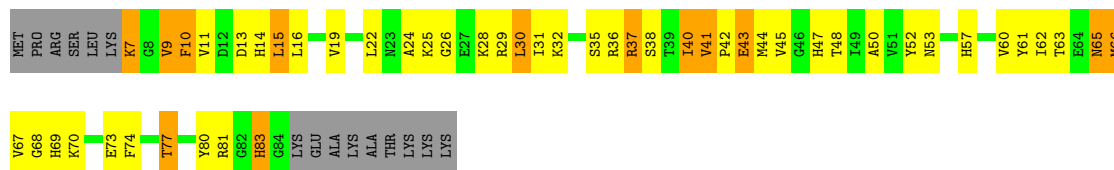
Chain CU:





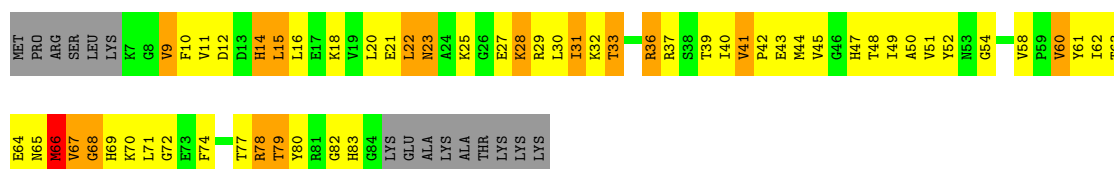
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AV:



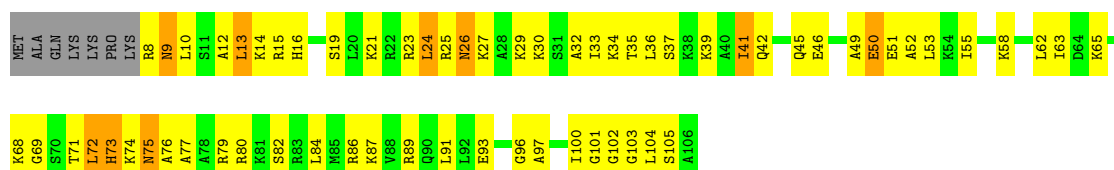
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CV:



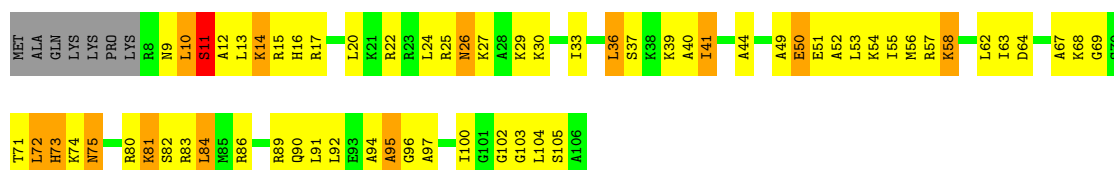
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW:



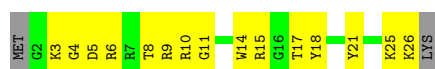
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX:



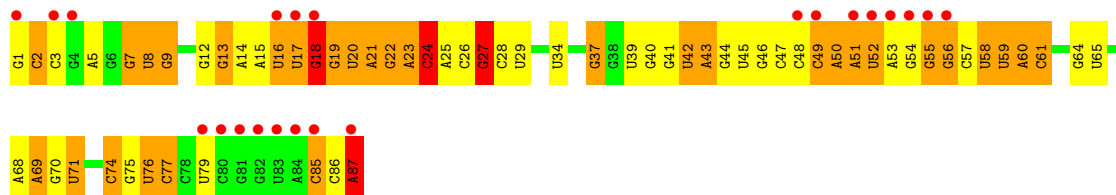
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:



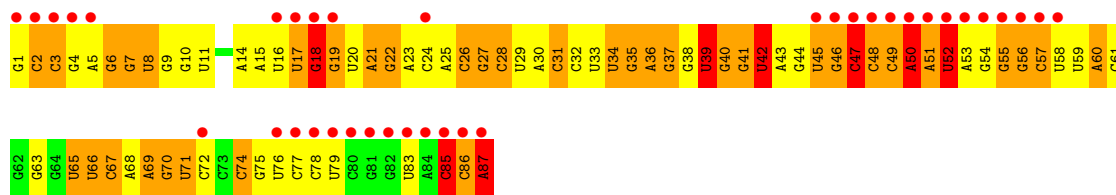
• Molecule 22: TRNA-LEU

Chain AB:



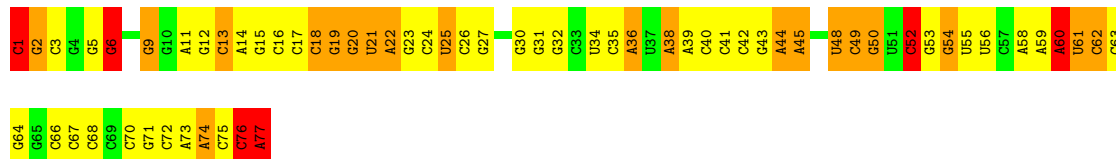
• Molecule 22: TRNA-LEU

Chain CB:



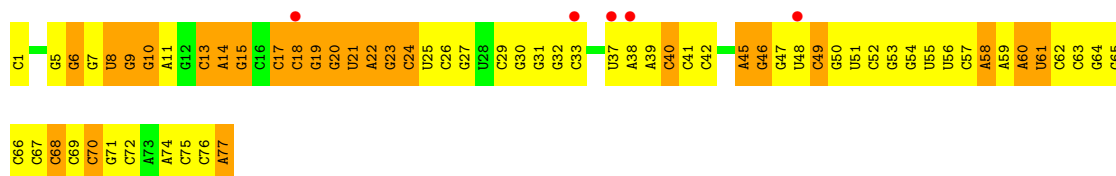
• Molecule 23: TRNA-FMET

Chain AC:



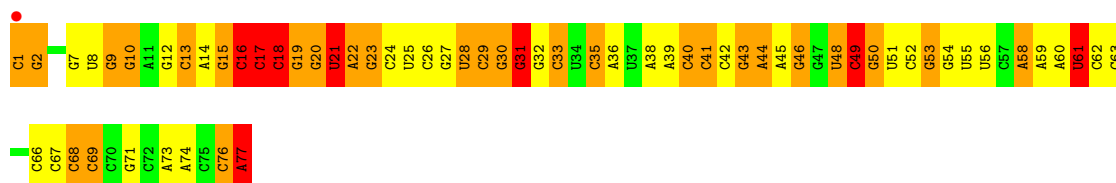
• Molecule 23: TRNA-FMET

Chain AD:



• Molecule 23: TRNA-FMET

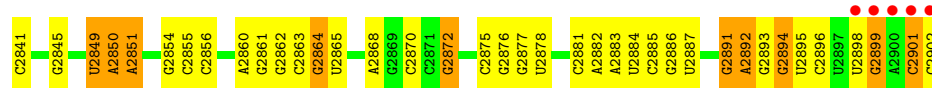
Chain CC:



• Molecule 23: TRNA-FMET

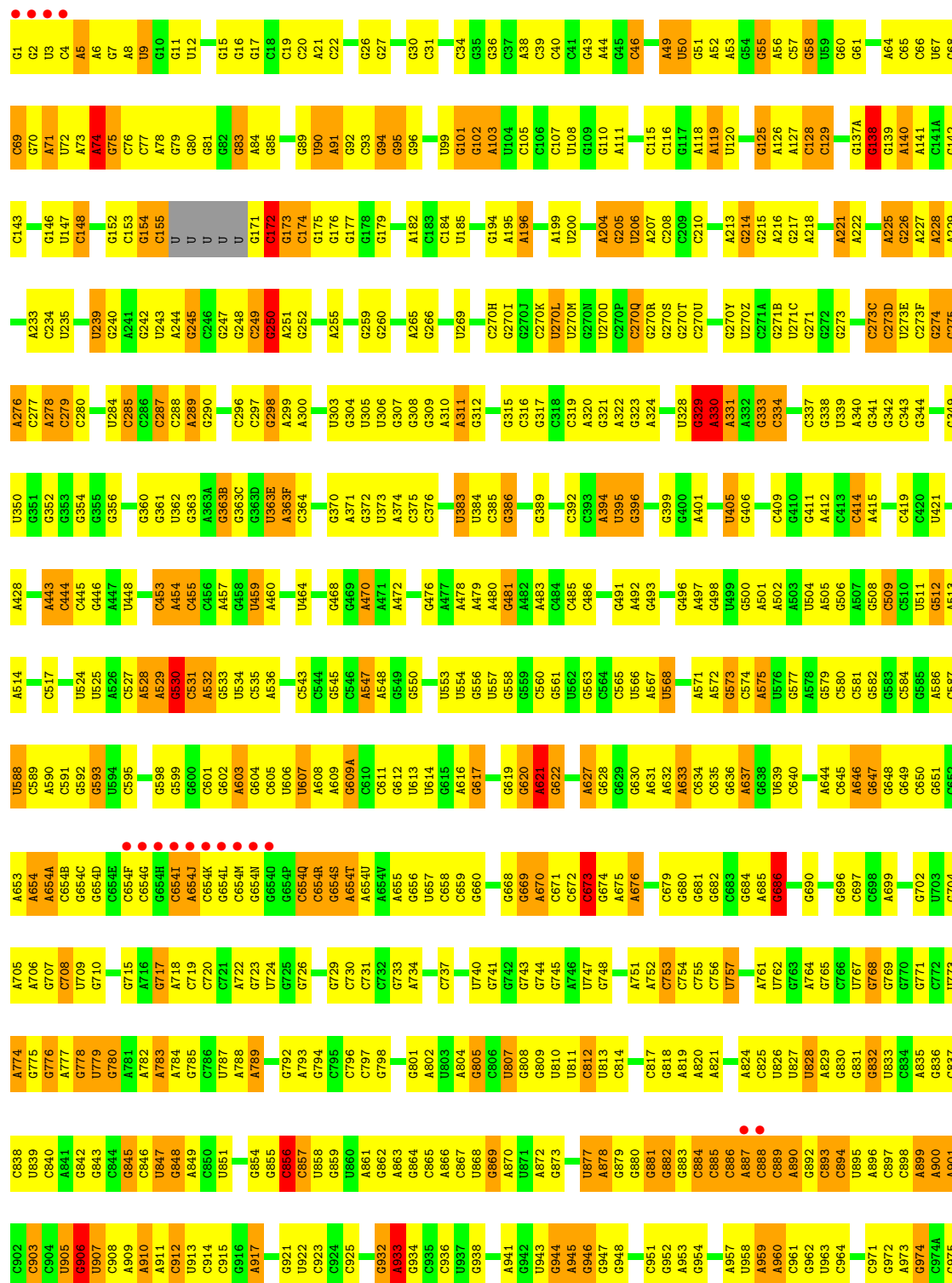
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
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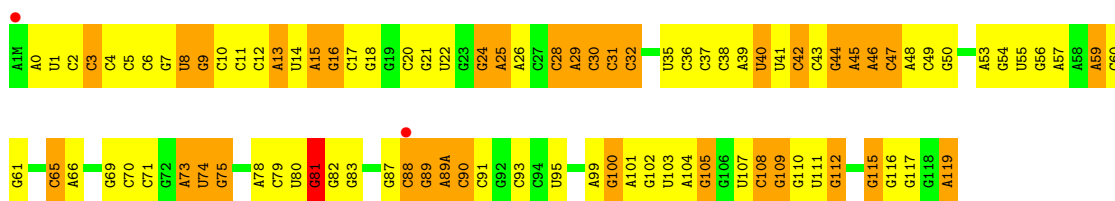
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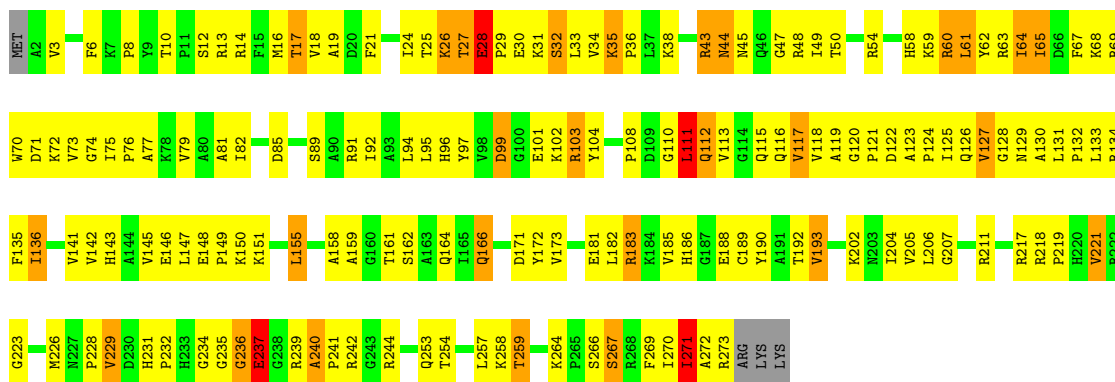
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| | A2030 | U1943 | G1869 | A1786 | C1694 | A1610 | A1537 | U1391 | A1241 | G1166 | A1096 | U1035 |
| C2111 | A2031 | U1944 | C1870 | | G1695 | C1611 | G1538 | A1392 | | U1167 | U1037 | G1036 |
| G2112 | G2032 | G1945 | A1871 | A1791 | G1696 | C1612 | G1539 | U1393 | G1244 | A1088 | G1037 | |
| U2113 | A2033 | U1946 | A1872 | | G1697 | G1613 | G1540 | U1397 | G1245 | G1169 | C1100 | |
| A2114 | | C1947 | G1878 | U1794 | A1698 | A1614 | U1541 | | A1246 | U1171 | U1101 | |
| G2115 | G2036 | U1948 | C1879 | C1795 | G1699 | G1615 | A1542 | | | | | |
| G2116 | G2037 | G1949 | C1880 | U1796 | A1700 | A1616 | G1543 | | | | | |
| A2117 | G2038 | U1950 | C1881 | C1797 | A1701 | | | | | | | |
| U2118 | C2039 | U1951 | C1882 | | G1702 | G1619 | C1544 | | | | | |





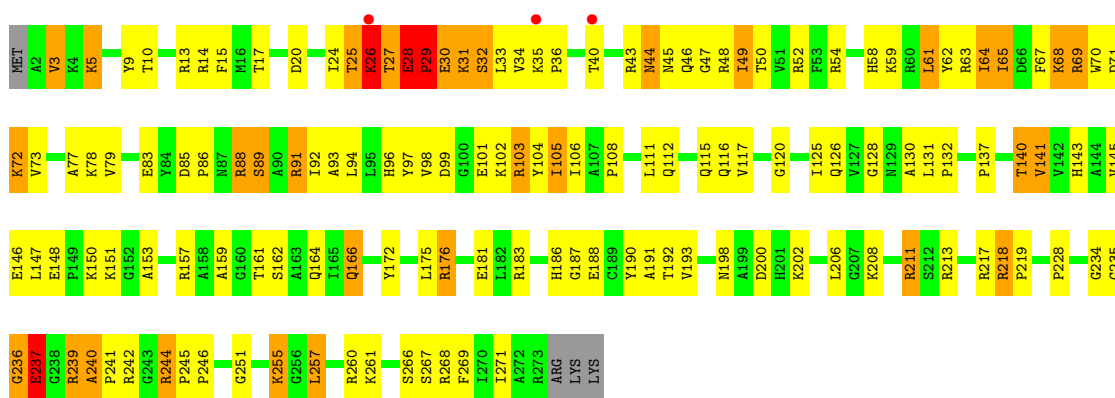
• Molecule 27: 50S ribosomal protein L2

Chain BD:



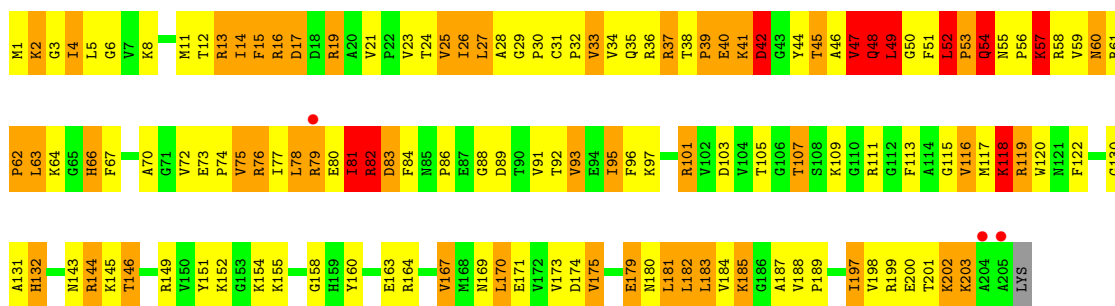
• Molecule 27: 50S ribosomal protein L2

Chain DD:



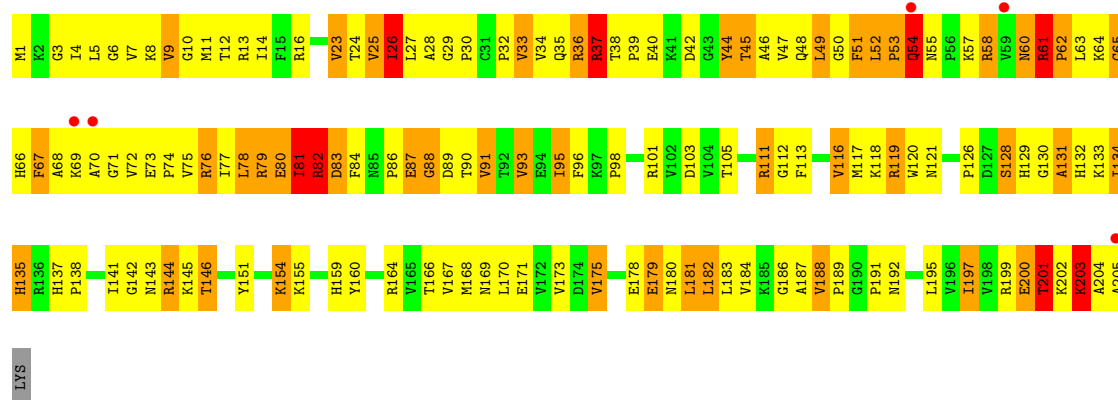
• Molecule 28: 50S ribosomal protein L3

Chain BE:



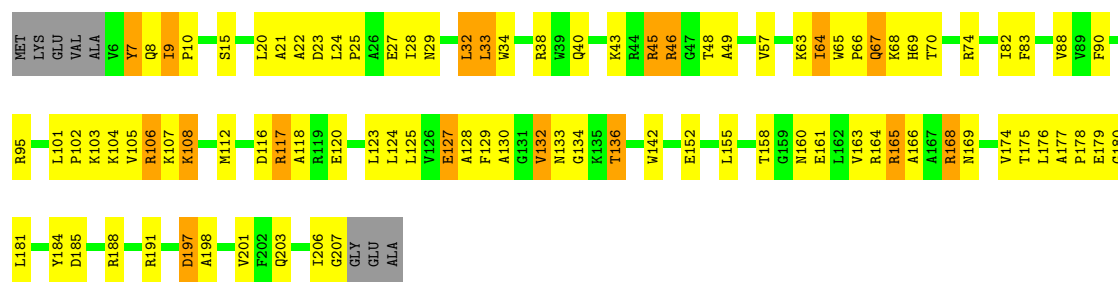
• Molecule 28: 50S ribosomal protein L3

Chain DE:



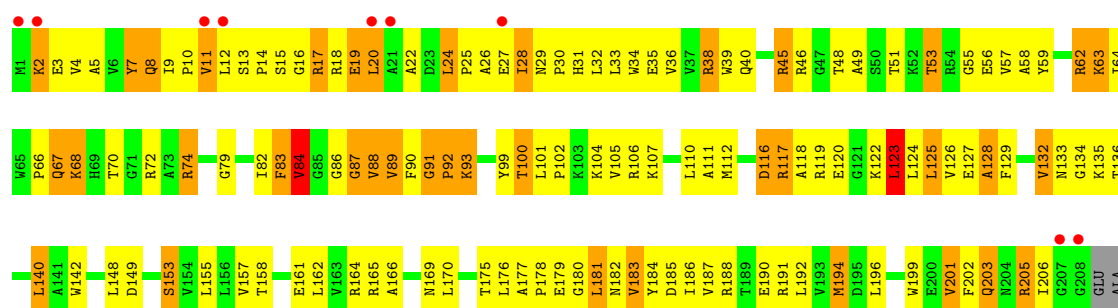
- Molecule 29: 50S ribosomal protein L4

Chain BF:



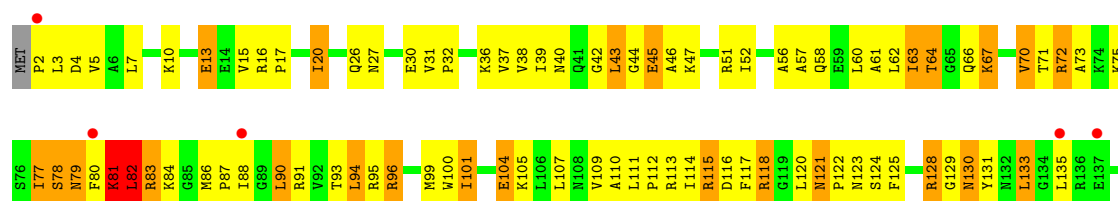
- Molecule 29: 50S ribosomal protein L4

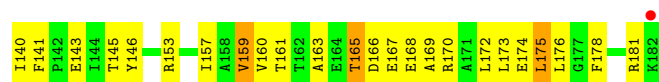
Chain DF:



- Molecule 30: 50S ribosomal protein L5

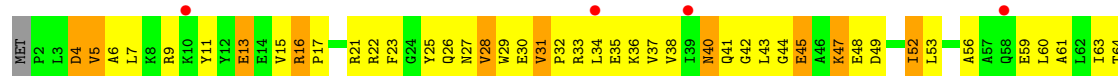
Chain BG:





- Molecule 30: 50S ribosomal protein L5

Chain DG:



- Molecule 31: 50S ribosomal protein L6

Chain BH:



- Molecule 31: 50S ribosomal protein L6

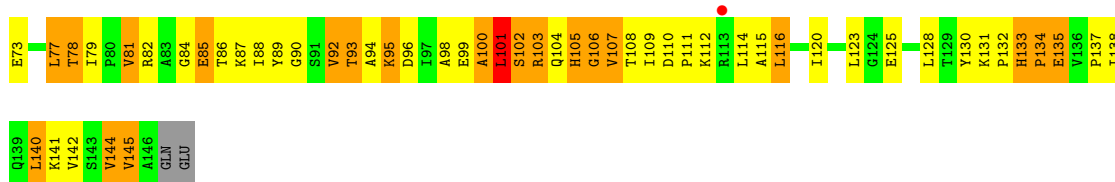
Chain DH:



- Molecule 32: 50S ribosomal protein L9

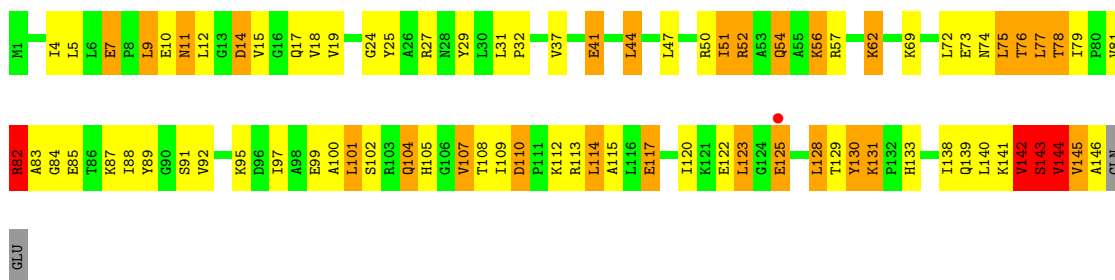
Chain BK:





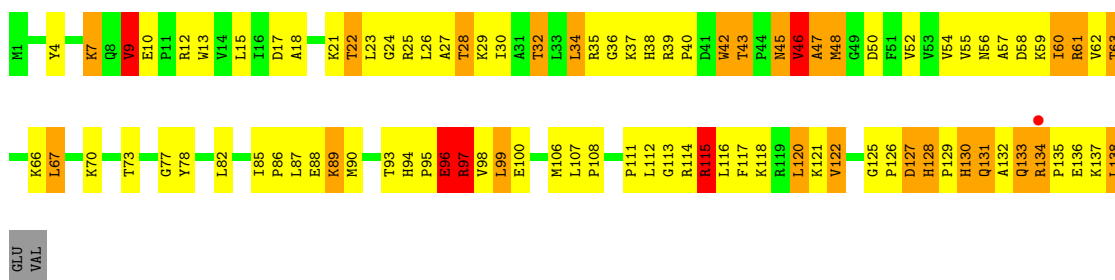
- Molecule 32: 50S ribosomal protein L9

Chain DK:



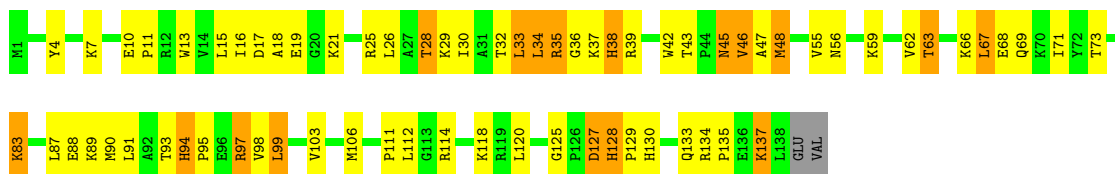
- Molecule 33: 50S ribosomal protein L13

Chain BM:



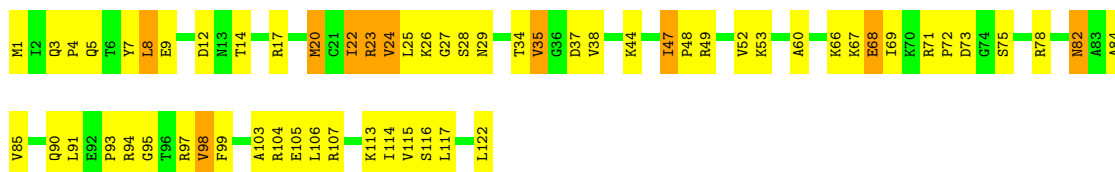
- Molecule 33: 50S ribosomal protein L13

Chain DM:



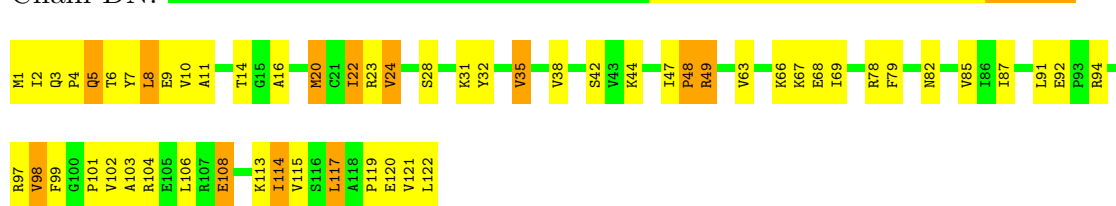
- Molecule 34: 50S ribosomal protein L14

Chain BN:



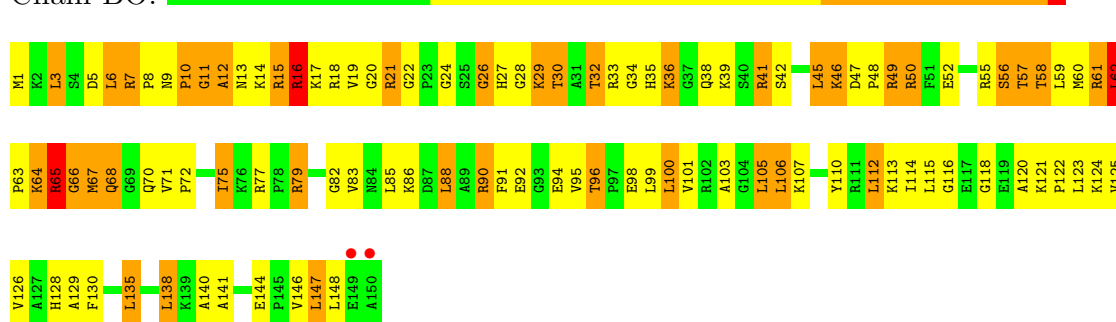
- Molecule 34: 50S ribosomal protein L14

Chain DN:



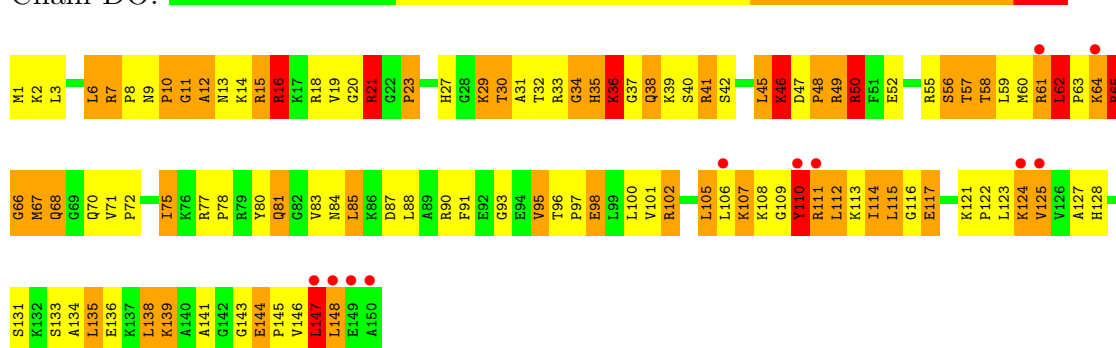
- Molecule 35: 50S ribosomal protein L15

Chain BO:



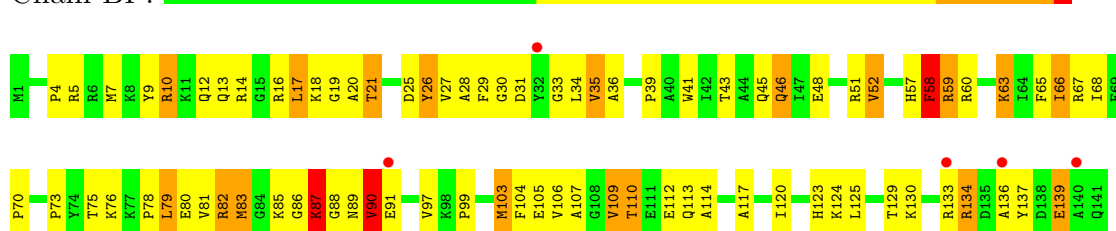
- Molecule 35: 50S ribosomal protein L15

Chain DO:



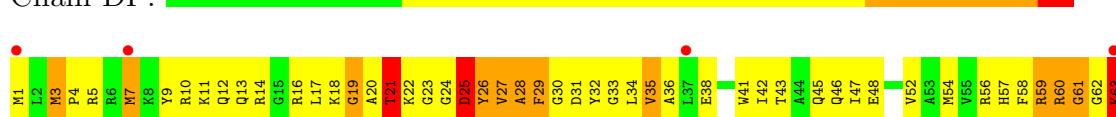
- Molecule 36: 50S ribosomal protein L16

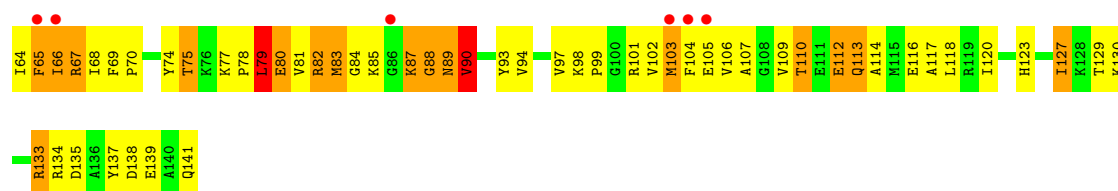
Chain BP:



- Molecule 36: 50S ribosomal protein L16

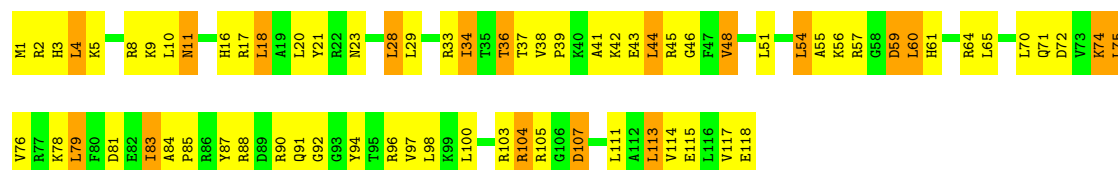
Chain DP:





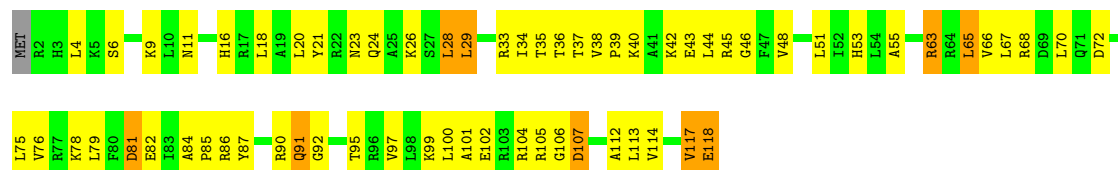
- Molecule 37: 50S ribosomal protein L17

Chain B0:



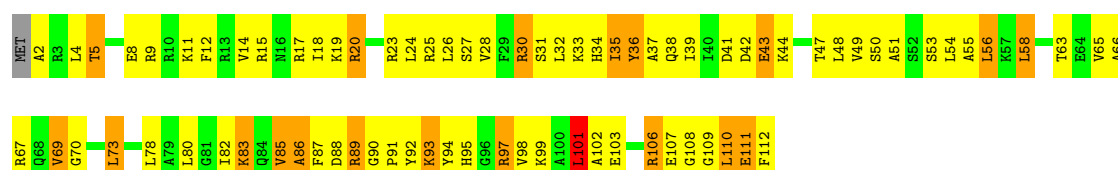
- Molecule 37: 50S ribosomal protein L17

Chain D0:



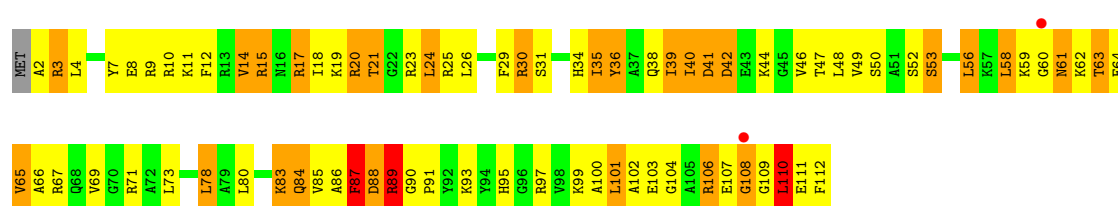
- Molecule 38: 50S ribosomal protein L18

Chain BQ:



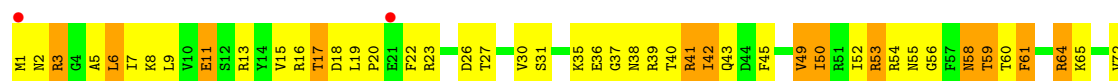
- Molecule 38: 50S ribosomal protein L18

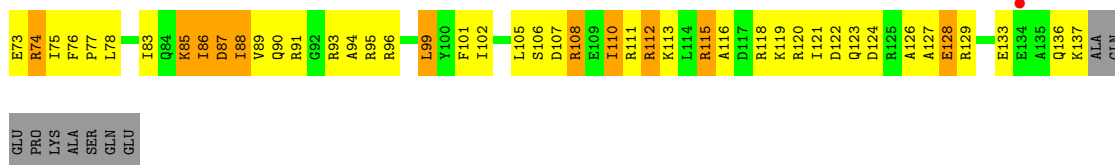
Chain DQ:



- Molecule 39: 50S ribosomal protein L19

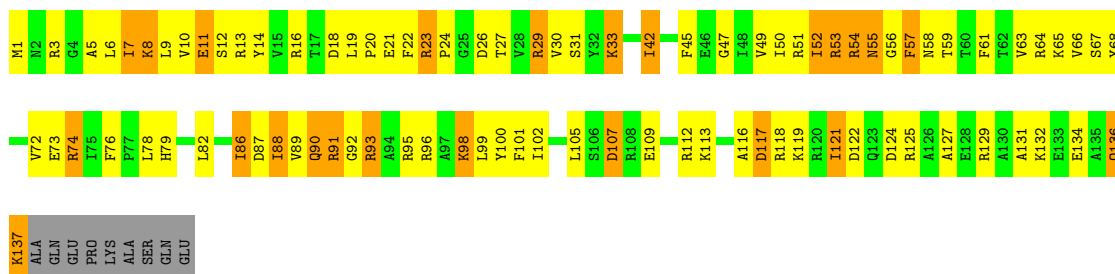
Chain BR:





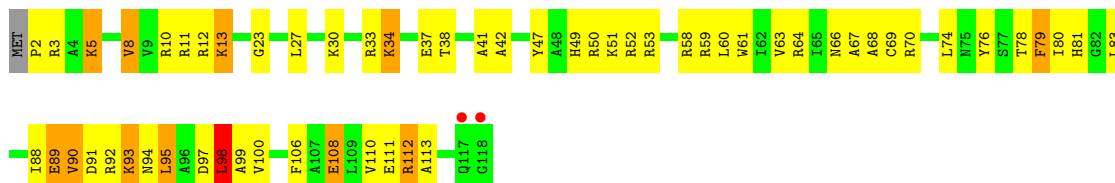
• Molecule 39: 50S ribosomal protein L19

Chain DR:



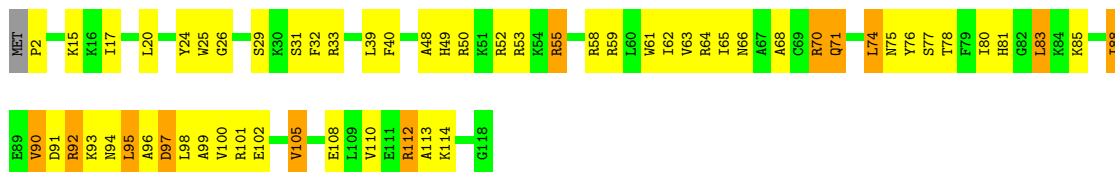
• Molecule 40: 50S ribosomal protein L20

Chain B1:



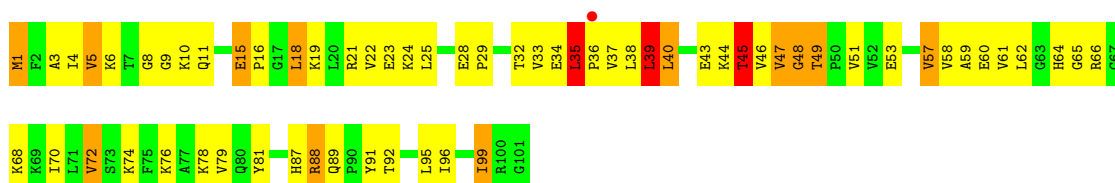
• Molecule 40: 50S ribosomal protein L20

Chain D1:



• Molecule 41: 50S ribosomal protein L21

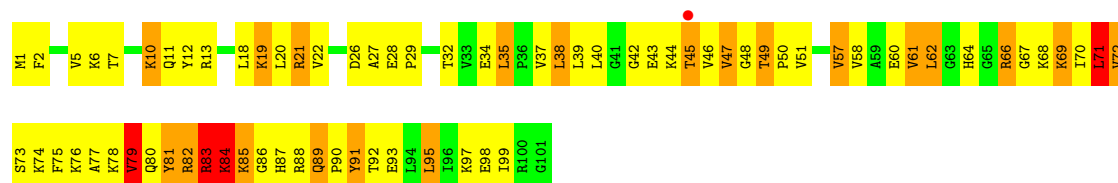
Chain B2:



• Molecule 41: 50S ribosomal protein L21

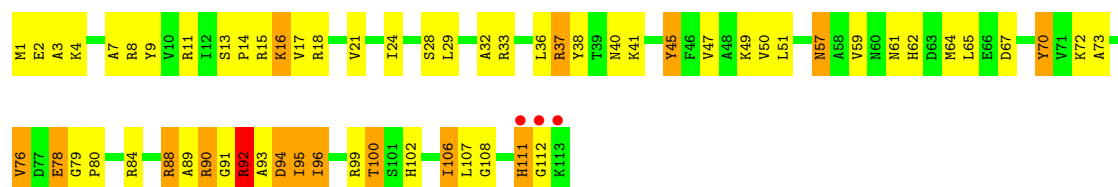
Chain D2:





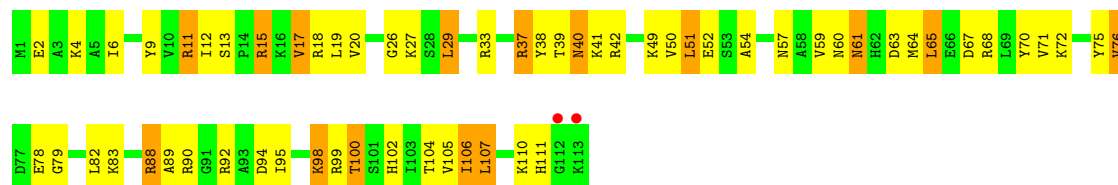
• Molecule 42: 50S ribosomal protein L22

Chain BS:



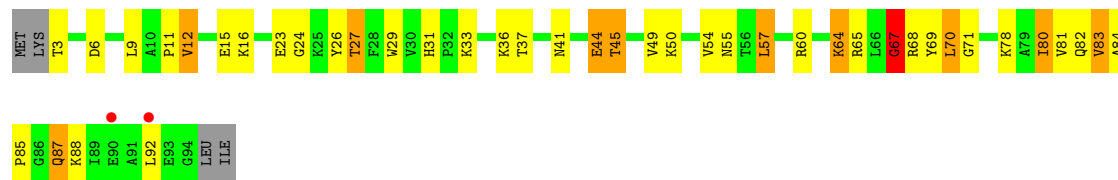
• Molecule 42: 50S ribosomal protein L22

Chain DS:



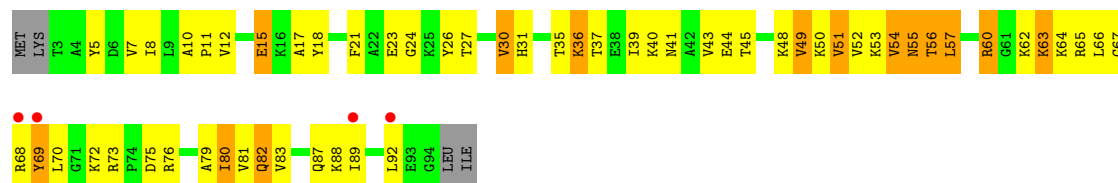
• Molecule 43: 50S ribosomal protein L23

Chain BT:



• Molecule 43: 50S ribosomal protein L23

Chain DT:



• Molecule 44: 50S ribosomal protein L24

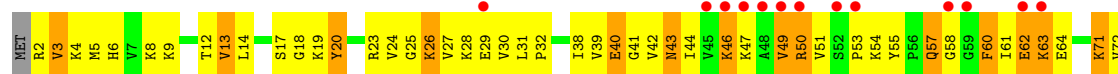
Chain BU:





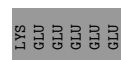
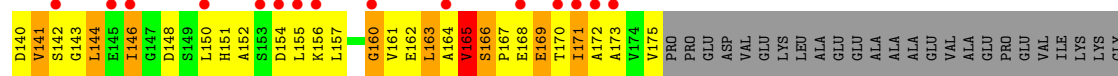
- Molecule 44: 50S ribosomal protein L24

Chain DU:



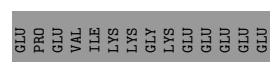
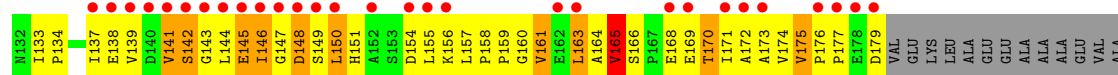
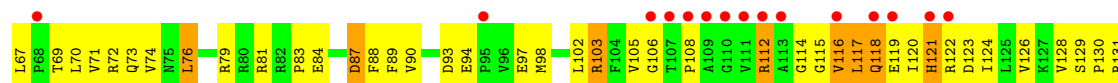
- Molecule 45: 50S ribosomal protein L25

Chain BV:



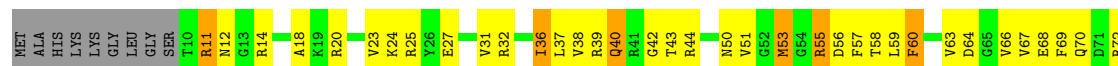
- Molecule 45: 50S ribosomal protein L25

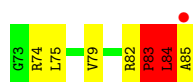
Chain DV:



- Molecule 46: 50S ribosomal protein L27

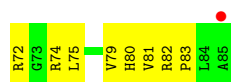
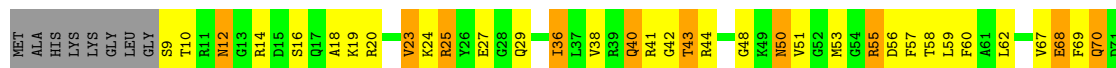
Chain B3:





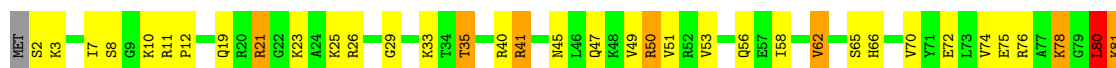
- Molecule 46: 50S ribosomal protein L27

Chain D3:



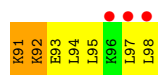
- Molecule 47: 50S ribosomal protein L28

Chain BZ:



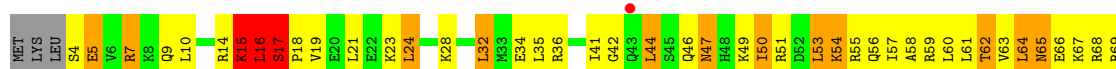
- Molecule 47: 50S ribosomal protein L28

Chain DZ:



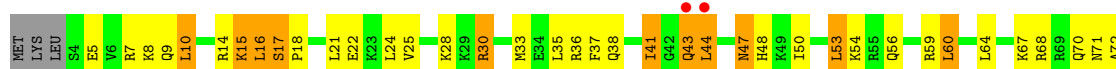
- Molecule 48: 50S ribosomal protein L29

Chain BW:



- Molecule 48: 50S ribosomal protein L29

Chain DW:



- Molecule 49: 50S ribosomal protein L30

Chain BX:



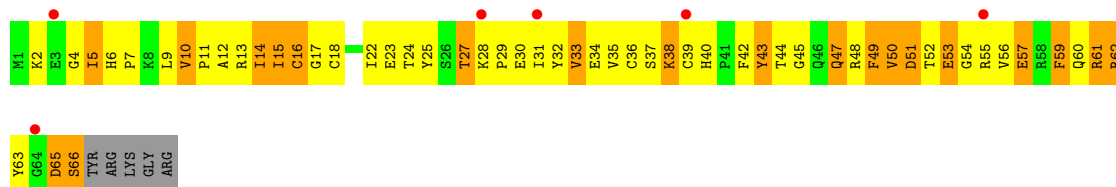
- Molecule 49: 50S ribosomal protein L30

Chain DX:



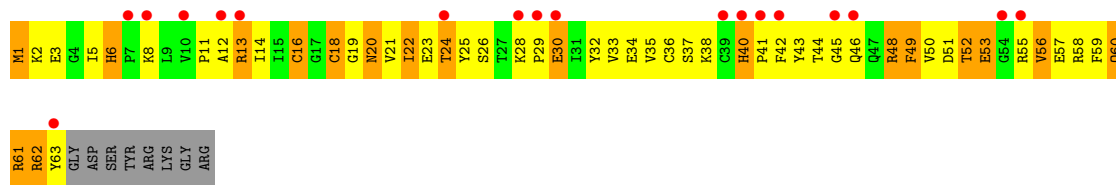
- Molecule 50: 50S ribosomal protein L31

Chain B4:



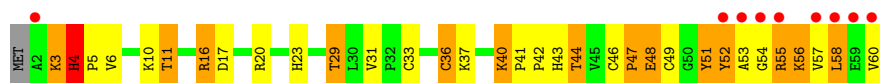
- Molecule 50: 50S ribosomal protein L31

Chain D4:



- Molecule 51: 50S ribosomal protein L32

Chain B5:



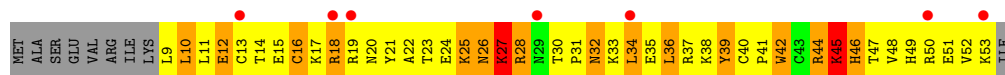
- Molecule 51: 50S ribosomal protein L32

Chain D5:



- Molecule 52: 50S ribosomal protein L33

Chain B6:



- Molecule 52: 50S ribosomal protein L33

Chain D6:



- Molecule 53: 50S ribosomal protein L34

Chain B7:



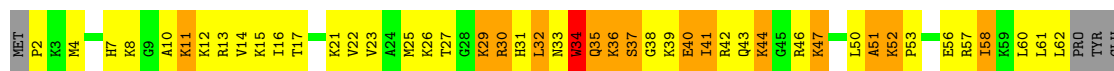
- Molecule 53: 50S ribosomal protein L34

Chain D7:



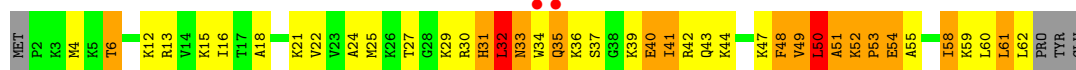
- Molecule 54: 50S ribosomal protein L35

Chain B8:



- Molecule 54: 50S ribosomal protein L35

Chain D8:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.00Å 450.05Å 621.46Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 153.53 – 3.00 153.53 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 94.1 (153.53-3.00) 93.7 (153.53-3.00) | Depositor EDS |
| R_{merge} | 0.25 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.44 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.1_743) | Depositor |
| R, R_{free} | 0.211 , 0.272 0.246 , 0.299 | Depositor DCC |
| R_{free} test set | 928 reflections (0.09%) | DCC |
| Wilson B-factor (Å ²) | 77.4 | Xtriage |
| Anisotropy | 0.190 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 52.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 0 of 1160172 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 299552 | wwPDB-VP |
| Average B, all atoms (Å ²) | 100.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.44 | 5/36234 (0.0%) | 0.91 | 68/56554 (0.1%) |
| 1 | CA | 0.42 | 1/36237 (0.0%) | 0.90 | 79/56558 (0.1%) |
| 2 | AE | 0.29 | 0/1959 | 0.56 | 0/2642 |
| 2 | CE | 0.28 | 0/1959 | 0.53 | 0/2642 |
| 3 | AF | 0.33 | 0/1629 | 0.53 | 0/2195 |
| 3 | CF | 0.31 | 0/1636 | 0.54 | 0/2205 |
| 4 | AG | 0.49 | 2/1733 (0.1%) | 0.62 | 1/2318 (0.0%) |
| 4 | CG | 0.38 | 0/1733 | 0.61 | 0/2318 |
| 5 | AH | 0.35 | 0/1171 | 0.58 | 0/1576 |
| 5 | CH | 0.34 | 0/1171 | 0.56 | 0/1576 |
| 6 | AI | 0.33 | 0/856 | 0.55 | 0/1154 |
| 6 | CI | 0.32 | 0/856 | 0.54 | 0/1154 |
| 7 | AJ | 0.29 | 0/1276 | 0.50 | 0/1709 |
| 7 | CJ | 0.28 | 0/1276 | 0.45 | 0/1709 |
| 8 | AK | 0.33 | 0/1136 | 0.60 | 0/1527 |
| 8 | CK | 0.27 | 0/1136 | 0.51 | 0/1527 |
| 9 | AL | 0.29 | 0/1029 | 0.52 | 0/1379 |
| 9 | CL | 0.29 | 0/1029 | 0.53 | 0/1379 |
| 10 | AM | 0.31 | 0/814 | 0.59 | 1/1095 (0.1%) |
| 10 | CM | 0.28 | 0/814 | 0.54 | 0/1095 |
| 11 | AN | 0.33 | 0/900 | 0.57 | 0/1213 |
| 11 | CN | 0.31 | 0/900 | 0.56 | 0/1213 |
| 12 | AO | 0.40 | 0/991 | 0.68 | 1/1327 (0.1%) |
| 12 | CO | 0.35 | 0/991 | 0.60 | 0/1327 |
| 13 | AP | 0.30 | 0/938 | 0.57 | 0/1258 |
| 13 | CP | 0.28 | 0/943 | 0.52 | 0/1265 |
| 14 | AQ | 0.42 | 0/501 | 0.66 | 1/664 (0.2%) |
| 14 | CQ | 0.29 | 0/501 | 0.58 | 0/664 |
| 15 | AR | 0.35 | 0/745 | 0.58 | 0/992 |
| 15 | CR | 0.30 | 0/745 | 0.51 | 0/992 |
| 16 | AS | 0.29 | 0/721 | 0.53 | 0/970 |
| 16 | CS | 0.31 | 0/721 | 0.58 | 0/970 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AT | 0.35 | 0/847 | 0.54 | 0/1131 |
| 17 | CT | 0.31 | 0/847 | 0.51 | 0/1131 |
| 18 | AU | 0.34 | 0/596 | 0.64 | 0/790 |
| 18 | CU | 0.35 | 0/596 | 0.59 | 0/790 |
| 19 | AV | 0.33 | 0/638 | 0.59 | 0/860 |
| 19 | CV | 0.31 | 0/638 | 0.65 | 0/860 |
| 20 | AW | 0.29 | 0/765 | 0.52 | 0/1007 |
| 20 | CW | 0.32 | 0/765 | 0.63 | 0/1007 |
| 21 | AX | 0.28 | 0/221 | 0.55 | 0/288 |
| 21 | CX | 0.28 | 0/221 | 0.49 | 0/288 |
| 22 | AB | 1.15 | 2/2080 (0.1%) | 1.41 | 25/3242 (0.8%) |
| 22 | CB | 1.34 | 6/2080 (0.3%) | 1.41 | 36/3242 (1.1%) |
| 23 | AC | 1.12 | 3/1835 (0.2%) | 1.69 | 56/2859 (2.0%) |
| 23 | AD | 0.57 | 0/1835 | 0.97 | 7/2859 (0.2%) |
| 23 | CC | 1.08 | 1/1835 (0.1%) | 1.52 | 44/2859 (1.5%) |
| 23 | CD | 0.61 | 0/1835 | 0.98 | 5/2859 (0.2%) |
| 24 | A1 | 1.43 | 2/226 (0.9%) | 1.60 | 7/348 (2.0%) |
| 24 | C1 | 1.57 | 1/226 (0.4%) | 1.73 | 5/348 (1.4%) |
| 25 | BA | 0.59 | 15/70233 (0.0%) | 1.07 | 285/109643 (0.3%) |
| 25 | DA | 0.52 | 13/70122 (0.0%) | 1.00 | 265/109469 (0.2%) |
| 26 | BB | 0.49 | 0/2928 | 0.97 | 9/4568 (0.2%) |
| 26 | DB | 0.44 | 0/2928 | 0.96 | 7/4568 (0.2%) |
| 27 | BD | 0.50 | 0/2165 | 0.80 | 2/2919 (0.1%) |
| 27 | DD | 0.46 | 0/2165 | 0.72 | 0/2919 |
| 28 | BE | 0.38 | 0/1601 | 0.67 | 2/2160 (0.1%) |
| 28 | DE | 0.38 | 0/1601 | 0.69 | 0/2160 |
| 29 | BF | 0.43 | 0/1620 | 0.67 | 0/2194 |
| 29 | DF | 0.36 | 0/1662 | 0.65 | 0/2249 |
| 30 | BG | 0.36 | 0/1499 | 0.60 | 0/2016 |
| 30 | DG | 0.29 | 0/1499 | 0.54 | 0/2016 |
| 31 | BH | 0.36 | 0/1332 | 0.67 | 1/1802 (0.1%) |
| 31 | DH | 0.28 | 0/1332 | 0.55 | 0/1802 |
| 32 | BK | 0.34 | 0/1151 | 0.68 | 1/1558 (0.1%) |
| 32 | DK | 0.33 | 0/1151 | 0.66 | 1/1558 (0.1%) |
| 33 | BM | 0.42 | 0/1131 | 0.69 | 0/1525 |
| 33 | DM | 0.29 | 0/1131 | 0.59 | 0/1525 |
| 34 | BN | 0.40 | 0/943 | 0.64 | 0/1269 |
| 34 | DN | 0.36 | 0/943 | 0.60 | 0/1269 |
| 35 | BO | 0.39 | 0/1162 | 0.76 | 0/1544 |
| 35 | DO | 0.32 | 0/1162 | 0.65 | 1/1544 (0.1%) |
| 36 | BP | 0.52 | 0/1143 | 0.80 | 0/1527 |
| 36 | DP | 0.32 | 0/1143 | 0.54 | 0/1527 |
| 37 | B0 | 0.39 | 0/982 | 0.69 | 0/1312 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 37 | D0 | 0.37 | 0/974 | 0.64 | 0/1302 |
| 38 | BQ | 0.42 | 0/892 | 0.70 | 1/1187 (0.1%) |
| 38 | DQ | 0.30 | 0/892 | 0.62 | 1/1187 (0.1%) |
| 39 | BR | 0.40 | 0/1155 | 0.66 | 0/1542 |
| 39 | DR | 0.37 | 0/1155 | 0.59 | 0/1542 |
| 40 | B1 | 0.42 | 0/982 | 0.67 | 1/1306 (0.1%) |
| 40 | D1 | 0.34 | 0/982 | 0.57 | 0/1306 |
| 41 | B2 | 0.42 | 0/790 | 0.74 | 2/1057 (0.2%) |
| 41 | D2 | 0.32 | 0/790 | 0.59 | 0/1057 |
| 42 | BS | 0.37 | 0/911 | 0.62 | 0/1220 |
| 42 | DS | 0.38 | 0/911 | 0.64 | 0/1220 |
| 43 | BT | 0.50 | 0/739 | 0.68 | 0/993 |
| 43 | DT | 0.47 | 0/739 | 0.62 | 0/993 |
| 44 | BU | 0.45 | 0/798 | 0.68 | 0/1064 |
| 44 | DU | 0.41 | 0/798 | 0.72 | 0/1064 |
| 45 | BV | 0.32 | 0/1427 | 0.63 | 0/1935 |
| 45 | DV | 0.28 | 0/1460 | 0.56 | 0/1982 |
| 46 | B3 | 0.44 | 0/615 | 0.67 | 0/819 |
| 46 | D3 | 0.39 | 0/621 | 0.61 | 0/827 |
| 47 | BZ | 0.42 | 0/770 | 0.73 | 1/1022 (0.1%) |
| 47 | DZ | 0.39 | 0/770 | 0.70 | 0/1022 |
| 48 | BW | 0.53 | 0/560 | 0.72 | 0/741 |
| 48 | DW | 0.37 | 0/583 | 0.63 | 0/771 |
| 49 | BX | 0.36 | 0/474 | 0.64 | 1/635 (0.2%) |
| 49 | DX | 0.32 | 0/474 | 0.53 | 0/635 |
| 50 | B4 | 0.34 | 0/545 | 0.72 | 1/733 (0.1%) |
| 50 | D4 | 0.32 | 0/527 | 0.67 | 0/709 |
| 51 | B5 | 0.43 | 0/473 | 0.69 | 0/639 |
| 51 | D5 | 0.34 | 0/468 | 0.70 | 0/632 |
| 52 | B6 | 0.43 | 0/396 | 0.70 | 0/529 |
| 52 | D6 | 0.33 | 0/396 | 0.63 | 0/529 |
| 53 | B7 | 0.46 | 0/438 | 0.68 | 0/575 |
| 53 | D7 | 0.40 | 0/438 | 0.59 | 0/575 |
| 54 | B8 | 0.52 | 0/494 | 0.71 | 0/649 |
| 54 | D8 | 0.38 | 0/494 | 0.71 | 1/649 (0.2%) |
| All | All | 0.51 | 51/324027 (0.0%) | 0.93 | 919/485226 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 2 | AE | 0 | 3 |
| 2 | CE | 0 | 5 |
| 3 | CF | 0 | 1 |
| 4 | AG | 0 | 1 |
| 8 | AK | 0 | 1 |
| 10 | AM | 0 | 1 |
| 12 | AO | 0 | 2 |
| 14 | AQ | 0 | 1 |
| 14 | CQ | 0 | 2 |
| 15 | AR | 0 | 1 |
| 19 | CV | 0 | 1 |
| 20 | CW | 0 | 1 |
| 27 | BD | 0 | 6 |
| 27 | DD | 0 | 3 |
| 28 | BE | 0 | 1 |
| 28 | DE | 0 | 6 |
| 29 | DF | 0 | 2 |
| 30 | BG | 0 | 1 |
| 30 | DG | 0 | 1 |
| 31 | BH | 0 | 2 |
| 31 | DH | 0 | 2 |
| 32 | BK | 0 | 3 |
| 32 | DK | 0 | 4 |
| 33 | BM | 0 | 1 |
| 35 | BO | 0 | 4 |
| 35 | DO | 0 | 3 |
| 36 | BP | 0 | 3 |
| 37 | D0 | 0 | 2 |
| 38 | BQ | 0 | 1 |
| 38 | DQ | 0 | 2 |
| 39 | BR | 0 | 2 |
| 40 | B1 | 0 | 1 |
| 40 | D1 | 0 | 1 |
| 41 | B2 | 0 | 1 |
| 43 | BT | 0 | 1 |
| 44 | DU | 0 | 2 |
| 45 | BV | 0 | 3 |
| 45 | DV | 0 | 2 |
| 46 | B3 | 0 | 2 |
| 48 | BW | 0 | 2 |
| 48 | DW | 0 | 1 |
| 50 | B4 | 0 | 4 |
| 50 | D4 | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 51 | B5 | 0 | 1 |
| 51 | D5 | 0 | 1 |
| 52 | B6 | 0 | 1 |
| 52 | D6 | 0 | 1 |
| 53 | B7 | 0 | 1 |
| 54 | B8 | 0 | 2 |
| 54 | D8 | 0 | 1 |
| All | All | 0 | 99 |

All (51) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 25 | DA | 1143 | A | N7-C5 | -11.10 | 1.32 | 1.39 |
| 4 | AG | 12 | CYS | CB-SG | 10.86 | 2.00 | 1.82 |
| 25 | DA | 2873 | A | N7-C5 | -10.30 | 1.33 | 1.39 |
| 25 | DA | 1342 | A | N7-C5 | -9.87 | 1.33 | 1.39 |
| 25 | BA | 2430 | A | N9-C4 | -9.40 | 1.32 | 1.37 |
| 22 | CB | 50 | A | N9-C4 | 8.39 | 1.42 | 1.37 |
| 4 | AG | 26 | CYS | CB-SG | 8.33 | 1.96 | 1.82 |
| 23 | CC | 77 | A | N9-C4 | -8.02 | 1.33 | 1.37 |
| 25 | BA | 774 | A | N9-C4 | -7.18 | 1.33 | 1.37 |
| 22 | CB | 36 | A | N9-C4 | 6.90 | 1.42 | 1.37 |
| 25 | DA | 783 | A | N9-C4 | -6.86 | 1.33 | 1.37 |
| 1 | AA | 1159 | U | N1-C2 | 6.80 | 1.44 | 1.38 |
| 1 | AA | 1177 | G | C5-C6 | 6.66 | 1.49 | 1.42 |
| 25 | BA | 783 | A | C5-C6 | -6.64 | 1.35 | 1.41 |
| 22 | AB | 69 | A | N9-C4 | 6.47 | 1.41 | 1.37 |
| 25 | BA | 2287 | A | N9-C4 | -6.46 | 1.33 | 1.37 |
| 25 | BA | 528 | A | N9-C4 | -6.43 | 1.33 | 1.37 |
| 25 | BA | 676 | A | N9-C4 | -6.41 | 1.34 | 1.37 |
| 24 | C1 | 13 | U | N1-C2 | 6.33 | 1.44 | 1.38 |
| 25 | DA | 2287 | A | N9-C4 | -6.29 | 1.34 | 1.37 |
| 25 | BA | 807 | U | C2-N3 | 6.26 | 1.42 | 1.37 |
| 25 | BA | 783 | A | N9-C4 | -6.26 | 1.34 | 1.37 |
| 23 | AC | 77 | A | N9-C4 | -6.08 | 1.34 | 1.37 |
| 25 | DA | 2681 | C | N3-C4 | -6.08 | 1.29 | 1.33 |
| 25 | BA | 1021 | A | N9-C4 | -6.07 | 1.34 | 1.37 |
| 24 | A1 | 14 | U | N1-C2 | 6.05 | 1.44 | 1.38 |
| 25 | DA | 2430 | A | N9-C4 | -6.01 | 1.34 | 1.37 |
| 23 | AC | 1 | C | N1-C6 | 5.98 | 1.40 | 1.37 |
| 25 | DA | 9 | U | C2-N3 | 5.93 | 1.42 | 1.37 |
| 1 | CA | 1177 | G | C5-C6 | 5.92 | 1.48 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 22 | AB | 87 | A | C5-C4 | 5.88 | 1.42 | 1.38 |
| 1 | AA | 1036 | G | C5-C6 | 5.82 | 1.48 | 1.42 |
| 1 | AA | 1025 | U | N3-C4 | 5.77 | 1.43 | 1.38 |
| 25 | DA | 807 | U | C2-N3 | 5.62 | 1.41 | 1.37 |
| 25 | BA | 1899 | G | N9-C4 | -5.61 | 1.33 | 1.38 |
| 1 | AA | 1036 | G | C6-O6 | 5.52 | 1.29 | 1.24 |
| 25 | DA | 2629 | A | N7-C5 | -5.52 | 1.35 | 1.39 |
| 25 | BA | 676 | A | N3-C4 | -5.46 | 1.31 | 1.34 |
| 25 | BA | 1899 | G | C8-N7 | 5.39 | 1.34 | 1.30 |
| 23 | AC | 70 | C | N1-C6 | 5.37 | 1.40 | 1.37 |
| 25 | BA | 783 | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 22 | CB | 69 | A | N9-C4 | 5.34 | 1.41 | 1.37 |
| 22 | CB | 52 | U | N1-C2 | 5.31 | 1.43 | 1.38 |
| 25 | DA | 2720 | U | C2-N3 | 5.29 | 1.41 | 1.37 |
| 25 | BA | 1142(A) | A | N9-C4 | -5.23 | 1.34 | 1.37 |
| 24 | A1 | 13 | U | N1-C2 | 5.21 | 1.43 | 1.38 |
| 22 | CB | 54 | G | N7-C5 | 5.15 | 1.42 | 1.39 |
| 22 | CB | 40 | G | C6-N1 | 5.08 | 1.43 | 1.39 |
| 25 | BA | 120 | U | N3-C4 | -5.08 | 1.33 | 1.38 |
| 25 | DA | 783 | A | C5-C6 | -5.04 | 1.36 | 1.41 |
| 25 | DA | 2503 | A | C8-N7 | 5.00 | 1.35 | 1.31 |

All (919) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 25 | BA | 1899 | G | N3-C4-N9 | -15.77 | 116.54 | 126.00 |
| 1 | AA | 1025 | U | C5-C4-O4 | -15.29 | 116.72 | 125.90 |
| 1 | AA | 1177 | G | N9-C4-C5 | 14.63 | 111.25 | 105.40 |
| 1 | AA | 1177 | G | C4-C5-N7 | -14.21 | 105.12 | 110.80 |
| 25 | DA | 1899 | G | N3-C4-N9 | -13.25 | 118.05 | 126.00 |
| 25 | BA | 783 | A | C5-N7-C8 | -13.12 | 97.34 | 103.90 |
| 25 | DA | 933 | A | C6-C5-N7 | -13.01 | 123.19 | 132.30 |
| 22 | AB | 87 | A | N7-C8-N9 | 13.00 | 120.30 | 113.80 |
| 25 | BA | 1899 | G | C8-N9-C1' | 12.84 | 143.69 | 127.00 |
| 25 | DA | 2873 | A | N1-C6-N6 | 12.47 | 126.08 | 118.60 |
| 1 | CA | 1036 | G | N9-C4-C5 | 12.37 | 110.35 | 105.40 |
| 1 | CA | 1036 | G | C5-C6-O6 | 12.37 | 136.02 | 128.60 |
| 25 | DA | 783 | A | C5-N7-C8 | -12.27 | 97.76 | 103.90 |
| 1 | AA | 1177 | G | N1-C6-O6 | -12.25 | 112.55 | 119.90 |
| 1 | CA | 1177 | G | N9-C4-C5 | 12.23 | 110.29 | 105.40 |
| 25 | DA | 1602 | U | C2-N3-C4 | -12.13 | 119.72 | 127.00 |
| 1 | CA | 1025 | U | C5-C4-O4 | -12.12 | 118.63 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | AA | 1036 | G | C5-C6-O6 | 12.06 | 135.84 | 128.60 |
| 25 | DA | 933 | A | C4-N9-C1' | 11.91 | 147.74 | 126.30 |
| 23 | AC | 6 | G | C8-N9-C4 | 11.81 | 111.13 | 106.40 |
| 1 | CA | 1177 | G | C4-C5-N7 | -11.64 | 106.14 | 110.80 |
| 1 | AA | 1036 | G | C8-N9-C4 | -11.63 | 101.75 | 106.40 |
| 1 | CA | 1036 | G | C4-C5-N7 | -11.60 | 106.16 | 110.80 |
| 25 | DA | 1899 | G | C8-N9-C1' | 11.53 | 141.99 | 127.00 |
| 1 | AA | 97 | U | N1-C2-O2 | 11.42 | 130.79 | 122.80 |
| 25 | BA | 1899 | G | N3-C4-C5 | 11.41 | 134.30 | 128.60 |
| 25 | DA | 2873 | A | C6-C5-N7 | -11.40 | 124.32 | 132.30 |
| 25 | BA | 633 | A | N1-C6-N6 | 11.38 | 125.43 | 118.60 |
| 1 | CA | 993 | G | N3-C4-N9 | 11.37 | 132.82 | 126.00 |
| 1 | AA | 1036 | G | N9-C4-C5 | 11.32 | 109.93 | 105.40 |
| 25 | DA | 933 | A | C8-N9-C1' | -11.29 | 107.38 | 127.70 |
| 22 | AB | 87 | A | C8-N9-C4 | -11.24 | 101.31 | 105.80 |
| 1 | CA | 1177 | G | N1-C6-O6 | -11.20 | 113.18 | 119.90 |
| 1 | CA | 1036 | G | N1-C6-O6 | -11.19 | 113.19 | 119.90 |
| 1 | AA | 1177 | G | C5-C6-O6 | 11.18 | 135.31 | 128.60 |
| 25 | BA | 2447 | G | C6-N1-C2 | -11.17 | 118.40 | 125.10 |
| 1 | AA | 1036 | G | C4-C5-N7 | -11.13 | 106.35 | 110.80 |
| 25 | DA | 1143 | A | C4-C5-C6 | 11.09 | 122.54 | 117.00 |
| 25 | DA | 2873 | A | C4-C5-C6 | 10.97 | 122.48 | 117.00 |
| 25 | BA | 1899 | G | C4-N9-C1' | -10.85 | 112.40 | 126.50 |
| 25 | DA | 1012 | U | C2-N3-C4 | -10.79 | 120.53 | 127.00 |
| 22 | AB | 87 | A | C5-N7-C8 | -10.79 | 98.51 | 103.90 |
| 25 | BA | 676 | A | C2-N3-C4 | -10.69 | 105.26 | 110.60 |
| 25 | DA | 1899 | G | C4-N9-C1' | -10.68 | 112.61 | 126.50 |
| 25 | BA | 2430 | A | C2-N3-C4 | -10.67 | 105.27 | 110.60 |
| 1 | CA | 1177 | G | C5-C6-O6 | 10.56 | 134.94 | 128.60 |
| 25 | DA | 1342 | A | N1-C6-N6 | 10.51 | 124.91 | 118.60 |
| 26 | BB | 95 | U | C5-C4-O4 | 10.49 | 132.20 | 125.90 |
| 25 | BA | 783 | A | C4-C5-N7 | 10.45 | 115.92 | 110.70 |
| 25 | DA | 2720 | U | C2-N3-C4 | -10.34 | 120.79 | 127.00 |
| 25 | BA | 673 | C | C2-N3-C4 | -10.31 | 114.75 | 119.90 |
| 25 | BA | 120 | U | C5-C4-O4 | 10.28 | 132.07 | 125.90 |
| 25 | DA | 933 | A | C4-C5-C6 | 10.24 | 122.12 | 117.00 |
| 25 | DA | 933 | A | N3-C4-N9 | 10.17 | 135.53 | 127.40 |
| 1 | AA | 1159 | U | N3-C2-O2 | -10.12 | 115.12 | 122.20 |
| 25 | BA | 673 | C | C5-C4-N4 | -10.05 | 113.16 | 120.20 |
| 25 | DA | 2598 | A | N1-C6-N6 | 10.02 | 124.61 | 118.60 |
| 1 | AA | 1036 | G | N1-C6-O6 | -10.01 | 113.89 | 119.90 |
| 25 | BA | 2430 | A | N3-C4-C5 | 9.83 | 133.68 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | BA | 1786 | A | C2-N3-C4 | -9.76 | 105.72 | 110.60 |
| 1 | CA | 993 | G | C4-N9-C1' | 9.73 | 139.15 | 126.50 |
| 1 | CA | 1177 | G | C8-N9-C4 | -9.69 | 102.52 | 106.40 |
| 25 | BA | 906 | G | C5-C6-O6 | 9.64 | 134.38 | 128.60 |
| 25 | DA | 933 | A | C6-N1-C2 | -9.63 | 112.82 | 118.60 |
| 25 | DA | 1143 | A | N1-C2-N3 | 9.52 | 134.06 | 129.30 |
| 25 | BA | 774 | A | C2-N3-C4 | -9.51 | 105.84 | 110.60 |
| 26 | DB | 95 | U | C5-C4-O4 | 9.51 | 131.61 | 125.90 |
| 1 | CA | 993 | G | C8-N9-C1' | -9.48 | 114.67 | 127.00 |
| 25 | DA | 1342 | A | C4-C5-C6 | 9.47 | 121.74 | 117.00 |
| 25 | BA | 783 | A | N1-C6-N6 | 9.46 | 124.27 | 118.60 |
| 1 | AA | 1495 | U | N1-C2-O2 | 9.45 | 129.42 | 122.80 |
| 25 | DA | 1342 | A | C6-C5-N7 | -9.44 | 125.69 | 132.30 |
| 25 | DA | 1781 | C | C2-N1-C1' | 9.42 | 129.16 | 118.80 |
| 25 | BA | 2447 | G | N3-C4-C5 | -9.41 | 123.89 | 128.60 |
| 25 | BA | 1899 | G | N9-C4-C5 | 9.37 | 109.15 | 105.40 |
| 25 | DA | 1899 | G | N3-C4-C5 | 9.23 | 133.22 | 128.60 |
| 25 | BA | 774 | A | N3-C4-N9 | -9.21 | 120.03 | 127.40 |
| 22 | CB | 35 | G | N1-C6-O6 | 9.17 | 125.40 | 119.90 |
| 22 | CB | 35 | G | C5-C6-O6 | -9.12 | 123.12 | 128.60 |
| 23 | AC | 6 | G | N3-C4-C5 | 9.10 | 133.15 | 128.60 |
| 25 | BA | 676 | A | C5-N7-C8 | -9.10 | 99.35 | 103.90 |
| 25 | BA | 2681 | C | C6-N1-C2 | -9.10 | 116.66 | 120.30 |
| 1 | AA | 1159 | U | N1-C2-O2 | 9.10 | 129.17 | 122.80 |
| 25 | DA | 783 | A | C4-C5-N7 | 9.05 | 115.23 | 110.70 |
| 1 | AA | 1054 | C | C2-N1-C1' | 9.05 | 128.75 | 118.80 |
| 25 | DA | 1786 | A | N7-C8-N9 | 9.03 | 118.31 | 113.80 |
| 1 | AA | 97 | U | N3-C2-O2 | -9.02 | 115.89 | 122.20 |
| 25 | DA | 1786 | A | C5-N7-C8 | -8.95 | 99.43 | 103.90 |
| 1 | CA | 1495 | U | N1-C2-O2 | 8.93 | 129.05 | 122.80 |
| 25 | BA | 1786 | A | N7-C8-N9 | 8.90 | 118.25 | 113.80 |
| 1 | CA | 1045 | C | N1-C2-O2 | 8.88 | 124.22 | 118.90 |
| 25 | DA | 2873 | A | C5-C6-N1 | -8.85 | 113.27 | 117.70 |
| 23 | AC | 76 | C | N1-C2-O2 | -8.83 | 113.60 | 118.90 |
| 25 | BA | 446 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 25 | BA | 1312 | U | C5-C4-O4 | 8.82 | 131.19 | 125.90 |
| 25 | DA | 933 | A | N9-C4-C5 | -8.82 | 102.27 | 105.80 |
| 1 | AA | 1177 | G | C8-N9-C4 | -8.81 | 102.88 | 106.40 |
| 22 | AB | 87 | A | C6-C5-N7 | -8.81 | 126.14 | 132.30 |
| 25 | BA | 2430 | A | N3-C4-N9 | -8.78 | 120.38 | 127.40 |
| 1 | AA | 1025 | U | N1-C2-O2 | 8.73 | 128.91 | 122.80 |
| 25 | BA | 783 | A | N7-C8-N9 | 8.72 | 118.16 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 2681 | C | C5-C4-N4 | 8.71 | 126.30 | 120.20 |
| 25 | BA | 807 | U | C2-N3-C4 | -8.70 | 121.78 | 127.00 |
| 25 | DA | 807 | U | C2-N3-C4 | -8.69 | 121.79 | 127.00 |
| 1 | AA | 1025 | U | C6-N1-C1' | -8.68 | 109.05 | 121.20 |
| 25 | DA | 1143 | A | C6-C5-N7 | -8.66 | 126.24 | 132.30 |
| 25 | DA | 2447 | G | N3-C4-C5 | -8.65 | 124.28 | 128.60 |
| 1 | AA | 1177 | G | C6-C5-N7 | 8.64 | 135.59 | 130.40 |
| 25 | BA | 1899 | G | C2-N3-C4 | -8.64 | 107.58 | 111.90 |
| 25 | DA | 9 | U | C2-N3-C4 | -8.58 | 121.85 | 127.00 |
| 1 | AA | 1025 | U | N3-C4-C5 | 8.53 | 119.72 | 114.60 |
| 1 | CA | 1036 | G | C8-N9-C4 | -8.53 | 102.99 | 106.40 |
| 25 | BA | 2287 | A | C2-N3-C4 | -8.53 | 106.34 | 110.60 |
| 1 | CA | 266 | G | N1-C6-O6 | -8.47 | 114.82 | 119.90 |
| 23 | CC | 21 | U | N3-C2-O2 | -8.47 | 116.27 | 122.20 |
| 25 | BA | 1786 | A | C5-N7-C8 | -8.46 | 99.67 | 103.90 |
| 25 | DA | 2503 | A | C8-N9-C4 | -8.46 | 102.42 | 105.80 |
| 25 | BA | 906 | G | N3-C4-N9 | -8.45 | 120.93 | 126.00 |
| 25 | BA | 1314 | C | C2-N1-C1' | 8.46 | 128.10 | 118.80 |
| 25 | DA | 1143 | A | N1-C6-N6 | 8.45 | 123.67 | 118.60 |
| 25 | BA | 783 | A | C6-C5-N7 | -8.44 | 126.39 | 132.30 |
| 25 | BA | 676 | A | N7-C8-N9 | 8.43 | 118.02 | 113.80 |
| 25 | DA | 103 | A | N1-C6-N6 | 8.43 | 123.66 | 118.60 |
| 25 | BA | 1332 | G | C2-N3-C4 | -8.43 | 107.69 | 111.90 |
| 1 | AA | 1436 | U | C2-N3-C4 | -8.38 | 121.97 | 127.00 |
| 25 | DA | 783 | A | N7-C8-N9 | 8.37 | 117.98 | 113.80 |
| 1 | AA | 1465 | C | C2-N3-C4 | -8.36 | 115.72 | 119.90 |
| 1 | CA | 1025 | U | C2-N1-C1' | 8.35 | 127.72 | 117.70 |
| 1 | CA | 993 | G | C6-C5-N7 | -8.35 | 125.39 | 130.40 |
| 25 | DA | 1899 | G | N9-C4-C5 | 8.33 | 108.73 | 105.40 |
| 22 | AB | 87 | A | C4-C5-N7 | 8.33 | 114.86 | 110.70 |
| 25 | BA | 673 | C | N1-C2-O2 | -8.31 | 113.92 | 118.90 |
| 1 | CA | 1045 | C | C2-N1-C1' | 8.30 | 127.93 | 118.80 |
| 25 | DA | 250 | G | N3-C2-N2 | 8.30 | 125.71 | 119.90 |
| 25 | DA | 933 | A | N1-C2-N3 | 8.27 | 133.44 | 129.30 |
| 25 | BA | 140 | A | N7-C8-N9 | 8.26 | 117.93 | 113.80 |
| 23 | CC | 77 | A | C8-N9-C4 | 8.23 | 109.09 | 105.80 |
| 25 | DA | 847 | U | C5-C4-O4 | 8.23 | 130.84 | 125.90 |
| 22 | AB | 18 | G | C4-N9-C1' | -8.19 | 115.85 | 126.50 |
| 25 | DA | 1332 | G | C2-N3-C4 | -8.16 | 107.82 | 111.90 |
| 1 | CA | 1025 | U | C6-N1-C1' | -8.15 | 109.79 | 121.20 |
| 23 | AC | 6 | G | N7-C8-N9 | -8.14 | 109.03 | 113.10 |
| 25 | BA | 774 | A | N3-C4-C5 | 8.13 | 132.49 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 25 | DA | 1143 | A | C8-N9-C4 | -8.13 | 102.55 | 105.80 |
| 25 | BA | 633 | A | C4-C5-C6 | 8.11 | 121.06 | 117.00 |
| 23 | CC | 77 | A | N3-C4-C5 | 8.09 | 132.46 | 126.80 |
| 22 | AB | 87 | A | N1-C6-N6 | 8.07 | 123.44 | 118.60 |
| 25 | DA | 2447 | G | C5-C6-O6 | -8.04 | 123.78 | 128.60 |
| 25 | BA | 847 | U | C5-C4-O4 | 8.03 | 130.72 | 125.90 |
| 25 | DA | 673 | C | C2-N3-C4 | -8.01 | 115.89 | 119.90 |
| 24 | C1 | 16 | A | N1-C6-N6 | 8.00 | 123.40 | 118.60 |
| 25 | DA | 2681 | C | N3-C4-N4 | -7.99 | 112.41 | 118.00 |
| 25 | DA | 933 | A | C4-C5-N7 | 7.97 | 114.68 | 110.70 |
| 25 | DA | 383 | U | N1-C2-O2 | 7.94 | 128.36 | 122.80 |
| 25 | BA | 140 | A | C5-N7-C8 | -7.93 | 99.93 | 103.90 |
| 25 | DA | 933 | A | C5-C6-N6 | -7.93 | 117.36 | 123.70 |
| 25 | BA | 1332 | G | C5-N7-C8 | -7.92 | 100.34 | 104.30 |
| 22 | CB | 85 | C | N1-C2-O2 | 7.91 | 123.64 | 118.90 |
| 23 | AC | 6 | G | C4-N9-C1' | -7.90 | 116.23 | 126.50 |
| 25 | BA | 676 | A | C8-N9-C4 | -7.87 | 102.65 | 105.80 |
| 25 | BA | 2447 | G | C5-C6-N1 | 7.84 | 115.42 | 111.50 |
| 23 | AC | 40 | C | C6-N1-C2 | -7.84 | 117.17 | 120.30 |
| 25 | DA | 2629 | A | N1-C6-N6 | 7.82 | 123.29 | 118.60 |
| 25 | DA | 1143 | A | C2-N3-C4 | -7.80 | 106.70 | 110.60 |
| 25 | BA | 633 | A | C6-C5-N7 | -7.79 | 126.84 | 132.30 |
| 25 | DA | 2430 | A | C2-N3-C4 | -7.77 | 106.71 | 110.60 |
| 1 | CA | 270 | A | C5-N7-C8 | -7.76 | 100.02 | 103.90 |
| 25 | BA | 780 | G | C5-C6-O6 | -7.75 | 123.95 | 128.60 |
| 25 | BA | 1142(A) | A | C5-N7-C8 | -7.75 | 100.03 | 103.90 |
| 25 | BA | 2375 | G | C8-N9-C4 | 7.70 | 109.48 | 106.40 |
| 1 | CA | 993 | G | N3-C4-C5 | -7.68 | 124.76 | 128.60 |
| 25 | DA | 9 | U | C5-C4-O4 | -7.67 | 121.30 | 125.90 |
| 25 | BA | 906 | G | N9-C4-C5 | 7.66 | 108.47 | 105.40 |
| 25 | BA | 676 | A | N3-C4-N9 | -7.64 | 121.29 | 127.40 |
| 25 | DA | 783 | A | N1-C6-N6 | 7.63 | 123.18 | 118.60 |
| 25 | BA | 138 | G | C8-N9-C4 | -7.62 | 103.35 | 106.40 |
| 25 | BA | 1786 | A | C8-N9-C4 | -7.62 | 102.75 | 105.80 |
| 25 | DA | 774 | A | C2-N3-C4 | -7.62 | 106.79 | 110.60 |
| 25 | DA | 2275 | C | C6-N1-C2 | -7.62 | 117.25 | 120.30 |
| 25 | BA | 893 | C | C2-N1-C1' | 7.60 | 127.16 | 118.80 |
| 25 | DA | 2873 | A | C2-N3-C4 | -7.58 | 106.81 | 110.60 |
| 25 | DA | 530 | G | C6-C5-N7 | -7.57 | 125.86 | 130.40 |
| 35 | DO | 147 | LEU | CA-CB-CG | 7.57 | 132.70 | 115.30 |
| 25 | BA | 210 | C | C6-N1-C2 | 7.56 | 123.33 | 120.30 |
| 4 | AG | 12 | CYS | CA-CB-SG | 7.54 | 127.56 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 906 | G | C5-C6-O6 | 7.53 | 133.12 | 128.60 |
| 1 | AA | 1053 | G | C4-N9-C1' | -7.49 | 116.76 | 126.50 |
| 1 | AA | 1036 | G | N3-C4-C5 | -7.48 | 124.86 | 128.60 |
| 25 | BA | 783 | A | C2-N3-C4 | -7.48 | 106.86 | 110.60 |
| 25 | BA | 1678 | G | C2-N3-C4 | -7.47 | 108.16 | 111.90 |
| 25 | BA | 528 | A | N3-C4-C5 | 7.47 | 132.03 | 126.80 |
| 25 | BA | 1496 | A | C8-N9-C4 | -7.47 | 102.81 | 105.80 |
| 1 | CA | 993 | G | N9-C4-C5 | -7.47 | 102.41 | 105.40 |
| 25 | DA | 530 | G | N1-C6-O6 | 7.46 | 124.38 | 119.90 |
| 24 | A1 | 16 | A | C8-N9-C4 | 7.43 | 108.77 | 105.80 |
| 25 | DA | 673 | C | C5-C4-N4 | -7.42 | 115.01 | 120.20 |
| 25 | DA | 1781 | C | C6-N1-C1' | -7.42 | 111.90 | 120.80 |
| 25 | DA | 933 | A | N7-C8-N9 | 7.42 | 117.51 | 113.80 |
| 25 | BA | 613 | U | C5-C4-O4 | 7.41 | 130.35 | 125.90 |
| 25 | DA | 530 | G | C4-C5-N7 | 7.41 | 113.77 | 110.80 |
| 25 | BA | 250 | G | N3-C2-N2 | 7.35 | 125.05 | 119.90 |
| 25 | BA | 933 | A | C6-N1-C2 | -7.34 | 114.20 | 118.60 |
| 38 | DQ | 110 | LEU | CA-CB-CG | 7.34 | 132.18 | 115.30 |
| 25 | BA | 1698 | A | C2-N3-C4 | -7.33 | 106.94 | 110.60 |
| 1 | CA | 1036 | G | C6-C5-N7 | 7.33 | 134.80 | 130.40 |
| 25 | DA | 9 | U | N1-C2-O2 | -7.33 | 117.67 | 122.80 |
| 25 | BA | 1678 | G | C5-N7-C8 | -7.32 | 100.64 | 104.30 |
| 1 | CA | 993 | G | N3-C2-N2 | 7.31 | 125.02 | 119.90 |
| 25 | BA | 528 | A | N3-C4-N9 | -7.30 | 121.56 | 127.40 |
| 23 | AC | 23 | G | C8-N9-C4 | -7.30 | 103.48 | 106.40 |
| 23 | CC | 15 | G | C5-C6-O6 | 7.29 | 132.98 | 128.60 |
| 25 | BA | 2375 | G | N9-C4-C5 | -7.29 | 102.49 | 105.40 |
| 25 | DA | 2447 | G | C6-N1-C2 | -7.28 | 120.73 | 125.10 |
| 25 | BA | 1314 | C | C6-N1-C1' | -7.26 | 112.09 | 120.80 |
| 26 | DB | 81 | G | C5-C6-O6 | -7.26 | 124.25 | 128.60 |
| 26 | BB | 81 | G | C5-C6-O6 | -7.25 | 124.25 | 128.60 |
| 25 | BA | 138 | G | N7-C8-N9 | 7.25 | 116.72 | 113.10 |
| 25 | DA | 2159 | G | N3-C4-N9 | 7.24 | 130.35 | 126.00 |
| 25 | BA | 2451 | A | C5-N7-C8 | -7.22 | 100.29 | 103.90 |
| 22 | CB | 85 | C | C2-N1-C1' | 7.21 | 126.73 | 118.80 |
| 25 | DA | 2451 | A | C5-N7-C8 | -7.19 | 100.30 | 103.90 |
| 25 | DA | 633 | A | C4-C5-C6 | 7.15 | 120.57 | 117.00 |
| 25 | BA | 446 | G | N9-C4-C5 | -7.14 | 102.54 | 105.40 |
| 25 | DA | 2447 | G | N1-C6-O6 | 7.14 | 124.19 | 119.90 |
| 25 | DA | 630 | G | C2-N3-C4 | -7.14 | 108.33 | 111.90 |
| 23 | AC | 25 | U | N3-C2-O2 | -7.12 | 117.22 | 122.20 |
| 25 | BA | 1506 | C | C2-N1-C1' | 7.11 | 126.63 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 1332 | G | N3-C4-N9 | -7.11 | 121.73 | 126.00 |
| 25 | DA | 2447 | G | N3-C4-N9 | 7.11 | 130.26 | 126.00 |
| 25 | BA | 1340 | U | C2-N3-C4 | -7.10 | 122.74 | 127.00 |
| 25 | DA | 1602 | U | C5-C6-N1 | -7.10 | 119.15 | 122.70 |
| 25 | BA | 1332 | G | C4-C5-N7 | 7.10 | 113.64 | 110.80 |
| 23 | AC | 72 | C | C6-N1-C2 | -7.09 | 117.46 | 120.30 |
| 25 | BA | 1332 | G | C6-C5-N7 | -7.08 | 126.15 | 130.40 |
| 23 | CC | 17 | C | N1-C2-O2 | 7.08 | 123.15 | 118.90 |
| 23 | AD | 18 | C | C2-N1-C1' | 7.06 | 126.57 | 118.80 |
| 25 | DA | 1012 | U | N1-C2-N3 | 7.06 | 119.14 | 114.90 |
| 25 | DA | 2451 | A | C8-N9-C4 | -7.05 | 102.98 | 105.80 |
| 25 | DA | 1992 | G | C8-N9-C4 | -7.04 | 103.58 | 106.40 |
| 25 | DA | 1786 | A | N1-C6-N6 | 7.04 | 122.83 | 118.60 |
| 22 | AB | 69 | A | C2-N3-C4 | 7.03 | 114.12 | 110.60 |
| 25 | DA | 933 | A | N1-C6-N6 | 7.03 | 122.82 | 118.60 |
| 25 | DA | 1143 | A | C5-C6-N1 | -7.03 | 114.19 | 117.70 |
| 25 | BA | 2447 | G | N3-C4-N9 | 7.03 | 130.22 | 126.00 |
| 23 | CC | 40 | C | C6-N1-C2 | -7.02 | 117.49 | 120.30 |
| 25 | BA | 621 | A | C2-N3-C4 | -7.02 | 107.09 | 110.60 |
| 25 | DA | 1786 | A | C6-C5-N7 | -7.02 | 127.39 | 132.30 |
| 22 | AB | 18 | G | C8-N9-C1' | 7.01 | 136.12 | 127.00 |
| 1 | CA | 1159 | U | N3-C2-O2 | -7.01 | 117.29 | 122.20 |
| 25 | DA | 783 | A | C2-N3-C4 | -7.01 | 107.09 | 110.60 |
| 25 | BA | 71 | A | C2-N3-C4 | -7.01 | 107.10 | 110.60 |
| 25 | BA | 783 | A | C8-N9-C4 | -7.00 | 103.00 | 105.80 |
| 1 | AA | 1406 | U | C2-N3-C4 | -7.00 | 122.80 | 127.00 |
| 22 | AB | 18 | G | N1-C2-N3 | -7.00 | 119.70 | 123.90 |
| 25 | DA | 633 | A | N1-C6-N6 | 6.99 | 122.80 | 118.60 |
| 25 | DA | 1602 | U | C5-C4-O4 | -6.99 | 121.71 | 125.90 |
| 22 | CB | 58 | U | C2-N1-C1' | 6.99 | 126.08 | 117.70 |
| 25 | BA | 103 | A | N1-C6-N6 | 6.99 | 122.79 | 118.60 |
| 25 | BA | 140 | A | C8-N9-C4 | -6.98 | 103.01 | 105.80 |
| 1 | AA | 1025 | U | C6-N1-C2 | 6.97 | 125.18 | 121.00 |
| 25 | DA | 530 | G | N9-C4-C5 | -6.96 | 102.61 | 105.40 |
| 25 | BA | 1079 | C | C2-N1-C1' | 6.95 | 126.44 | 118.80 |
| 1 | AA | 1495 | U | N3-C2-O2 | -6.94 | 117.34 | 122.20 |
| 25 | BA | 1786 | A | C6-C5-N7 | -6.93 | 127.45 | 132.30 |
| 23 | CC | 26 | C | C6-N1-C2 | 6.93 | 123.07 | 120.30 |
| 25 | BA | 630 | G | C2-N3-C4 | -6.92 | 108.44 | 111.90 |
| 25 | DA | 1064 | C | C6-N1-C1' | 6.91 | 129.10 | 120.80 |
| 1 | CA | 1036 | G | C8-N9-C1' | 6.91 | 135.98 | 127.00 |
| 25 | BA | 1332 | G | N1-C6-O6 | 6.90 | 124.04 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 2287 | A | C5-N7-C8 | -6.89 | 100.45 | 103.90 |
| 23 | CC | 26 | C | C2-N1-C1' | -6.88 | 111.23 | 118.80 |
| 25 | DA | 1064 | C | C2-N1-C1' | -6.88 | 111.23 | 118.80 |
| 25 | DA | 250 | G | N3-C4-N9 | 6.88 | 130.13 | 126.00 |
| 25 | DA | 2447 | G | C4-C5-C6 | 6.87 | 122.92 | 118.80 |
| 25 | BA | 2501 | C | C2-N1-C1' | -6.86 | 111.25 | 118.80 |
| 25 | DA | 2378 | A | N1-C6-N6 | 6.86 | 122.72 | 118.60 |
| 25 | BA | 906 | G | C6-C5-N7 | 6.86 | 134.51 | 130.40 |
| 25 | BA | 83 | G | C2-N3-C4 | -6.84 | 108.48 | 111.90 |
| 25 | DA | 2598 | A | C6-C5-N7 | -6.84 | 127.51 | 132.30 |
| 25 | DA | 140 | A | N7-C8-N9 | 6.84 | 117.22 | 113.80 |
| 1 | CA | 266 | G | C5-C6-O6 | 6.82 | 132.69 | 128.60 |
| 25 | BA | 2447 | G | C5-C6-O6 | -6.81 | 124.52 | 128.60 |
| 1 | AA | 1177 | G | C8-N9-C1' | 6.80 | 135.84 | 127.00 |
| 25 | BA | 1496 | A | N7-C8-N9 | 6.80 | 117.20 | 113.80 |
| 25 | BA | 2287 | A | C5-N7-C8 | -6.80 | 100.50 | 103.90 |
| 25 | DA | 2287 | A | C2-N3-C4 | -6.79 | 107.21 | 110.60 |
| 25 | BA | 1021 | A | C5-N7-C8 | -6.79 | 100.51 | 103.90 |
| 25 | BA | 788 | A | N1-C6-N6 | 6.75 | 122.65 | 118.60 |
| 25 | BA | 1658 | C | C6-N1-C2 | -6.75 | 117.60 | 120.30 |
| 25 | DA | 2282 | G | C8-N9-C4 | -6.74 | 103.70 | 106.40 |
| 25 | BA | 673 | C | N3-C4-N4 | 6.73 | 122.71 | 118.00 |
| 25 | DA | 1963 | U | C2-N1-C1' | 6.73 | 125.78 | 117.70 |
| 1 | AA | 1025 | U | C2-N1-C1' | 6.72 | 125.77 | 117.70 |
| 22 | CB | 35 | G | C6-C5-N7 | -6.72 | 126.37 | 130.40 |
| 25 | DA | 2287 | A | N3-C4-C5 | 6.71 | 131.50 | 126.80 |
| 1 | CA | 1045 | C | C6-N1-C1' | -6.71 | 112.74 | 120.80 |
| 25 | DA | 1950 | G | C4-C5-N7 | 6.71 | 113.48 | 110.80 |
| 23 | AC | 13 | C | C5-C6-N1 | 6.70 | 124.35 | 121.00 |
| 22 | CB | 87 | A | N7-C8-N9 | 6.70 | 117.15 | 113.80 |
| 1 | CA | 1530 | G | C4-N9-C1' | -6.70 | 117.79 | 126.50 |
| 1 | AA | 1054 | C | C5-C6-N1 | 6.70 | 124.35 | 121.00 |
| 23 | CC | 21 | U | N1-C2-O2 | 6.69 | 127.48 | 122.80 |
| 25 | DA | 1332 | G | N3-C4-C5 | 6.69 | 131.95 | 128.60 |
| 25 | DA | 2061 | G | N1-C6-O6 | 6.67 | 123.90 | 119.90 |
| 25 | BA | 1204 | A | C2-N3-C4 | -6.66 | 107.27 | 110.60 |
| 25 | DA | 933 | A | N3-C4-C5 | -6.66 | 122.14 | 126.80 |
| 25 | BA | 847 | U | N3-C4-O4 | -6.65 | 114.75 | 119.40 |
| 50 | B4 | 45 | GLY | N-CA-C | -6.65 | 96.47 | 113.10 |
| 25 | DA | 2139 | C | C2-N1-C1' | 6.65 | 126.12 | 118.80 |
| 22 | AB | 87 | A | C5-C6-N6 | -6.64 | 118.38 | 123.70 |
| 25 | BA | 1678 | G | C4-C5-N7 | 6.64 | 113.45 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | BA | 1614 | A | C5-N7-C8 | -6.62 | 100.59 | 103.90 |
| 25 | BA | 49 | A | C5-N7-C8 | -6.61 | 100.59 | 103.90 |
| 25 | BA | 446 | G | C5-C6-O6 | -6.61 | 124.63 | 128.60 |
| 25 | DA | 1899 | G | C6-C5-N7 | 6.61 | 134.37 | 130.40 |
| 25 | BA | 728 | G | C8-N9-C4 | 6.61 | 109.04 | 106.40 |
| 25 | BA | 446 | G | C6-C5-N7 | -6.61 | 126.44 | 130.40 |
| 25 | DA | 1678 | G | C5-N7-C8 | -6.60 | 101.00 | 104.30 |
| 25 | BA | 783 | A | C5-C6-N6 | -6.59 | 118.43 | 123.70 |
| 25 | BA | 676 | A | N3-C4-C5 | 6.58 | 131.40 | 126.80 |
| 23 | CC | 41 | C | C6-N1-C2 | -6.57 | 117.67 | 120.30 |
| 25 | BA | 780 | G | N1-C6-O6 | 6.55 | 123.83 | 119.90 |
| 25 | BA | 2490 | G | C4-C5-N7 | 6.54 | 113.42 | 110.80 |
| 25 | DA | 2287 | A | N3-C4-N9 | -6.54 | 122.17 | 127.40 |
| 23 | AC | 11 | A | C8-N9-C4 | -6.54 | 103.19 | 105.80 |
| 25 | BA | 409 | C | C6-N1-C2 | 6.53 | 122.91 | 120.30 |
| 25 | DA | 676 | A | C2-N3-C4 | -6.53 | 107.33 | 110.60 |
| 25 | BA | 807 | U | N1-C2-O2 | -6.53 | 118.23 | 122.80 |
| 22 | AB | 77 | C | C5-C6-N1 | 6.52 | 124.26 | 121.00 |
| 25 | BA | 906 | G | C4-C5-N7 | -6.51 | 108.20 | 110.80 |
| 26 | BB | 81 | G | C6-C5-N7 | -6.50 | 126.50 | 130.40 |
| 1 | CA | 1495 | U | N3-C2-O2 | -6.50 | 117.65 | 122.20 |
| 1 | AA | 1336 | C | C2-N1-C1' | 6.49 | 125.94 | 118.80 |
| 23 | AC | 25 | U | N1-C2-O2 | 6.49 | 127.34 | 122.80 |
| 25 | DA | 1678 | G | N3-C4-C5 | 6.49 | 131.84 | 128.60 |
| 1 | CA | 108 | G | C4-N9-C1' | 6.48 | 134.92 | 126.50 |
| 1 | AA | 1054 | C | C6-N1-C1' | -6.48 | 113.03 | 120.80 |
| 1 | CA | 1465 | C | C2-N3-C4 | -6.47 | 116.66 | 119.90 |
| 23 | AC | 72 | C | C5-C6-N1 | 6.46 | 124.23 | 121.00 |
| 25 | BA | 2430 | A | C4-N9-C1' | -6.46 | 114.66 | 126.30 |
| 1 | CA | 1025 | U | N1-C2-O2 | 6.46 | 127.32 | 122.80 |
| 25 | BA | 807 | U | N1-C2-N3 | 6.45 | 118.77 | 114.90 |
| 25 | BA | 1950 | G | C5-N7-C8 | -6.45 | 101.07 | 104.30 |
| 25 | BA | 2430 | A | C8-N9-C1' | 6.45 | 139.31 | 127.70 |
| 25 | BA | 1332 | G | N7-C8-N9 | 6.45 | 116.32 | 113.10 |
| 25 | BA | 528 | A | C2-N3-C4 | -6.45 | 107.38 | 110.60 |
| 25 | BA | 906 | G | N1-C6-O6 | -6.45 | 116.03 | 119.90 |
| 23 | AC | 74 | A | N1-C6-N6 | 6.44 | 122.46 | 118.60 |
| 25 | DA | 2629 | A | C6-C5-N7 | -6.43 | 127.80 | 132.30 |
| 25 | DA | 226 | G | N3-C4-N9 | -6.42 | 122.14 | 126.00 |
| 25 | DA | 774 | A | N3-C4-N9 | -6.42 | 122.26 | 127.40 |
| 25 | DA | 1786 | A | C8-N9-C4 | -6.42 | 103.23 | 105.80 |
| 1 | AA | 1025 | U | C2-N3-C4 | -6.42 | 123.15 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 1301 | U | C2-N1-C1' | 6.41 | 125.39 | 117.70 |
| 25 | DA | 528 | A | C2-N3-C4 | -6.41 | 107.39 | 110.60 |
| 25 | DA | 676 | A | C8-N9-C4 | -6.41 | 103.24 | 105.80 |
| 22 | CB | 18 | G | N3-C4-N9 | 6.41 | 129.84 | 126.00 |
| 23 | CC | 15 | G | C5-C6-N1 | -6.41 | 108.30 | 111.50 |
| 22 | CB | 85 | C | C6-N1-C1' | -6.40 | 113.12 | 120.80 |
| 1 | CA | 993 | G | C4-C5-N7 | 6.40 | 113.36 | 110.80 |
| 26 | DB | 59 | A | C6-N1-C2 | -6.39 | 114.77 | 118.60 |
| 23 | CC | 18 | C | N3-C2-O2 | -6.39 | 117.43 | 121.90 |
| 23 | CC | 35 | C | C2-N1-C1' | 6.39 | 125.83 | 118.80 |
| 25 | BA | 2598 | A | N1-C6-N6 | 6.38 | 122.43 | 118.60 |
| 22 | AB | 27 | G | C2-N3-C4 | 6.37 | 115.08 | 111.90 |
| 25 | BA | 2442 | C | N1-C2-O2 | -6.36 | 115.08 | 118.90 |
| 1 | AA | 1436 | U | C5-C4-O4 | -6.36 | 122.09 | 125.90 |
| 22 | CB | 36 | A | C8-N9-C4 | -6.35 | 103.26 | 105.80 |
| 1 | AA | 1177 | G | N3-C2-N2 | -6.35 | 115.46 | 119.90 |
| 25 | BA | 1079 | C | C6-N1-C1' | -6.35 | 113.19 | 120.80 |
| 22 | CB | 35 | G | C4-C5-N7 | 6.34 | 113.33 | 110.80 |
| 25 | DA | 1678 | G | N3-C4-N9 | -6.34 | 122.20 | 126.00 |
| 1 | AA | 1177 | G | C5-N7-C8 | 6.34 | 107.47 | 104.30 |
| 25 | DA | 138 | G | C4-N9-C1' | 6.34 | 134.74 | 126.50 |
| 23 | CC | 44 | A | C2-N3-C4 | 6.33 | 113.77 | 110.60 |
| 22 | CB | 18 | G | N9-C4-C5 | -6.33 | 102.87 | 105.40 |
| 25 | DA | 1786 | A | C4-C5-N7 | 6.32 | 113.86 | 110.70 |
| 25 | BA | 74 | A | C2-N3-C4 | -6.31 | 107.44 | 110.60 |
| 23 | CC | 77 | A | C4-C5-C6 | -6.31 | 113.85 | 117.00 |
| 22 | AB | 27 | G | C5-C6-N1 | 6.29 | 114.65 | 111.50 |
| 22 | CB | 50 | A | C8-N9-C4 | -6.29 | 103.28 | 105.80 |
| 25 | DA | 1496 | A | N7-C8-N9 | 6.29 | 116.94 | 113.80 |
| 23 | AD | 77 | A | C5-C6-N6 | -6.28 | 118.68 | 123.70 |
| 1 | CA | 993 | G | N1-C2-N2 | -6.28 | 110.55 | 116.20 |
| 25 | BA | 1022 | G | C8-N9-C4 | -6.27 | 103.89 | 106.40 |
| 25 | BA | 812 | C | N1-C2-O2 | -6.27 | 115.14 | 118.90 |
| 25 | BA | 621 | A | C5-N7-C8 | -6.26 | 100.77 | 103.90 |
| 25 | BA | 1616 | A | C5-N7-C8 | -6.26 | 100.77 | 103.90 |
| 25 | BA | 1899 | G | C8-N9-C4 | -6.25 | 103.90 | 106.40 |
| 1 | CA | 108 | G | C8-N9-C1' | -6.25 | 118.87 | 127.00 |
| 25 | BA | 140 | A | C6-C5-N7 | -6.25 | 127.93 | 132.30 |
| 25 | BA | 141 | A | C5-N7-C8 | -6.25 | 100.78 | 103.90 |
| 25 | DA | 329 | G | N1-C6-O6 | -6.24 | 116.15 | 119.90 |
| 1 | CA | 897 | C | N1-C2-O2 | -6.24 | 115.16 | 118.90 |
| 1 | CA | 91 | C | C2-N1-C1' | 6.23 | 125.66 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 25 | DA | 2629 | A | C5-C6-N6 | -6.22 | 118.72 | 123.70 |
| 1 | AA | 530 | G | C4-N9-C1' | 6.22 | 134.59 | 126.50 |
| 25 | BA | 893 | C | C6-N1-C1' | -6.22 | 113.34 | 120.80 |
| 23 | AC | 45 | A | N1-C6-N6 | 6.21 | 122.33 | 118.60 |
| 1 | CA | 1177 | G | N3-C4-C5 | -6.21 | 125.49 | 128.60 |
| 25 | BA | 1617 | C | N3-C2-O2 | 6.21 | 126.25 | 121.90 |
| 1 | CA | 270 | A | N1-C6-N6 | 6.21 | 122.33 | 118.60 |
| 25 | DA | 210 | C | N1-C2-O2 | -6.19 | 115.19 | 118.90 |
| 25 | DA | 2902 | C | N1-C2-O2 | 6.19 | 122.62 | 118.90 |
| 25 | DA | 2720 | U | C5-C4-O4 | -6.19 | 122.19 | 125.90 |
| 22 | AB | 27 | G | N3-C4-C5 | -6.19 | 125.51 | 128.60 |
| 25 | BA | 530 | G | N3-C4-N9 | -6.19 | 122.29 | 126.00 |
| 25 | BA | 528 | A | C6-N1-C2 | 6.18 | 122.31 | 118.60 |
| 25 | DA | 1340 | U | C2-N3-C4 | -6.18 | 123.29 | 127.00 |
| 25 | DA | 330 | A | C2-N3-C4 | -6.18 | 107.51 | 110.60 |
| 25 | DA | 2501 | C | C2-N1-C1' | -6.18 | 112.00 | 118.80 |
| 24 | A1 | 17 | U | C5-C4-O4 | -6.18 | 122.19 | 125.90 |
| 25 | DA | 1602 | U | N1-C2-N3 | 6.17 | 118.60 | 114.90 |
| 25 | DA | 2451 | A | N7-C8-N9 | 6.16 | 116.88 | 113.80 |
| 23 | CD | 18 | C | C2-N1-C1' | 6.16 | 125.58 | 118.80 |
| 25 | DA | 807 | U | N1-C2-N3 | 6.16 | 118.59 | 114.90 |
| 23 | CC | 61 | U | C2-N1-C1' | 6.15 | 125.08 | 117.70 |
| 25 | DA | 2503 | A | C5-N7-C8 | -6.14 | 100.83 | 103.90 |
| 25 | BA | 1021 | A | C2-N3-C4 | -6.14 | 107.53 | 110.60 |
| 25 | BA | 271(B) | G | C4-N9-C1' | 6.14 | 134.48 | 126.50 |
| 25 | BA | 2392 | A | N7-C8-N9 | 6.14 | 116.87 | 113.80 |
| 1 | AA | 383 | A | N1-C6-N6 | 6.12 | 122.27 | 118.60 |
| 1 | CA | 1025 | U | N3-C4-O4 | 6.12 | 123.68 | 119.40 |
| 25 | DA | 2598 | A | N9-C4-C5 | -6.12 | 103.35 | 105.80 |
| 22 | AB | 44 | G | N3-C4-C5 | 6.11 | 131.66 | 128.60 |
| 25 | DA | 783 | A | C8-N9-C4 | -6.11 | 103.36 | 105.80 |
| 25 | DA | 1616 | A | N7-C8-N9 | 6.10 | 116.85 | 113.80 |
| 22 | AB | 40 | G | N1-C6-O6 | 6.10 | 123.56 | 119.90 |
| 23 | AC | 23 | G | N9-C4-C5 | 6.10 | 107.84 | 105.40 |
| 25 | DA | 2062 | A | N1-C6-N6 | 6.09 | 122.26 | 118.60 |
| 23 | AC | 40 | C | C5-C6-N1 | 6.09 | 124.05 | 121.00 |
| 25 | DA | 1 | G | N3-C4-N9 | 6.08 | 129.65 | 126.00 |
| 23 | AC | 76 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 25 | DA | 780 | G | C2-N3-C4 | 6.07 | 114.94 | 111.90 |
| 25 | DA | 676 | A | N7-C8-N9 | 6.07 | 116.83 | 113.80 |
| 25 | BA | 120 | U | N3-C4-O4 | -6.06 | 115.16 | 119.40 |
| 25 | DA | 383 | U | N3-C2-O2 | -6.06 | 117.96 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | BA | 2392 | A | C8-N9-C4 | -6.06 | 103.38 | 105.80 |
| 23 | CC | 30 | G | N3-C4-N9 | 6.06 | 129.64 | 126.00 |
| 25 | DA | 2490 | G | C4-N9-C1' | 6.06 | 134.37 | 126.50 |
| 25 | BA | 2443 | C | N1-C2-O2 | -6.05 | 115.27 | 118.90 |
| 24 | A1 | 13 | U | N1-C2-O2 | 6.05 | 127.04 | 122.80 |
| 23 | AC | 31 | G | C5-C6-N1 | -6.05 | 108.48 | 111.50 |
| 1 | CA | 270 | A | C4-C5-N7 | 6.04 | 113.72 | 110.70 |
| 25 | BA | 2287 | A | N3-C4-C5 | 6.04 | 131.03 | 126.80 |
| 1 | CA | 898 | G | C2-N3-C4 | -6.04 | 108.88 | 111.90 |
| 25 | BA | 140 | A | C2-N3-C4 | -6.04 | 107.58 | 110.60 |
| 25 | BA | 2346 | A | C2-N3-C4 | -6.03 | 107.58 | 110.60 |
| 25 | DA | 774 | A | N3-C4-C5 | 6.03 | 131.02 | 126.80 |
| 25 | BA | 103 | A | N9-C4-C5 | -6.02 | 103.39 | 105.80 |
| 26 | BB | 81 | G | C6-N1-C2 | -6.02 | 121.49 | 125.10 |
| 25 | DA | 933 | A | C5-N7-C8 | -6.02 | 100.89 | 103.90 |
| 25 | BA | 2490 | G | C5-N7-C8 | -6.01 | 101.30 | 104.30 |
| 25 | BA | 1210 | A | N7-C8-N9 | 6.01 | 116.80 | 113.80 |
| 25 | DA | 530 | G | C5-C6-O6 | -6.01 | 125.00 | 128.60 |
| 25 | DA | 676 | A | C5-N7-C8 | -6.01 | 100.90 | 103.90 |
| 25 | DA | 807 | U | C5-C4-O4 | -6.00 | 122.30 | 125.90 |
| 23 | AC | 5 | G | N3-C4-C5 | 6.00 | 131.60 | 128.60 |
| 25 | BA | 1141 | U | N1-C2-O2 | -6.00 | 118.60 | 122.80 |
| 22 | CB | 31 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 25 | DA | 2598 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 1 | CA | 1159 | U | N1-C2-O2 | 5.99 | 126.99 | 122.80 |
| 1 | CA | 1177 | G | C6-C5-N7 | 5.99 | 133.99 | 130.40 |
| 23 | CC | 77 | A | C2-N3-C4 | -5.98 | 107.61 | 110.60 |
| 25 | BA | 917 | A | C2-N3-C4 | -5.98 | 107.61 | 110.60 |
| 25 | DA | 74 | A | C2-N3-C4 | -5.97 | 107.61 | 110.60 |
| 25 | DA | 2598 | A | C5-C6-N6 | -5.97 | 118.92 | 123.70 |
| 25 | DA | 906 | G | N1-C6-O6 | -5.97 | 116.32 | 119.90 |
| 25 | DA | 1312 | U | C5-C4-O4 | 5.97 | 129.48 | 125.90 |
| 25 | DA | 1678 | G | C2-N3-C4 | -5.97 | 108.92 | 111.90 |
| 25 | BA | 1617 | C | C6-N1-C2 | 5.96 | 122.69 | 120.30 |
| 25 | DA | 530 | G | C8-N9-C1' | -5.96 | 119.25 | 127.00 |
| 25 | DA | 2873 | A | N1-C2-N3 | 5.96 | 132.28 | 129.30 |
| 25 | DA | 2503 | A | N7-C8-N9 | 5.96 | 116.78 | 113.80 |
| 1 | AA | 1177 | G | N3-C4-N9 | -5.95 | 122.43 | 126.00 |
| 25 | BA | 2430 | A | N1-C6-N6 | 5.95 | 122.17 | 118.60 |
| 1 | CA | 108 | G | C4-C5-N7 | 5.94 | 113.18 | 110.80 |
| 23 | AC | 25 | U | N3-C4-O4 | -5.94 | 115.24 | 119.40 |
| 23 | CC | 10 | G | C8-N9-C1' | -5.94 | 119.27 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | DA | 2344 | U | C2-N3-C4 | -5.94 | 123.43 | 127.00 |
| 25 | DA | 2139 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 22 | CB | 48 | C | C5-C6-N1 | 5.94 | 123.97 | 121.00 |
| 1 | AA | 1025 | U | N3-C4-O4 | 5.93 | 123.56 | 119.40 |
| 24 | A1 | 13 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 25 | BA | 1810 | A | N1-C6-N6 | 5.93 | 122.16 | 118.60 |
| 25 | DA | 1616 | A | C5-N7-C8 | -5.93 | 100.93 | 103.90 |
| 25 | BA | 2392 | A | C5-N7-C8 | -5.93 | 100.93 | 103.90 |
| 24 | C1 | 13 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 25 | DA | 140 | A | C8-N9-C4 | -5.93 | 103.43 | 105.80 |
| 25 | BA | 774 | A | C8-N9-C1' | 5.93 | 138.37 | 127.70 |
| 25 | BA | 1514 | U | C2-N1-C1' | 5.92 | 124.81 | 117.70 |
| 23 | AC | 39 | A | N1-C6-N6 | 5.92 | 122.15 | 118.60 |
| 25 | DA | 194 | G | N1-C6-O6 | 5.92 | 123.45 | 119.90 |
| 1 | CA | 1495 | U | C2-N1-C1' | 5.92 | 124.80 | 117.70 |
| 1 | AA | 1177 | G | C6-N1-C2 | -5.92 | 121.55 | 125.10 |
| 25 | BA | 1617 | C | N1-C2-O2 | -5.91 | 115.35 | 118.90 |
| 22 | AB | 24 | C | C5-C6-N1 | 5.91 | 123.96 | 121.00 |
| 1 | CA | 1529 | G | C4-N9-C1' | 5.91 | 134.18 | 126.50 |
| 24 | A1 | 14 | U | N3-C2-O2 | -5.90 | 118.07 | 122.20 |
| 25 | BA | 2318 | G | C8-N9-C4 | -5.89 | 104.04 | 106.40 |
| 25 | DA | 2713 | A | C5-N7-C8 | -5.89 | 100.95 | 103.90 |
| 25 | DA | 2490 | G | N7-C8-N9 | 5.89 | 116.04 | 113.10 |
| 23 | AD | 77 | A | N1-C6-N6 | 5.88 | 122.13 | 118.60 |
| 1 | AA | 1495 | U | C2-N3-C4 | 5.88 | 130.53 | 127.00 |
| 10 | AM | 86 | MET | N-CA-C | -5.87 | 95.14 | 111.00 |
| 23 | AC | 35 | C | C5-C6-N1 | 5.87 | 123.94 | 121.00 |
| 23 | AC | 68 | C | C2-N1-C1' | 5.87 | 125.26 | 118.80 |
| 25 | BA | 83 | G | N9-C4-C5 | -5.87 | 103.05 | 105.40 |
| 25 | BA | 1189 | A | N1-C6-N6 | 5.87 | 122.12 | 118.60 |
| 26 | DB | 81 | G | C6-N1-C2 | -5.87 | 121.58 | 125.10 |
| 28 | BE | 132 | HIS | N-CA-C | 5.87 | 126.85 | 111.00 |
| 22 | CB | 3 | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 1 | CA | 1406 | U | C2-N3-C4 | -5.87 | 123.48 | 127.00 |
| 1 | CA | 1498 | U | C2-N1-C1' | 5.87 | 124.74 | 117.70 |
| 25 | BA | 2032 | G | C2-N3-C4 | -5.86 | 108.97 | 111.90 |
| 25 | BA | 140 | A | N1-C6-N6 | 5.86 | 122.11 | 118.60 |
| 25 | BA | 1992 | G | N3-C4-C5 | -5.86 | 125.67 | 128.60 |
| 23 | AC | 12 | G | C5-C6-O6 | -5.85 | 125.09 | 128.60 |
| 1 | AA | 1053 | G | C6-C5-N7 | 5.85 | 133.91 | 130.40 |
| 22 | CB | 39 | U | C5-C6-N1 | 5.85 | 125.62 | 122.70 |
| 25 | DA | 138 | G | C8-N9-C4 | -5.85 | 104.06 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 25 | DA | 2430 | A | N1-C6-N6 | 5.84 | 122.10 | 118.60 |
| 25 | BA | 1786 | A | C5-C6-N1 | -5.84 | 114.78 | 117.70 |
| 25 | BA | 1506 | C | C6-N1-C1' | -5.84 | 113.80 | 120.80 |
| 23 | CC | 77 | A | N1-C6-N6 | 5.83 | 122.10 | 118.60 |
| 1 | AA | 97 | U | C2-N1-C1' | 5.83 | 124.69 | 117.70 |
| 25 | DA | 1496 | A | C8-N9-C4 | -5.83 | 103.47 | 105.80 |
| 23 | AC | 31 | G | C5-C6-O6 | 5.83 | 132.09 | 128.60 |
| 23 | AC | 35 | C | C2-N3-C4 | 5.82 | 122.81 | 119.90 |
| 25 | DA | 1533 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 26 | BB | 95 | U | N3-C4-O4 | -5.82 | 115.33 | 119.40 |
| 25 | DA | 2725 | A | C4-C5-C6 | 5.81 | 119.91 | 117.00 |
| 25 | BA | 1931 | U | N1-C2-N3 | 5.81 | 118.39 | 114.90 |
| 23 | AD | 18 | C | C6-N1-C2 | -5.81 | 117.98 | 120.30 |
| 25 | BA | 1506 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 25 | DA | 783 | A | C6-C5-N7 | -5.81 | 128.24 | 132.30 |
| 25 | BA | 1142(A) | A | C2-N3-C4 | -5.81 | 107.70 | 110.60 |
| 25 | BA | 492 | A | N1-C6-N6 | 5.80 | 122.08 | 118.60 |
| 25 | DA | 103 | A | N9-C4-C5 | -5.80 | 103.48 | 105.80 |
| 25 | BA | 2318 | G | N7-C8-N9 | 5.80 | 116.00 | 113.10 |
| 24 | A1 | 16 | A | N1-C6-N6 | 5.79 | 122.08 | 118.60 |
| 25 | BA | 247 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 25 | DA | 1614 | A | N7-C8-N9 | 5.79 | 116.69 | 113.80 |
| 24 | A1 | 16 | A | N9-C4-C5 | -5.79 | 103.49 | 105.80 |
| 25 | DA | 1950 | G | C5-N7-C8 | -5.78 | 101.41 | 104.30 |
| 25 | BA | 2439 | A | N1-C6-N6 | 5.78 | 122.07 | 118.60 |
| 22 | CB | 47 | C | C5-C6-N1 | 5.78 | 123.89 | 121.00 |
| 25 | DA | 1332 | G | C5-N7-C8 | -5.78 | 101.41 | 104.30 |
| 25 | BA | 201 | C | C2-N3-C4 | -5.77 | 117.01 | 119.90 |
| 25 | BA | 391 | G | C6-N1-C2 | -5.77 | 121.64 | 125.10 |
| 25 | BA | 2501 | C | C6-N1-C1' | 5.77 | 127.72 | 120.80 |
| 25 | BA | 2378 | A | N1-C6-N6 | 5.77 | 122.06 | 118.60 |
| 25 | BA | 2346 | A | N1-C2-N3 | 5.77 | 132.18 | 129.30 |
| 25 | DA | 856 | C | C6-N1-C2 | -5.76 | 117.99 | 120.30 |
| 1 | AA | 1465 | C | N3-C4-C5 | 5.76 | 124.20 | 121.90 |
| 1 | AA | 1053 | G | C8-N9-C1' | 5.76 | 134.48 | 127.00 |
| 54 | D8 | 32 | LEU | CA-CB-CG | 5.75 | 128.52 | 115.30 |
| 25 | BA | 2498 | C | N1-C2-O2 | -5.74 | 115.45 | 118.90 |
| 25 | BA | 774 | A | C5-N7-C8 | -5.74 | 101.03 | 103.90 |
| 25 | DA | 250 | G | N3-C4-C5 | -5.73 | 125.73 | 128.60 |
| 25 | BA | 1786 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 25 | DA | 103 | A | C6-C5-N7 | -5.72 | 128.29 | 132.30 |
| 25 | DA | 2344 | U | N1-C2-O2 | -5.72 | 118.80 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | CC | 29 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 23 | CD | 18 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 25 | BA | 1678 | G | N7-C8-N9 | 5.71 | 115.96 | 113.10 |
| 25 | BA | 1950 | G | N7-C8-N9 | 5.71 | 115.96 | 113.10 |
| 22 | CB | 58 | U | C6-N1-C1' | -5.71 | 113.20 | 121.20 |
| 1 | AA | 1159 | U | C2-N1-C1' | 5.71 | 124.55 | 117.70 |
| 22 | AB | 87 | A | C4-N9-C1' | 5.71 | 136.57 | 126.30 |
| 25 | BA | 1433 | U | C2-N1-C1' | 5.71 | 124.55 | 117.70 |
| 25 | BA | 2344 | U | N1-C2-O2 | -5.70 | 118.81 | 122.80 |
| 25 | BA | 103 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 25 | DA | 2139 | C | C6-N1-C1' | -5.70 | 113.97 | 120.80 |
| 25 | DA | 2152 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |
| 23 | CC | 30 | G | N3-C4-C5 | -5.69 | 125.75 | 128.60 |
| 25 | BA | 391 | G | N3-C4-N9 | 5.69 | 129.41 | 126.00 |
| 14 | AQ | 24 | CYS | CA-CB-SG | 5.68 | 124.23 | 114.00 |
| 25 | BA | 1380 | G | C8-N9-C1' | -5.68 | 119.61 | 127.00 |
| 23 | CD | 75 | C | C2-N1-C1' | 5.68 | 125.05 | 118.80 |
| 25 | DA | 801 | G | N1-C6-O6 | -5.68 | 116.49 | 119.90 |
| 25 | BA | 1210 | A | C6-C5-N7 | -5.68 | 128.32 | 132.30 |
| 25 | BA | 2451 | A | C4-C5-C6 | -5.68 | 114.16 | 117.00 |
| 23 | AC | 11 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 25 | BA | 189 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 25 | BA | 859 | G | N3-C4-C5 | 5.67 | 131.43 | 128.60 |
| 25 | DA | 530 | G | C2-N3-C4 | -5.66 | 109.07 | 111.90 |
| 22 | AB | 27 | G | N3-C4-N9 | 5.66 | 129.40 | 126.00 |
| 1 | CA | 1436 | U | C2-N3-C4 | -5.66 | 123.60 | 127.00 |
| 25 | DA | 2595 | G | C2-N3-C4 | -5.66 | 109.07 | 111.90 |
| 25 | BA | 71 | A | C5-N7-C8 | -5.66 | 101.07 | 103.90 |
| 23 | CC | 77 | A | C4-C5-N7 | 5.66 | 113.53 | 110.70 |
| 25 | BA | 1213 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 25 | BA | 2134 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 25 | DA | 630 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 12 | AO | 88 | GLY | N-CA-C | -5.64 | 98.99 | 113.10 |
| 25 | BA | 541 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 25 | BA | 633 | A | C5-C6-N1 | -5.64 | 114.88 | 117.70 |
| 25 | DA | 2725 | A | N1-C6-N6 | 5.64 | 121.98 | 118.60 |
| 1 | CA | 383 | A | N1-C6-N6 | 5.63 | 121.98 | 118.60 |
| 1 | CA | 1045 | C | N3-C2-O2 | -5.63 | 117.95 | 121.90 |
| 1 | AA | 723 | U | C2-N1-C1' | 5.63 | 124.46 | 117.70 |
| 1 | CA | 1036 | G | N3-C4-N9 | -5.63 | 122.62 | 126.00 |
| 1 | AA | 115 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 25 | DA | 737 | C | N1-C2-O2 | -5.62 | 115.53 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | AB | 40 | G | C5-C6-N1 | -5.61 | 108.69 | 111.50 |
| 1 | AA | 530 | G | C8-N9-C1' | -5.60 | 119.72 | 127.00 |
| 25 | BA | 676 | A | C5-C6-N1 | -5.60 | 114.90 | 117.70 |
| 23 | CC | 77 | A | C4-N9-C1' | -5.60 | 116.22 | 126.30 |
| 25 | DA | 83 | G | N9-C4-C5 | -5.60 | 103.16 | 105.40 |
| 25 | BA | 858 | U | N1-C2-O2 | 5.60 | 126.72 | 122.80 |
| 25 | BA | 784 | A | N1-C6-N6 | -5.59 | 115.24 | 118.60 |
| 23 | CC | 18 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 25 | DA | 138 | G | N7-C8-N9 | 5.58 | 115.89 | 113.10 |
| 25 | BA | 1210 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 25 | DA | 1698 | A | C5-N7-C8 | -5.58 | 101.11 | 103.90 |
| 25 | DA | 140 | A | C5-N7-C8 | -5.58 | 101.11 | 103.90 |
| 32 | DK | 131 | LYS | C-N-CD | -5.58 | 108.33 | 120.60 |
| 25 | BA | 2071 | A | C2-N3-C4 | -5.58 | 107.81 | 110.60 |
| 25 | BA | 333 | G | C4-N9-C1' | 5.57 | 133.75 | 126.50 |
| 25 | DA | 788 | A | N1-C6-N6 | 5.57 | 121.94 | 118.60 |
| 1 | CA | 266 | G | C8-N9-C4 | -5.57 | 104.17 | 106.40 |
| 22 | CB | 87 | A | C5-N7-C8 | -5.57 | 101.12 | 103.90 |
| 23 | CC | 35 | C | N3-C4-C5 | -5.57 | 119.67 | 121.90 |
| 25 | BA | 2430 | A | C5-N7-C8 | -5.57 | 101.12 | 103.90 |
| 25 | DA | 83 | G | C6-C5-N7 | -5.57 | 127.06 | 130.40 |
| 1 | AA | 97 | U | C2-N3-C4 | 5.56 | 130.34 | 127.00 |
| 25 | BA | 1786 | A | N1-C6-N6 | 5.56 | 121.94 | 118.60 |
| 25 | BA | 2451 | A | N1-C6-N6 | -5.56 | 115.26 | 118.60 |
| 1 | CA | 266 | G | N3-C4-C5 | -5.56 | 125.82 | 128.60 |
| 23 | AC | 68 | C | N1-C2-O2 | 5.56 | 122.24 | 118.90 |
| 25 | BA | 49 | A | N7-C8-N9 | 5.56 | 116.58 | 113.80 |
| 25 | DA | 1950 | G | C6-C5-N7 | -5.56 | 127.06 | 130.40 |
| 22 | CB | 63 | G | C4-N9-C1' | -5.56 | 119.27 | 126.50 |
| 22 | AB | 18 | G | C4-C5-C6 | -5.56 | 115.47 | 118.80 |
| 25 | BA | 330 | A | C2-N3-C4 | -5.56 | 107.82 | 110.60 |
| 25 | DA | 2720 | U | N1-C2-N3 | 5.56 | 118.23 | 114.90 |
| 25 | DA | 74 | A | C5-C6-N1 | -5.56 | 114.92 | 117.70 |
| 1 | AA | 1498 | U | C2-N1-C1' | 5.55 | 124.36 | 117.70 |
| 23 | AC | 77 | A | N3-C4-C5 | 5.55 | 130.69 | 126.80 |
| 25 | BA | 673 | C | N3-C4-C5 | 5.55 | 124.12 | 121.90 |
| 27 | BD | 28 | GLU | N-CA-C | -5.55 | 96.03 | 111.00 |
| 25 | DA | 226 | G | N3-C2-N2 | -5.55 | 116.02 | 119.90 |
| 25 | BA | 201 | C | C5-C4-N4 | -5.54 | 116.32 | 120.20 |
| 25 | DA | 2062 | A | N9-C4-C5 | -5.54 | 103.58 | 105.80 |
| 26 | BB | 95 | U | C6-N1-C1' | 5.54 | 128.95 | 121.20 |
| 25 | DA | 1930 | G | C4-N9-C1' | -5.54 | 119.30 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 25 | DA | 783 | A | C5-C6-N6 | -5.53 | 119.27 | 123.70 |
| 25 | BA | 797 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 26 | BB | 89(A) | A | N1-C6-N6 | 5.53 | 121.92 | 118.60 |
| 25 | BA | 391 | G | C4-N9-C1' | 5.53 | 133.69 | 126.50 |
| 23 | AC | 39 | A | C6-C5-N7 | -5.53 | 128.43 | 132.30 |
| 41 | B2 | 39 | LEU | CA-CB-CG | 5.53 | 128.01 | 115.30 |
| 22 | CB | 57 | C | C6-N1-C2 | -5.52 | 118.09 | 120.30 |
| 25 | BA | 1528 | A | N7-C8-N9 | 5.52 | 116.56 | 113.80 |
| 25 | BA | 2287 | A | N3-C4-N9 | -5.52 | 122.98 | 127.40 |
| 25 | BA | 2318 | G | C4-N9-C1' | 5.52 | 133.68 | 126.50 |
| 23 | AC | 38 | A | C8-N9-C4 | -5.52 | 103.59 | 105.80 |
| 22 | AB | 47 | C | C5-C6-N1 | 5.52 | 123.76 | 121.00 |
| 25 | BA | 1616 | A | C4-C5-N7 | 5.52 | 113.46 | 110.70 |
| 25 | BA | 621 | A | N1-C6-N6 | 5.51 | 121.91 | 118.60 |
| 1 | CA | 1530 | G | C8-N9-C1' | 5.51 | 134.16 | 127.00 |
| 23 | CC | 33 | C | C2-N1-C1' | 5.51 | 124.86 | 118.80 |
| 23 | CC | 46 | G | C5-C6-N1 | -5.50 | 108.75 | 111.50 |
| 23 | CC | 31 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 25 | DA | 633 | A | C5-C6-N1 | -5.50 | 114.95 | 117.70 |
| 25 | DA | 1786 | A | C2-N3-C4 | -5.50 | 107.85 | 110.60 |
| 23 | AC | 9 | G | C4-N9-C1' | 5.49 | 133.64 | 126.50 |
| 25 | BA | 1156 | A | N1-C6-N6 | 5.49 | 121.89 | 118.60 |
| 25 | DA | 686 | G | N3-C4-N9 | 5.49 | 129.29 | 126.00 |
| 22 | CB | 58 | U | N1-C2-O2 | 5.49 | 126.64 | 122.80 |
| 25 | DA | 812 | C | N1-C2-O2 | -5.48 | 115.61 | 118.90 |
| 1 | AA | 1053 | G | C8-N9-C4 | 5.48 | 108.59 | 106.40 |
| 1 | AA | 1053 | G | N7-C8-N9 | -5.47 | 110.36 | 113.10 |
| 25 | DA | 1614 | A | C5-N7-C8 | -5.47 | 101.16 | 103.90 |
| 25 | BA | 2451 | A | C5-C6-N1 | 5.47 | 120.44 | 117.70 |
| 23 | CC | 76 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 25 | BA | 528 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 25 | BA | 140 | A | C4-C5-N7 | 5.46 | 113.43 | 110.70 |
| 1 | CA | 91 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 25 | DA | 1992 | G | N3-C4-C5 | -5.46 | 125.87 | 128.60 |
| 25 | BA | 807 | U | C5-C4-O4 | -5.46 | 122.62 | 125.90 |
| 23 | CC | 10 | G | C4-N9-C1' | 5.45 | 133.58 | 126.50 |
| 25 | DA | 226 | G | C8-N9-C1' | 5.44 | 134.07 | 127.00 |
| 25 | BA | 1220 | A | C8-N9-C4 | -5.44 | 103.62 | 105.80 |
| 25 | DA | 633 | A | C6-C5-N7 | -5.44 | 128.49 | 132.30 |
| 25 | BA | 2557 | G | C4-N9-C1' | 5.44 | 133.57 | 126.50 |
| 24 | C1 | 13 | U | N1-C2-O2 | 5.43 | 126.60 | 122.80 |
| 25 | DA | 226 | G | C4-N9-C1' | -5.43 | 119.44 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 25 | BA | 860 | U | C2-N1-C1' | 5.42 | 124.21 | 117.70 |
| 25 | BA | 2443 | C | N3-C4-N4 | 5.42 | 121.80 | 118.00 |
| 23 | AC | 68 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 25 | BA | 1427 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 25 | DA | 453 | C | C6-N1-C2 | 5.41 | 122.46 | 120.30 |
| 23 | AC | 12 | G | N1-C6-O6 | 5.41 | 123.14 | 119.90 |
| 25 | BA | 2211 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 23 | AC | 30 | G | C2-N3-C4 | -5.41 | 109.20 | 111.90 |
| 23 | AC | 43 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 25 | BA | 138 | G | C5-N7-C8 | -5.40 | 101.60 | 104.30 |
| 23 | CD | 2 | G | N1-C6-O6 | 5.40 | 123.14 | 119.90 |
| 25 | DA | 1602 | U | N3-C4-C5 | 5.39 | 117.84 | 114.60 |
| 25 | DA | 1142(A) | A | C5-N7-C8 | -5.39 | 101.20 | 103.90 |
| 26 | DB | 81 | G | N3-C4-N9 | 5.39 | 129.23 | 126.00 |
| 23 | CD | 18 | C | C5-C6-N1 | 5.39 | 123.69 | 121.00 |
| 25 | DA | 172 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 25 | BA | 383 | U | N1-C2-O2 | 5.38 | 126.57 | 122.80 |
| 25 | BA | 859 | G | C4-N9-C1' | -5.38 | 119.50 | 126.50 |
| 25 | DA | 1407 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 25 | BA | 2595 | G | C2-N3-C4 | -5.38 | 109.21 | 111.90 |
| 25 | DA | 1762 | A | C1'-O4'-C4' | -5.38 | 105.60 | 109.90 |
| 25 | DA | 2595 | G | N9-C4-C5 | -5.38 | 103.25 | 105.40 |
| 23 | AC | 23 | G | N7-C8-N9 | 5.37 | 115.79 | 113.10 |
| 1 | AA | 163 | C | C6-N1-C1' | 5.37 | 127.24 | 120.80 |
| 25 | DA | 1021 | A | C5-N7-C8 | -5.37 | 101.22 | 103.90 |
| 25 | BA | 2681 | C | C5-C6-N1 | 5.37 | 123.68 | 121.00 |
| 25 | DA | 2720 | U | N3-C4-C5 | 5.37 | 117.82 | 114.60 |
| 25 | DA | 2776 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 25 | BA | 2344 | U | C2-N3-C4 | -5.36 | 123.78 | 127.00 |
| 25 | BA | 1691 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 23 | AC | 44 | A | C5-C6-N6 | -5.36 | 119.42 | 123.70 |
| 26 | BB | 95 | U | C2-N1-C1' | -5.36 | 111.27 | 117.70 |
| 22 | CB | 18 | G | C8-N9-C4 | 5.36 | 108.54 | 106.40 |
| 25 | DA | 912 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 25 | BA | 1380 | G | C4-N9-C1' | 5.35 | 133.46 | 126.50 |
| 1 | CA | 898 | G | N3-C4-C5 | 5.35 | 131.28 | 128.60 |
| 25 | DA | 1610 | A | N9-C4-C5 | -5.35 | 103.66 | 105.80 |
| 32 | BK | 12 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 25 | DA | 1612 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 25 | BA | 1614 | A | C2-N3-C4 | -5.34 | 107.93 | 110.60 |
| 26 | BB | 81 | G | C4-C5-N7 | 5.34 | 112.94 | 110.80 |
| 25 | DA | 2048 | G | C8-N9-C4 | -5.34 | 104.26 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 26 | DB | 95 | U | N3-C4-O4 | -5.34 | 115.66 | 119.40 |
| 25 | BA | 1312 | U | N3-C4-C5 | -5.34 | 111.40 | 114.60 |
| 23 | CC | 17 | C | N3-C2-O2 | -5.33 | 118.17 | 121.90 |
| 22 | CB | 65 | U | C6-N1-C2 | -5.33 | 117.80 | 121.00 |
| 23 | AC | 62 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 25 | BA | 1678 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 22 | CB | 28 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 25 | DA | 2159 | G | C4-N9-C1' | 5.33 | 133.43 | 126.50 |
| 23 | AC | 60 | A | C4-C5-C6 | 5.33 | 119.66 | 117.00 |
| 25 | BA | 1698 | A | N3-C4-N9 | -5.33 | 123.14 | 127.40 |
| 25 | DA | 2573 | C | C2-N1-C1' | 5.32 | 124.65 | 118.80 |
| 1 | AA | 1495 | U | C2-N1-C1' | 5.32 | 124.08 | 117.70 |
| 25 | DA | 2502 | G | C8-N9-C4 | -5.31 | 104.28 | 106.40 |
| 25 | BA | 1141 | U | C2-N3-C4 | -5.31 | 123.82 | 127.00 |
| 23 | CC | 61 | U | C6-N1-C1' | -5.31 | 113.77 | 121.20 |
| 25 | BA | 633 | A | N9-C4-C5 | -5.30 | 103.68 | 105.80 |
| 25 | BA | 2510 | C | N1-C2-O2 | -5.30 | 115.72 | 118.90 |
| 23 | CC | 77 | A | C5-N7-C8 | -5.30 | 101.25 | 103.90 |
| 22 | CB | 42 | U | C5-C6-N1 | 5.29 | 125.35 | 122.70 |
| 25 | DA | 1623 | G | N9-C4-C5 | 5.29 | 107.52 | 105.40 |
| 23 | CC | 16 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 22 | CB | 40 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 25 | BA | 103 | A | C8-N9-C1' | -5.29 | 118.18 | 127.70 |
| 25 | BA | 933 | A | N1-C2-N3 | 5.28 | 131.94 | 129.30 |
| 1 | CA | 1319 | A | N1-C6-N6 | -5.28 | 115.44 | 118.60 |
| 25 | BA | 391 | G | C8-N9-C1' | -5.27 | 120.15 | 127.00 |
| 25 | BA | 271(B) | G | N3-C4-C5 | -5.27 | 125.97 | 128.60 |
| 25 | BA | 1678 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 23 | CC | 33 | C | C6-N1-C1' | -5.26 | 114.48 | 120.80 |
| 23 | AC | 13 | C | C2-N3-C4 | 5.26 | 122.53 | 119.90 |
| 41 | B2 | 35 | LEU | CA-CB-CG | 5.26 | 127.39 | 115.30 |
| 23 | CC | 58 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 25 | DA | 1342 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 23 | AD | 1 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 1 | CA | 270 | A | C5-C6-N6 | -5.25 | 119.50 | 123.70 |
| 25 | DA | 1204 | A | C2-N3-C4 | -5.25 | 107.98 | 110.60 |
| 25 | BA | 1937 | A | N9-C4-C5 | 5.24 | 107.89 | 105.80 |
| 25 | BA | 541 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 25 | BA | 828 | U | C5-C4-O4 | 5.24 | 129.04 | 125.90 |
| 25 | DA | 2378 | A | C4-C5-C6 | 5.23 | 119.62 | 117.00 |
| 25 | BA | 1614 | A | N7-C8-N9 | 5.23 | 116.42 | 113.80 |
| 23 | AC | 71 | G | N3-C4-C5 | 5.23 | 131.22 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | BA | 885 | C | C2-N1-C1' | -5.23 | 113.05 | 118.80 |
| 25 | BA | 2452 | C | C2-N1-C1' | 5.23 | 124.55 | 118.80 |
| 25 | DA | 2346 | A | C2-N3-C4 | -5.23 | 107.98 | 110.60 |
| 1 | AA | 807 | A | C8-N9-C4 | -5.23 | 103.71 | 105.80 |
| 25 | BA | 2497 | A | C4-C5-C6 | 5.23 | 119.61 | 117.00 |
| 25 | DA | 1930 | G | C8-N9-C1' | 5.23 | 133.80 | 127.00 |
| 25 | BA | 2610 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 25 | DA | 885 | C | C2-N1-C1' | -5.22 | 113.06 | 118.80 |
| 23 | AC | 15 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |
| 25 | DA | 530 | G | C4-N9-C1' | 5.22 | 133.28 | 126.50 |
| 1 | CA | 1177 | G | C5-N7-C8 | 5.22 | 106.91 | 104.30 |
| 23 | AC | 36 | A | N1-C6-N6 | 5.21 | 121.73 | 118.60 |
| 25 | DA | 2159 | G | C8-N9-C1' | -5.21 | 120.22 | 127.00 |
| 25 | BA | 2681 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 22 | CB | 48 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 25 | DA | 103 | A | C8-N9-C1' | -5.21 | 118.32 | 127.70 |
| 1 | AA | 1054 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 25 | BA | 146 | G | N3-C4-C5 | 5.21 | 131.21 | 128.60 |
| 1 | AA | 789 | U | C5-C4-O4 | 5.21 | 129.03 | 125.90 |
| 25 | DA | 1342 | A | C5-C6-N6 | -5.21 | 119.53 | 123.70 |
| 1 | CA | 1267 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 23 | CC | 35 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 28 | BE | 132 | HIS | N-CA-CB | -5.20 | 101.23 | 110.60 |
| 25 | BA | 1332 | G | N3-C4-C5 | 5.20 | 131.20 | 128.60 |
| 23 | AC | 30 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 25 | BA | 1616 | A | N7-C8-N9 | 5.20 | 116.40 | 113.80 |
| 1 | CA | 898 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 22 | CB | 74 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 25 | DA | 1475 | G | C4-N9-C1' | 5.20 | 133.25 | 126.50 |
| 23 | AC | 13 | C | C4-C5-C6 | -5.19 | 114.80 | 117.40 |
| 25 | BA | 74 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 25 | DA | 621 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 25 | DA | 1533 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 25 | BA | 2062 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 23 | AC | 6 | G | C6-C5-N7 | 5.19 | 133.51 | 130.40 |
| 22 | CB | 35 | G | C4-N9-C1' | 5.19 | 133.24 | 126.50 |
| 22 | CB | 40 | G | N7-C8-N9 | 5.19 | 115.69 | 113.10 |
| 23 | CC | 41 | C | N3-C4-C5 | -5.19 | 119.83 | 121.90 |
| 25 | BA | 2375 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 25 | BA | 1950 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 38 | BQ | 101 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 25 | DA | 1210 | A | C3'-C2'-C1' | 5.18 | 105.65 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25 | BA | 780 | G | C2-N3-C4 | 5.18 | 114.49 | 111.90 |
| 25 | DA | 2501 | C | C6-N1-C1' | 5.18 | 127.02 | 120.80 |
| 25 | BA | 446 | G | C4-C5-N7 | 5.18 | 112.87 | 110.80 |
| 25 | DA | 2490 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 1 | CA | 150 | C | C2-N3-C4 | 5.18 | 122.49 | 119.90 |
| 25 | DA | 1427 | A | C8-N9-C4 | -5.17 | 103.73 | 105.80 |
| 25 | DA | 676 | A | N3-C4-N9 | -5.17 | 123.26 | 127.40 |
| 25 | DA | 1786 | A | C4-N9-C1' | 5.17 | 135.61 | 126.30 |
| 23 | CC | 22 | A | N1-C6-N6 | -5.17 | 115.50 | 118.60 |
| 25 | DA | 630 | G | N9-C4-C5 | -5.17 | 103.33 | 105.40 |
| 25 | DA | 1616 | A | C8-N9-C4 | -5.17 | 103.73 | 105.80 |
| 25 | DA | 1899 | G | C2-N3-C4 | -5.17 | 109.32 | 111.90 |
| 1 | AA | 1465 | C | C5-C4-N4 | -5.16 | 116.59 | 120.20 |
| 23 | AC | 62 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 40 | B1 | 98 | LEU | CA-CB-CG | 5.16 | 127.16 | 115.30 |
| 25 | DA | 1585 | C | C2-N1-C1' | 5.16 | 124.47 | 118.80 |
| 25 | BA | 1914 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 1 | AA | 163 | C | C2-N1-C1' | -5.16 | 113.13 | 118.80 |
| 25 | BA | 1698 | A | N3-C4-C5 | 5.16 | 130.41 | 126.80 |
| 1 | CA | 1025 | U | N3-C4-C5 | 5.15 | 117.69 | 114.60 |
| 25 | BA | 1964 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 25 | DA | 885 | C | C6-N1-C1' | 5.15 | 126.98 | 120.80 |
| 25 | BA | 1022 | G | N9-C4-C5 | 5.14 | 107.46 | 105.40 |
| 25 | DA | 1141 | U | N1-C2-N3 | 5.14 | 117.99 | 114.90 |
| 1 | CA | 1278 | U | C2-N1-C1' | 5.14 | 123.87 | 117.70 |
| 25 | DA | 1309 | G | N1-C6-O6 | 5.14 | 122.98 | 119.90 |
| 25 | BA | 1950 | G | N3-C4-N9 | -5.14 | 122.92 | 126.00 |
| 24 | C1 | 16 | A | C4-C5-C6 | 5.14 | 119.57 | 117.00 |
| 23 | AC | 45 | A | C5-C6-N6 | -5.14 | 119.59 | 123.70 |
| 25 | BA | 2609 | U | C2-N1-C1' | -5.14 | 111.53 | 117.70 |
| 1 | CA | 91 | C | C6-N1-C1' | -5.13 | 114.64 | 120.80 |
| 25 | DA | 2129 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 1 | CA | 631 | G | C3'-C2'-C1' | 5.13 | 105.60 | 101.50 |
| 1 | AA | 1530 | G | C4-N9-C1' | -5.13 | 119.84 | 126.50 |
| 25 | BA | 1658 | C | N3-C4-C5 | -5.13 | 119.85 | 121.90 |
| 22 | CB | 48 | C | C2-N3-C4 | 5.13 | 122.46 | 119.90 |
| 25 | BA | 1653 | G | N3-C4-C5 | -5.12 | 126.04 | 128.60 |
| 25 | BA | 271(B) | G | C8-N9-C1' | -5.12 | 120.34 | 127.00 |
| 1 | CA | 897 | C | C2-N1-C1' | -5.12 | 113.17 | 118.80 |
| 23 | AC | 68 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 25 | BA | 216 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 22 | CB | 87 | A | C8-N9-C4 | -5.12 | 103.75 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 25 | DA | 1725 | G | C4-N9-C1' | 5.12 | 133.15 | 126.50 |
| 25 | BA | 2751 | G | C4-N9-C1' | 5.12 | 133.15 | 126.50 |
| 1 | CA | 1036 | G | C5-N7-C8 | 5.12 | 106.86 | 104.30 |
| 22 | CB | 36 | A | C2-N3-C4 | 5.12 | 113.16 | 110.60 |
| 25 | DA | 783 | A | N3-C4-C5 | 5.11 | 130.38 | 126.80 |
| 25 | BA | 1992 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 25 | BA | 2713 | A | C2-N3-C4 | -5.10 | 108.05 | 110.60 |
| 24 | C1 | 16 | A | N9-C4-C5 | -5.10 | 103.76 | 105.80 |
| 25 | DA | 2502 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 26 | DB | 95 | U | C6-N1-C1' | 5.09 | 128.33 | 121.20 |
| 25 | BA | 856 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 27 | BD | 111 | LEU | CA-CB-CG | 5.09 | 127.00 | 115.30 |
| 49 | BX | 8 | LEU | CA-CB-CG | 5.08 | 127.00 | 115.30 |
| 1 | CA | 700 | G | C8-N9-C1' | 5.08 | 133.61 | 127.00 |
| 25 | DA | 801 | G | N9-C4-C5 | 5.08 | 107.43 | 105.40 |
| 25 | DA | 1502 | C | C2-N1-C1' | 5.08 | 124.39 | 118.80 |
| 25 | BA | 2566 | A | C8-N9-C4 | -5.08 | 103.77 | 105.80 |
| 25 | DA | 1899 | G | N3-C2-N2 | -5.08 | 116.35 | 119.90 |
| 22 | AB | 18 | G | C6-C5-N7 | 5.07 | 133.44 | 130.40 |
| 25 | BA | 210 | C | C5-C6-N1 | -5.07 | 118.46 | 121.00 |
| 1 | CA | 328 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 25 | BA | 1142(A) | A | N3-C4-N9 | -5.07 | 123.35 | 127.40 |
| 23 | CC | 49 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 25 | DA | 2287 | A | C8-N9-C1' | 5.07 | 136.82 | 127.70 |
| 25 | DA | 2754 | U | C2-N1-C1' | 5.07 | 123.78 | 117.70 |
| 31 | BH | 167 | GLU | C-N-CD | -5.07 | 109.46 | 120.60 |
| 23 | CC | 71 | G | C4-C5-N7 | 5.07 | 112.83 | 110.80 |
| 23 | AC | 76 | C | C4-C5-C6 | 5.06 | 119.93 | 117.40 |
| 25 | DA | 1602 | U | N1-C2-O2 | -5.06 | 119.25 | 122.80 |
| 23 | AC | 61 | U | N3-C4-O4 | 5.06 | 122.94 | 119.40 |
| 23 | AC | 52 | C | C2-N1-C1' | 5.06 | 124.36 | 118.80 |
| 25 | DA | 2049 | G | N3-C4-C5 | 5.06 | 131.13 | 128.60 |
| 23 | AD | 77 | A | N3-C4-C5 | -5.06 | 123.26 | 126.80 |
| 25 | DA | 673 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 1 | AA | 1177 | G | N1-C2-N3 | 5.05 | 126.93 | 123.90 |
| 25 | BA | 2688 | U | C5-C4-O4 | 5.05 | 128.93 | 125.90 |
| 25 | BA | 1678 | G | N3-C4-C5 | 5.05 | 131.12 | 128.60 |
| 25 | DA | 2490 | G | C6-C5-N7 | -5.04 | 127.38 | 130.40 |
| 47 | BZ | 80 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 25 | DA | 856 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 1 | AA | 898 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 1 | CA | 901 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | BA | 1079 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 23 | CC | 28 | U | N3-C2-O2 | 5.04 | 125.73 | 122.20 |
| 25 | BA | 530 | G | C8-N9-C1' | 5.03 | 133.54 | 127.00 |
| 22 | AB | 9 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |
| 1 | AA | 812 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 1 | AA | 1495 | U | C5-C6-N1 | 5.02 | 125.21 | 122.70 |
| 25 | BA | 906 | G | C8-N9-C1' | 5.02 | 133.53 | 127.00 |
| 1 | CA | 108 | G | C6-C5-N7 | -5.02 | 127.39 | 130.40 |
| 1 | CA | 754 | C | C2-N1-C1' | 5.02 | 124.32 | 118.80 |
| 25 | DA | 1963 | U | C6-N1-C1' | -5.02 | 114.17 | 121.20 |
| 1 | AA | 898 | G | N3-C4-C5 | 5.02 | 131.11 | 128.60 |
| 23 | AC | 43 | G | N7-C8-N9 | 5.02 | 115.61 | 113.10 |
| 22 | CB | 85 | C | C4-C5-C6 | -5.02 | 114.89 | 117.40 |
| 23 | AC | 30 | G | N1-C2-N3 | 5.01 | 126.91 | 123.90 |
| 25 | BA | 633 | A | C5-C6-N6 | -5.01 | 119.69 | 123.70 |
| 23 | AD | 77 | A | N3-C4-N9 | 5.01 | 131.41 | 127.40 |
| 23 | CC | 13 | C | C5-C6-N1 | 5.01 | 123.51 | 121.00 |
| 25 | DA | 1616 | A | C6-C5-N7 | -5.01 | 128.80 | 132.30 |
| 25 | BA | 580 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |
| 25 | DA | 2713 | A | N7-C8-N9 | 5.00 | 116.30 | 113.80 |

There are no chirality outliers.

All (99) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | AE | 14 | GLY | Peptide |
| 2 | AE | 194 | PRO | Peptide |
| 2 | AE | 71 | VAL | Peptide |
| 4 | AG | 29 | PRO | Peptide |
| 8 | AK | 102 | ARG | Peptide |
| 10 | AM | 55 | LYS | Peptide |
| 12 | AO | 17 | LYS | Peptide |
| 12 | AO | 47 | LYS | Peptide |
| 14 | AQ | 13 | THR | Peptide |
| 15 | AR | 87 | ILE | Peptide |
| 40 | B1 | 90 | VAL | Peptide |
| 41 | B2 | 48 | GLY | Peptide |
| 46 | B3 | 83 | PRO | Peptide |
| 46 | B3 | 84 | LEU | Peptide |
| 50 | B4 | 38 | LYS | Peptide |
| 50 | B4 | 40 | HIS | Peptide |
| 50 | B4 | 44 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 50 | B4 | 51 | ASP | Peptide |
| 51 | B5 | 47 | PRO | Peptide |
| 52 | B6 | 27 | LYS | Peptide |
| 53 | B7 | 48 | LYS | Peptide |
| 54 | B8 | 51 | ALA | Peptide |
| 54 | B8 | 52 | LYS | Peptide |
| 27 | BD | 122 | ASP | Peptide |
| 27 | BD | 236 | GLY | Peptide |
| 27 | BD | 237 | GLU | Peptide |
| 27 | BD | 27 | THR | Peptide |
| 27 | BD | 28 | GLU | Peptide |
| 27 | BD | 47 | GLY | Peptide |
| 28 | BE | 131 | ALA | Peptide |
| 30 | BG | 13 | GLU | Peptide |
| 31 | BH | 153 | LYS | Peptide |
| 31 | BH | 7 | LEU | Peptide |
| 32 | BK | 10 | GLU | Peptide |
| 32 | BK | 116 | LEU | Peptide |
| 32 | BK | 134 | PRO | Peptide |
| 33 | BM | 96 | GLU | Peptide |
| 35 | BO | 115 | LEU | Peptide |
| 35 | BO | 26 | GLY | Peptide |
| 35 | BO | 36 | LYS | Peptide |
| 35 | BO | 5 | ASP | Peptide |
| 36 | BP | 21 | THR | Peptide |
| 36 | BP | 58 | PHE | Peptide |
| 36 | BP | 87 | LYS | Peptide |
| 38 | BQ | 110 | LEU | Peptide |
| 39 | BR | 115 | ARG | Peptide |
| 39 | BR | 3 | ARG | Peptide |
| 43 | BT | 67 | GLY | Peptide |
| 45 | BV | 160 | GLY | Peptide |
| 45 | BV | 5 | LEU | Peptide |
| 45 | BV | 63 | ASP | Peptide |
| 48 | BW | 15 | LYS | Peptide |
| 48 | BW | 17 | SER | Peptide |
| 2 | CE | 231 | GLU | Peptide |
| 2 | CE | 237 | ALA | Peptide |
| 2 | CE | 71 | VAL | Peptide |
| 2 | CE | 73 | THR | Peptide |
| 2 | CE | 74 | LYS | Peptide |
| 3 | CF | 47 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 14 | CQ | 14 | PRO | Peptide |
| 14 | CQ | 27 | CYS | Peptide |
| 19 | CV | 66 | MET | Peptide |
| 20 | CW | 11 | SER | Peptide |
| 37 | D0 | 106 | GLY | Peptide |
| 37 | D0 | 81 | ASP | Peptide |
| 40 | D1 | 90 | VAL | Peptide |
| 50 | D4 | 40 | HIS | Peptide |
| 50 | D4 | 56 | VAL | Peptide |
| 51 | D5 | 56 | LYS | Peptide |
| 52 | D6 | 18 | ARG | Peptide |
| 54 | D8 | 31 | HIS | Peptide |
| 27 | DD | 236 | GLY | Peptide |
| 27 | DD | 237 | GLU | Peptide |
| 27 | DD | 29 | PRO | Peptide |
| 28 | DE | 186 | GLY | Peptide |
| 28 | DE | 201 | THR | Peptide |
| 28 | DE | 203 | LYS | Peptide |
| 28 | DE | 61 | ARG | Peptide |
| 28 | DE | 65 | GLY | Peptide |
| 28 | DE | 88 | GLY | Peptide |
| 29 | DF | 123 | LEU | Peptide |
| 29 | DF | 2 | LYS | Peptide |
| 30 | DG | 13 | GLU | Peptide |
| 31 | DH | 124 | GLU | Peptide |
| 31 | DH | 125 | VAL | Peptide |
| 32 | DK | 112 | LYS | Peptide |
| 32 | DK | 142 | VAL | Peptide |
| 32 | DK | 143 | SER | Peptide |
| 32 | DK | 82 | ARG | Peptide |
| 35 | DO | 110 | TYR | Peptide |
| 35 | DO | 115 | LEU | Peptide |
| 35 | DO | 139 | LYS | Peptide |
| 38 | DQ | 108 | GLY | Peptide |
| 38 | DQ | 56 | LEU | Peptide |
| 44 | DU | 46 | LYS | Peptide |
| 44 | DU | 76 | CYS | Peptide |
| 45 | DV | 175 | VAL | Peptide |
| 45 | DV | 60 | GLU | Peptide |
| 48 | DW | 43 | GLN | Peptide |

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32369 | 0 | 16339 | 1207 | 1 |
| 1 | CA | 32372 | 0 | 16338 | 1298 | 1 |
| 2 | AE | 1924 | 0 | 1975 | 158 | 0 |
| 2 | CE | 1924 | 0 | 1975 | 180 | 0 |
| 3 | AF | 1605 | 0 | 1668 | 111 | 0 |
| 3 | CF | 1612 | 0 | 1677 | 144 | 0 |
| 4 | AG | 1703 | 0 | 1764 | 146 | 0 |
| 4 | CG | 1703 | 0 | 1763 | 140 | 1 |
| 5 | AH | 1155 | 0 | 1213 | 74 | 0 |
| 5 | CH | 1155 | 0 | 1213 | 91 | 0 |
| 6 | AI | 843 | 0 | 857 | 39 | 1 |
| 6 | CI | 843 | 0 | 857 | 45 | 0 |
| 7 | AJ | 1257 | 0 | 1296 | 68 | 0 |
| 7 | CJ | 1257 | 0 | 1296 | 74 | 0 |
| 8 | AK | 1116 | 0 | 1177 | 75 | 0 |
| 8 | CK | 1116 | 0 | 1177 | 66 | 0 |
| 9 | AL | 1010 | 0 | 1037 | 99 | 0 |
| 9 | CL | 1010 | 0 | 1037 | 121 | 0 |
| 10 | AM | 801 | 0 | 849 | 78 | 0 |
| 10 | CM | 801 | 0 | 849 | 114 | 0 |
| 11 | AN | 885 | 0 | 904 | 65 | 0 |
| 11 | CN | 885 | 0 | 904 | 45 | 0 |
| 12 | AO | 975 | 0 | 1062 | 62 | 0 |
| 12 | CO | 975 | 0 | 1062 | 75 | 0 |
| 13 | AP | 928 | 0 | 987 | 66 | 0 |
| 13 | CP | 933 | 0 | 992 | 107 | 0 |
| 14 | AQ | 492 | 0 | 529 | 47 | 0 |
| 14 | CQ | 492 | 0 | 531 | 68 | 0 |
| 15 | AR | 734 | 0 | 771 | 38 | 0 |
| 15 | CR | 734 | 0 | 771 | 35 | 0 |
| 16 | AS | 705 | 0 | 725 | 79 | 0 |
| 16 | CS | 705 | 0 | 725 | 45 | 0 |
| 17 | AT | 834 | 0 | 904 | 55 | 0 |
| 17 | CT | 834 | 0 | 904 | 41 | 0 |
| 18 | AU | 591 | 0 | 662 | 30 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18 | CU | 591 | 0 | 662 | 47 | 0 |
| 19 | AV | 624 | 0 | 636 | 71 | 0 |
| 19 | CV | 624 | 0 | 636 | 91 | 0 |
| 20 | AW | 763 | 0 | 859 | 73 | 0 |
| 20 | CW | 763 | 0 | 861 | 56 | 0 |
| 21 | AX | 217 | 0 | 234 | 17 | 0 |
| 21 | CX | 217 | 0 | 234 | 23 | 0 |
| 22 | AB | 1861 | 0 | 938 | 85 | 0 |
| 22 | CB | 1861 | 0 | 938 | 99 | 0 |
| 23 | AC | 1643 | 0 | 837 | 75 | 0 |
| 23 | AD | 1643 | 0 | 837 | 97 | 0 |
| 23 | CC | 1643 | 0 | 837 | 91 | 0 |
| 23 | CD | 1643 | 0 | 837 | 108 | 0 |
| 24 | A1 | 205 | 0 | 103 | 12 | 0 |
| 24 | C1 | 205 | 0 | 103 | 10 | 0 |
| 25 | BA | 62707 | 0 | 31613 | 2105 | 0 |
| 25 | DA | 62607 | 0 | 31565 | 2108 | 1 |
| 26 | BB | 2617 | 0 | 1328 | 94 | 0 |
| 26 | DB | 2617 | 0 | 1328 | 135 | 0 |
| 27 | BD | 2115 | 0 | 2195 | 238 | 0 |
| 27 | DD | 2115 | 0 | 2195 | 211 | 0 |
| 28 | BE | 1568 | 0 | 1634 | 334 | 0 |
| 28 | DE | 1568 | 0 | 1634 | 256 | 0 |
| 29 | BF | 1585 | 0 | 1632 | 119 | 0 |
| 29 | DF | 1627 | 0 | 1680 | 184 | 0 |
| 30 | BG | 1474 | 0 | 1535 | 171 | 0 |
| 30 | DG | 1474 | 0 | 1535 | 148 | 0 |
| 31 | BH | 1307 | 0 | 1382 | 135 | 0 |
| 31 | DH | 1307 | 0 | 1382 | 156 | 1 |
| 32 | BK | 1136 | 0 | 1223 | 99 | 0 |
| 32 | DK | 1136 | 0 | 1223 | 84 | 0 |
| 33 | BM | 1104 | 0 | 1180 | 142 | 0 |
| 33 | DM | 1104 | 0 | 1180 | 87 | 0 |
| 34 | BN | 933 | 0 | 996 | 63 | 0 |
| 34 | DN | 933 | 0 | 996 | 51 | 0 |
| 35 | BO | 1145 | 0 | 1228 | 200 | 0 |
| 35 | DO | 1145 | 0 | 1227 | 240 | 0 |
| 36 | BP | 1122 | 0 | 1179 | 95 | 0 |
| 36 | DP | 1122 | 0 | 1179 | 208 | 0 |
| 37 | B0 | 968 | 0 | 1033 | 78 | 0 |
| 37 | D0 | 960 | 0 | 1021 | 60 | 0 |
| 38 | BQ | 882 | 0 | 943 | 106 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38 | DQ | 882 | 0 | 943 | 120 | 0 |
| 39 | BR | 1141 | 0 | 1202 | 116 | 0 |
| 39 | DR | 1141 | 0 | 1202 | 125 | 0 |
| 40 | B1 | 964 | 0 | 1022 | 98 | 0 |
| 40 | D1 | 964 | 0 | 1022 | 94 | 0 |
| 41 | B2 | 779 | 0 | 852 | 80 | 0 |
| 41 | D2 | 779 | 0 | 852 | 129 | 0 |
| 42 | BS | 900 | 0 | 964 | 71 | 0 |
| 42 | DS | 900 | 0 | 964 | 42 | 0 |
| 43 | BT | 725 | 0 | 778 | 53 | 0 |
| 43 | DT | 725 | 0 | 778 | 75 | 0 |
| 44 | BU | 785 | 0 | 878 | 75 | 0 |
| 44 | DU | 785 | 0 | 878 | 98 | 0 |
| 45 | BV | 1397 | 0 | 1430 | 120 | 0 |
| 45 | DV | 1428 | 0 | 1454 | 162 | 0 |
| 46 | B3 | 607 | 0 | 628 | 50 | 0 |
| 46 | D3 | 613 | 0 | 633 | 52 | 0 |
| 47 | BZ | 763 | 0 | 848 | 50 | 0 |
| 47 | DZ | 763 | 0 | 848 | 46 | 0 |
| 48 | BW | 558 | 0 | 610 | 44 | 0 |
| 48 | DW | 581 | 0 | 629 | 49 | 0 |
| 49 | BX | 469 | 0 | 518 | 35 | 0 |
| 49 | DX | 469 | 0 | 518 | 24 | 0 |
| 50 | B4 | 533 | 0 | 522 | 84 | 0 |
| 50 | D4 | 515 | 0 | 510 | 84 | 0 |
| 51 | B5 | 459 | 0 | 480 | 54 | 0 |
| 51 | D5 | 454 | 0 | 475 | 44 | 0 |
| 52 | B6 | 389 | 0 | 404 | 80 | 0 |
| 52 | D6 | 389 | 0 | 404 | 84 | 0 |
| 53 | B7 | 430 | 0 | 480 | 30 | 0 |
| 53 | D7 | 430 | 0 | 480 | 36 | 0 |
| 54 | B8 | 488 | 0 | 558 | 110 | 0 |
| 54 | D8 | 488 | 0 | 558 | 113 | 0 |
| 55 | A1 | 2 | 0 | 0 | 0 | 0 |
| 55 | AA | 242 | 0 | 0 | 0 | 0 |
| 55 | AB | 5 | 0 | 0 | 0 | 0 |
| 55 | AC | 9 | 0 | 0 | 0 | 0 |
| 55 | AD | 1 | 0 | 0 | 0 | 0 |
| 55 | AG | 1 | 0 | 0 | 0 | 0 |
| 55 | AH | 1 | 0 | 0 | 0 | 0 |
| 55 | AN | 2 | 0 | 0 | 0 | 0 |
| 55 | AQ | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55 | B0 | 1 | 0 | 0 | 0 | 0 |
| 55 | B1 | 1 | 0 | 0 | 0 | 0 |
| 55 | B2 | 1 | 0 | 0 | 0 | 0 |
| 55 | B3 | 1 | 0 | 0 | 0 | 0 |
| 55 | B5 | 1 | 0 | 0 | 0 | 0 |
| 55 | B7 | 1 | 0 | 0 | 0 | 0 |
| 55 | B8 | 1 | 0 | 0 | 0 | 0 |
| 55 | BA | 623 | 0 | 0 | 0 | 0 |
| 55 | BB | 17 | 0 | 0 | 0 | 0 |
| 55 | BD | 1 | 0 | 0 | 0 | 0 |
| 55 | BE | 5 | 0 | 0 | 0 | 0 |
| 55 | BF | 3 | 0 | 0 | 0 | 0 |
| 55 | BO | 2 | 0 | 0 | 0 | 0 |
| 55 | BU | 2 | 0 | 0 | 0 | 0 |
| 55 | CA | 207 | 0 | 0 | 0 | 0 |
| 55 | CB | 3 | 0 | 0 | 0 | 0 |
| 55 | CC | 8 | 0 | 0 | 0 | 0 |
| 55 | CG | 2 | 0 | 0 | 0 | 0 |
| 55 | CN | 1 | 0 | 0 | 0 | 0 |
| 55 | CS | 1 | 0 | 0 | 0 | 0 |
| 55 | D1 | 2 | 0 | 0 | 0 | 0 |
| 55 | D3 | 1 | 0 | 0 | 0 | 0 |
| 55 | D5 | 1 | 0 | 0 | 0 | 0 |
| 55 | DA | 526 | 0 | 0 | 0 | 0 |
| 55 | DB | 14 | 0 | 0 | 0 | 0 |
| 55 | DE | 3 | 0 | 0 | 0 | 0 |
| 55 | DP | 1 | 0 | 0 | 0 | 0 |
| 55 | DR | 1 | 0 | 0 | 0 | 0 |
| 55 | DU | 1 | 0 | 0 | 0 | 0 |
| 56 | AG | 1 | 0 | 0 | 0 | 0 |
| 56 | AQ | 1 | 0 | 0 | 0 | 0 |
| 56 | CG | 1 | 0 | 0 | 0 | 0 |
| 56 | CQ | 1 | 0 | 0 | 0 | 0 |
| All | All | 299552 | 0 | 200910 | 14872 | 3 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (14872) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:AA:625:G:H4' | 16:AS:16:HIS:CD2 | 1.33 | 1.61 |
| 28:DE:46:ALA:CB | 28:DE:82:ARG:HA | 1.37 | 1.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 30:BG:83:ARG:H | 30:BG:86:MET:CE | 1.24 | 1.47 |
| 36:DP:26:TYR:CE1 | 36:DP:139:GLU:HB2 | 1.48 | 1.45 |
| 25:BA:1056:G:N2 | 25:BA:1103:A:H62 | 1.13 | 1.44 |
| 28:DE:46:ALA:HB2 | 28:DE:82:ARG:CA | 1.50 | 1.41 |
| 47:BZ:85:LEU:C | 47:BZ:87:PRO:HD2 | 1.38 | 1.40 |
| 1:AA:625:G:C4' | 16:AS:16:HIS:HD2 | 1.32 | 1.40 |
| 25:DA:226:G:N2 | 25:DA:228:A:H61 | 1.21 | 1.39 |
| 25:BA:2467:C:C2' | 25:BA:2468:G:H5' | 1.53 | 1.39 |
| 25:BA:49:A:N7 | 25:BA:120:U:H5 | 1.20 | 1.38 |
| 36:DP:24:GLY:HA3 | 36:DP:25:ASP:CB | 1.42 | 1.35 |
| 35:BO:61:ARG:HB2 | 35:BO:61:ARG:NH2 | 1.39 | 1.35 |
| 25:DA:226:G:H21 | 25:DA:228:A:N6 | 0.88 | 1.35 |
| 51:D5:4:HIS:HB3 | 51:D5:5:PRO:CD | 1.39 | 1.35 |
| 35:DO:61:ARG:HB2 | 35:DO:61:ARG:NH2 | 1.39 | 1.35 |
| 25:DA:226:G:N2 | 25:DA:228:A:N6 | 1.73 | 1.34 |
| 25:DA:847:U:C5 | 25:DA:933:A:N6 | 1.95 | 1.34 |
| 25:BA:631:A:OP2 | 54:B8:46:ARG:NH2 | 1.60 | 1.33 |
| 28:BE:79:ARG:CD | 28:BE:197:ILE:HG21 | 1.59 | 1.31 |
| 27:BD:272:ALA:HB1 | 27:BD:273:ARG:CA | 1.62 | 1.30 |
| 1:AA:1160:G:H1 | 1:AA:1177:G:N2 | 1.29 | 1.30 |
| 28:DE:46:ALA:CB | 28:DE:82:ARG:CA | 2.08 | 1.29 |
| 38:BQ:23:ARG:HD3 | 38:BQ:85:VAL:O | 1.28 | 1.28 |
| 20:AW:10:LEU:CD2 | 20:AW:12:ALA:HB3 | 1.62 | 1.28 |
| 54:D8:49:VAL:C | 54:D8:50:LEU:HD12 | 1.53 | 1.27 |
| 35:DO:19:VAL:CG2 | 35:DO:27:HIS:HB3 | 1.62 | 1.27 |
| 27:BD:272:ALA:CB | 27:BD:273:ARG:HA | 1.53 | 1.27 |
| 38:BQ:83:LYS:O | 38:BQ:109:GLY:HA2 | 1.24 | 1.27 |
| 25:DA:9:U:H3 | 25:DA:2629:A:N6 | 1.31 | 1.27 |
| 27:DD:35:LYS:HD2 | 27:DD:104:TYR:CD1 | 1.70 | 1.27 |
| 36:DP:29:PHE:CD2 | 36:DP:65:PHE:CE1 | 2.22 | 1.26 |
| 38:DQ:87:PHE:CE1 | 38:DQ:102:ALA:HB2 | 1.71 | 1.25 |
| 28:BE:23:VAL:HG12 | 28:BE:185:LYS:CB | 1.66 | 1.25 |
| 25:BA:49:A:N7 | 25:BA:120:U:C5 | 2.03 | 1.25 |
| 25:DA:847:U:C4 | 25:DA:933:A:N6 | 2.03 | 1.24 |
| 25:BA:2310:A:N3 | 30:BG:77:ILE:HD11 | 1.50 | 1.24 |
| 30:BG:83:ARG:HG3 | 30:BG:86:MET:CE | 1.65 | 1.24 |
| 27:DD:43:ARG:HH11 | 27:DD:44:ASN:ND2 | 1.33 | 1.24 |
| 41:D2:81:TYR:O | 41:D2:82:ARG:HG3 | 1.37 | 1.23 |
| 28:BE:23:VAL:HB | 28:BE:184:VAL:O | 1.10 | 1.23 |
| 27:BD:43:ARG:NH1 | 27:BD:44:ASN:OD1 | 1.70 | 1.22 |
| 27:BD:35:LYS:HD2 | 27:BD:104:TYR:CD1 | 1.74 | 1.22 |
| 16:AS:20:VAL:HG21 | 16:AS:32:TYR:CD1 | 1.74 | 1.22 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:2681:C:C5 | 25:DA:2725:A:N6 | 2.06 | 1.21 |
| 36:DP:26:TYR:CD1 | 36:DP:139:GLU:CG | 2.24 | 1.21 |
| 28:BE:19:ARG:NH1 | 34:BN:72:PRO:HB3 | 1.55 | 1.21 |
| 35:DO:19:VAL:HG23 | 35:DO:27:HIS:CB | 1.69 | 1.20 |
| 36:DP:26:TYR:HD1 | 36:DP:139:GLU:CG | 1.55 | 1.20 |
| 54:D8:34:TRP:O | 54:D8:36:LYS:HG3 | 1.37 | 1.20 |
| 36:DP:66:ILE:HD12 | 36:DP:67:ARG:N | 1.55 | 1.19 |
| 25:DA:2371:G:O4' | 52:D6:45:LYS:HE2 | 1.39 | 1.19 |
| 36:DP:29:PHE:CD2 | 36:DP:65:PHE:HE1 | 1.56 | 1.19 |
| 16:AS:20:VAL:HG21 | 16:AS:32:TYR:CG | 1.77 | 1.18 |
| 16:AS:19:ILE:CG2 | 16:AS:36:ILE:CG1 | 2.21 | 1.18 |
| 36:DP:66:ILE:CD1 | 36:DP:67:ARG:H | 1.55 | 1.18 |
| 33:DM:47:ALA:HB2 | 33:DM:112:LEU:HD11 | 1.23 | 1.18 |
| 38:BQ:83:LYS:O | 38:BQ:109:GLY:CA | 1.92 | 1.18 |
| 28:BE:35:GLN:CB | 28:BE:48:GLN:HG3 | 1.74 | 1.18 |
| 25:BA:2309:A:H2' | 25:BA:2310:A:C5' | 1.74 | 1.17 |
| 28:BE:81:ILE:HG21 | 28:BE:84:PHE:CD1 | 1.78 | 1.17 |
| 23:AC:17:C:H3' | 23:AC:18:C:H5'' | 1.25 | 1.17 |
| 1:CA:1004:A:H1' | 1:CA:1036:G:N1 | 1.59 | 1.17 |
| 1:AA:625:G:C4' | 16:AS:16:HIS:CD2 | 2.14 | 1.17 |
| 25:BA:1899:G:H22 | 25:BA:1902:C:N4 | 1.41 | 1.17 |
| 39:DR:74:ARG:HG2 | 39:DR:74:ARG:HH11 | 1.10 | 1.17 |
| 30:BG:83:ARG:N | 30:BG:86:MET:CE | 2.08 | 1.16 |
| 28:BE:14:ILE:HG22 | 28:BE:15:PHE:N | 1.54 | 1.16 |
| 25:DA:1257:C:O2' | 29:DF:84:VAL:CG1 | 1.93 | 1.16 |
| 35:BO:15:ARG:HH11 | 35:BO:15:ARG:HG2 | 1.10 | 1.16 |
| 25:BA:2317:C:H2' | 25:BA:2318:G:H5' | 1.28 | 1.16 |
| 35:BO:65:ARG:HG3 | 35:BO:65:ARG:HH11 | 1.07 | 1.16 |
| 25:BA:2309:A:C2' | 25:BA:2310:A:H5' | 1.76 | 1.15 |
| 52:D6:48:VAL:HG13 | 52:D6:49:HIS:N | 1.57 | 1.15 |
| 25:DA:672:C:H2' | 25:DA:673:C:H5'' | 1.22 | 1.15 |
| 25:BA:1056:G:N2 | 25:BA:1103:A:N6 | 1.93 | 1.15 |
| 1:AA:1053:G:H5' | 1:AA:1054:C:H5' | 1.24 | 1.14 |
| 33:BM:47:ALA:HB2 | 33:BM:112:LEU:HD11 | 1.27 | 1.14 |
| 23:CC:30:G:C2' | 23:CC:31:G:H5' | 1.77 | 1.14 |
| 27:BD:35:LYS:HD3 | 27:BD:63:ARG:HB3 | 1.30 | 1.14 |
| 16:AS:19:ILE:HG23 | 16:AS:36:ILE:CG1 | 1.76 | 1.14 |
| 38:DQ:14:VAL:HG21 | 38:DQ:89:ARG:CD | 1.77 | 1.14 |
| 16:AS:19:ILE:HG23 | 16:AS:36:ILE:HG12 | 1.15 | 1.14 |
| 28:BE:52:LEU:HB2 | 28:BE:75:VAL:CG2 | 1.77 | 1.14 |
| 51:D5:4:HIS:CB | 51:D5:5:PRO:HD3 | 1.78 | 1.13 |
| 4:AG:9:CYS:O | 4:AG:13:ARG:HG2 | 1.46 | 1.13 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 38:DQ:87:PHE:HE1 | 38:DQ:102:ALA:HB2 | 0.97 | 1.13 |
| 28:BE:52:LEU:H | 28:BE:52:LEU:HD23 | 1.13 | 1.13 |
| 25:DA:2306:C:H3' | 25:DA:2307:G:H5'' | 1.29 | 1.13 |
| 28:BE:23:VAL:HG12 | 28:BE:185:LYS:CA | 1.79 | 1.12 |
| 29:DF:89:VAL:HG12 | 29:DF:90:PHE:N | 1.54 | 1.12 |
| 16:AS:19:ILE:HG21 | 16:AS:36:ILE:HG13 | 1.30 | 1.12 |
| 1:CA:975:A:H4' | 1:CA:976:G:H5'' | 1.25 | 1.12 |
| 28:DE:46:ALA:HB1 | 28:DE:82:ARG:N | 1.65 | 1.11 |
| 28:BE:19:ARG:NH1 | 34:BN:72:PRO:CB | 2.12 | 1.11 |
| 1:AA:1139:G:N2 | 1:AA:1143:G:O6 | 1.81 | 1.11 |
| 25:DA:2393:A:H5' | 35:DO:62:LEU:HB3 | 1.16 | 1.11 |
| 41:D2:85:LYS:HG3 | 41:D2:87:HIS:H | 1.10 | 1.11 |
| 25:DA:2060:A:OP1 | 29:DF:68:LYS:O | 1.67 | 1.11 |
| 25:DA:2636:U:OP1 | 28:DE:79:ARG:O | 1.69 | 1.11 |
| 30:BG:83:ARG:H | 30:BG:86:MET:HE1 | 1.07 | 1.11 |
| 23:CC:60:A:H2' | 23:CC:61:U:H5' | 1.17 | 1.11 |
| 31:DH:125:VAL:HG22 | 31:DH:126:PRO:HD3 | 1.12 | 1.11 |
| 27:BD:181:GLU:HA | 27:BD:272:ALA:CB | 1.80 | 1.10 |
| 26:BB:15:A:H5' | 26:BB:16:G:C8 | 1.86 | 1.10 |
| 39:DR:54:ARG:HG2 | 39:DR:54:ARG:HH11 | 1.07 | 1.10 |
| 28:BE:78:LEU:HD12 | 28:BE:79:ARG:N | 1.67 | 1.10 |
| 33:DM:45:ASN:O | 33:DM:46:VAL:HG23 | 1.52 | 1.10 |
| 28:BE:51:PHE:CD1 | 28:BE:52:LEU:HD23 | 1.87 | 1.10 |
| 41:D2:76:LYS:O | 41:D2:79:VAL:HG23 | 1.51 | 1.10 |
| 31:DH:151:ILE:O | 31:DH:152:ARG:HG3 | 1.49 | 1.10 |
| 30:BG:67:LYS:HE2 | 50:B4:6:HIS:CE1 | 1.86 | 1.10 |
| 23:CC:17:C:H3' | 23:CC:18:C:H5'' | 1.32 | 1.10 |
| 38:DQ:14:VAL:CG2 | 38:DQ:89:ARG:HD3 | 1.81 | 1.09 |
| 28:BE:4:ILE:HD13 | 28:BE:28:ALA:HB1 | 1.14 | 1.09 |
| 53:D7:8:ASN:ND2 | 53:D7:11:LYS:H | 1.50 | 1.09 |
| 23:AD:5:G:N2 | 23:AD:70:C:N3 | 2.00 | 1.09 |
| 44:BU:79:CYS:SG | 44:BU:80:GLY:N | 2.25 | 1.09 |
| 33:BM:42:TRP:HA | 33:BM:48:MET:HE1 | 1.17 | 1.09 |
| 27:DD:27:THR:HG21 | 27:DD:83:GLU:HG2 | 1.30 | 1.09 |
| 36:DP:26:TYR:CE1 | 36:DP:139:GLU:CB | 2.33 | 1.09 |
| 1:CA:1223:C:H5'' | 1:CA:1224:G:H5'' | 1.11 | 1.09 |
| 45:DV:146:ILE:HG13 | 45:DV:147:GLY:H | 1.11 | 1.09 |
| 36:DP:24:GLY:CA | 36:DP:25:ASP:CB | 2.30 | 1.09 |
| 1:AA:1305:G:H22 | 1:AA:1331:G:H2' | 1.15 | 1.09 |
| 25:BA:2310:A:C2 | 30:BG:77:ILE:CG1 | 2.36 | 1.09 |
| 5:AH:126:ARG:HG3 | 5:AH:126:ARG:HH11 | 1.14 | 1.09 |
| 26:DB:74:U:H2' | 26:DB:75:G:H5'' | 1.19 | 1.09 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:CF:111:LEU:HD11 | 3:CF:145:GLY:HA3 | 1.34 | 1.08 |
| 20:AW:10:LEU:HD21 | 20:AW:12:ALA:CB | 1.83 | 1.08 |
| 25:BA:2310:A:N3 | 30:BG:77:ILE:CD1 | 2.17 | 1.08 |
| 35:DO:64:LYS:CB | 54:D8:25:MET:HG3 | 1.82 | 1.08 |
| 30:BG:83:ARG:HG3 | 30:BG:86:MET:HE2 | 1.26 | 1.08 |
| 28:BE:79:ARG:HD2 | 28:BE:197:ILE:CG2 | 1.84 | 1.08 |
| 20:AW:10:LEU:HD21 | 20:AW:12:ALA:HB3 | 1.22 | 1.08 |
| 36:DP:27:VAL:HG13 | 36:DP:105:GLU:OE2 | 1.53 | 1.08 |
| 16:AS:19:ILE:CG2 | 16:AS:36:ILE:HG12 | 1.82 | 1.08 |
| 28:BE:35:GLN:HB3 | 28:BE:48:GLN:HG3 | 1.30 | 1.08 |
| 25:BA:1026:U:H1' | 25:BA:1027:A:O5' | 1.50 | 1.08 |
| 25:DA:2415:G:H4' | 35:DO:67:MET:H | 1.10 | 1.08 |
| 27:DD:35:LYS:HE2 | 27:DD:104:TYR:HB2 | 1.13 | 1.08 |
| 52:D6:48:VAL:CG1 | 52:D6:49:HIS:H | 1.62 | 1.08 |
| 28:BE:81:ILE:CG2 | 28:BE:84:PHE:HB2 | 1.83 | 1.08 |
| 28:BE:81:ILE:HG22 | 28:BE:84:PHE:HB2 | 1.27 | 1.08 |
| 52:B6:47:THR:HG22 | 52:B6:48:VAL:H | 0.93 | 1.08 |
| 1:CA:963:G:H21 | 10:CM:55:LYS:HD3 | 1.13 | 1.08 |
| 35:DO:15:ARG:HH11 | 35:DO:15:ARG:CG | 1.67 | 1.08 |
| 25:DA:2371:G:C4' | 52:D6:45:LYS:HE2 | 1.83 | 1.08 |
| 25:BA:1899:G:N2 | 25:BA:1902:C:H41 | 1.52 | 1.08 |
| 28:BE:23:VAL:CB | 28:BE:184:VAL:O | 2.01 | 1.07 |
| 52:D6:48:VAL:O | 52:D6:49:HIS:HB2 | 1.51 | 1.07 |
| 23:CC:30:G:H2' | 23:CC:31:G:H5' | 1.29 | 1.07 |
| 35:DO:65:ARG:HG3 | 35:DO:65:ARG:HH11 | 1.07 | 1.07 |
| 25:BA:2310:A:C2 | 30:BG:77:ILE:HG12 | 1.88 | 1.07 |
| 29:DF:83:PHE:O | 29:DF:84:VAL:HG13 | 1.53 | 1.07 |
| 25:DA:9:U:N3 | 25:DA:2629:A:N6 | 2.01 | 1.07 |
| 1:CA:448:A:OP2 | 1:CA:485:G:N2 | 1.86 | 1.07 |
| 38:DQ:14:VAL:HG21 | 38:DQ:89:ARG:HD3 | 1.07 | 1.07 |
| 28:BE:23:VAL:CG1 | 28:BE:185:LYS:HB3 | 1.84 | 1.07 |
| 28:BE:19:ARG:HH11 | 34:BN:72:PRO:HB3 | 0.92 | 1.07 |
| 28:BE:36:ARG:HH22 | 28:BE:88:GLY:HA2 | 1.19 | 1.07 |
| 48:BW:4:SER:HB2 | 48:BW:5:GLU:OE2 | 1.54 | 1.07 |
| 15:CR:17:ARG:HG3 | 15:CR:17:ARG:HH11 | 1.17 | 1.07 |
| 4:CG:13:ARG:HG2 | 4:CG:14:ARG:H | 1.18 | 1.07 |
| 36:DP:29:PHE:HD2 | 36:DP:65:PHE:CE1 | 1.63 | 1.07 |
| 28:BE:23:VAL:HG12 | 28:BE:185:LYS:HB3 | 1.14 | 1.07 |
| 28:BE:38:THR:HB | 28:BE:39:PRO:HD2 | 1.36 | 1.07 |
| 25:BA:2394:C:OP1 | 35:BO:63:PRO:HD2 | 1.55 | 1.06 |
| 41:D2:83:ARG:N | 41:D2:83:ARG:HD2 | 1.67 | 1.06 |
| 31:DH:127:GLU:HG2 | 31:DH:128:PRO:HD2 | 1.32 | 1.06 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 52:D6:25:LYS:HB3 | 54:D8:34:TRP:HZ3 | 1.14 | 1.06 |
| 36:BP:76:LYS:H | 36:BP:88:GLY:HA3 | 1.00 | 1.06 |
| 36:DP:63:LYS:HD3 | 36:DP:63:LYS:C | 1.75 | 1.06 |
| 25:DA:2420:C:OP1 | 54:D8:34:TRP:HB3 | 1.55 | 1.06 |
| 28:DE:47:VAL:O | 28:DE:80:GLU:HA | 1.53 | 1.06 |
| 35:DO:64:LYS:HB3 | 54:D8:25:MET:CG | 1.83 | 1.06 |
| 22:CB:59:U:O2' | 22:CB:70:G:H4' | 1.55 | 1.06 |
| 25:BA:1884:A:H2' | 25:BA:1885:A:H5'' | 1.32 | 1.06 |
| 27:BD:35:LYS:HB3 | 27:BD:63:ARG:HA | 1.38 | 1.06 |
| 28:BE:14:ILE:CG2 | 28:BE:15:PHE:H | 1.60 | 1.06 |
| 38:DQ:87:PHE:HE1 | 38:DQ:102:ALA:CB | 1.69 | 1.05 |
| 35:BO:15:ARG:CG | 35:BO:15:ARG:HH11 | 1.67 | 1.05 |
| 31:DH:152:ARG:O | 31:DH:153:LYS:HB2 | 1.46 | 1.05 |
| 29:BF:178:PRO:HB2 | 29:BF:201:VAL:HG11 | 1.38 | 1.05 |
| 47:DZ:91:LYS:NZ | 47:DZ:91:LYS:HB2 | 1.66 | 1.05 |
| 25:BA:2371:G:O4' | 52:B6:45:LYS:HG3 | 1.55 | 1.05 |
| 39:BR:74:ARG:HH11 | 39:BR:74:ARG:HG2 | 1.16 | 1.05 |
| 27:BD:35:LYS:NZ | 27:BD:104:TYR:HB2 | 1.72 | 1.05 |
| 28:BE:56:PRO:O | 28:BE:57:LYS:HB2 | 1.48 | 1.05 |
| 25:BA:2393:A:H5' | 35:BO:62:LEU:HB3 | 1.37 | 1.05 |
| 41:D2:82:ARG:HG2 | 41:D2:82:ARG:HH11 | 0.91 | 1.04 |
| 30:BG:83:ARG:N | 30:BG:86:MET:HE1 | 1.66 | 1.04 |
| 25:BA:2469:A:N6 | 25:BA:2481:G:N3 | 2.03 | 1.04 |
| 31:BH:171:LEU:O | 31:BH:171:LEU:HD12 | 1.55 | 1.04 |
| 25:DA:9:U:N3 | 25:DA:2629:A:C6 | 2.25 | 1.04 |
| 28:BE:81:ILE:CG2 | 28:BE:84:PHE:CB | 2.34 | 1.04 |
| 25:BA:620:G:H4' | 25:BA:621:A:H5'' | 1.35 | 1.04 |
| 25:DA:2748:A:N7 | 25:DA:2754:U:O4 | 1.88 | 1.04 |
| 1:AA:1004:A:H1' | 1:AA:1036:G:C6 | 1.91 | 1.04 |
| 39:DR:52:ILE:HG22 | 39:DR:52:ILE:O | 1.58 | 1.04 |
| 35:DO:15:ARG:HG2 | 35:DO:15:ARG:HH11 | 1.10 | 1.04 |
| 25:BA:860:U:H5 | 25:BA:917:A:C2 | 1.74 | 1.04 |
| 28:DE:52:LEU:O | 28:DE:74:PRO:HA | 1.58 | 1.03 |
| 35:BO:9:ASN:HB3 | 35:BO:10:PRO:HD2 | 1.36 | 1.03 |
| 28:BE:19:ARG:HH11 | 34:BN:72:PRO:CB | 1.71 | 1.03 |
| 28:BE:52:LEU:HB2 | 28:BE:75:VAL:HG22 | 1.38 | 1.03 |
| 23:AC:17:C:H3' | 23:AC:18:C:C5' | 1.87 | 1.03 |
| 22:CB:37:G:N2 | 24:C1:19:U:O2 | 1.89 | 1.03 |
| 50:B4:62:ARG:O | 50:B4:66:SER:HA | 1.58 | 1.03 |
| 21:AX:15:ARG:HG2 | 21:AX:15:ARG:HH11 | 1.18 | 1.03 |
| 25:DA:74:A:H4' | 25:DA:75:G:O5' | 1.55 | 1.03 |
| 25:DA:1342:A:N1 | 25:DA:1602:U:N3 | 2.06 | 1.03 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 36:DP:24:GLY:HA3 | 36:DP:25:ASP:HB2 | 1.04 | 1.03 |
| 16:AS:19:ILE:CG2 | 16:AS:36:ILE:HG13 | 1.82 | 1.03 |
| 28:BE:27:LEU:C | 28:BE:27:LEU:HD23 | 1.78 | 1.03 |
| 29:BF:198:ALA:HA | 29:BF:201:VAL:HG12 | 1.40 | 1.03 |
| 11:AN:79:SER:O | 11:AN:80:VAL:HG13 | 1.59 | 1.03 |
| 27:DD:44:ASN:HB3 | 27:DD:49:ILE:HA | 1.40 | 1.03 |
| 36:BP:66:ILE:HG13 | 36:BP:67:ARG:H | 1.19 | 1.03 |
| 25:BA:71:A:C2 | 43:BT:31:HIS:HE1 | 1.77 | 1.03 |
| 51:D5:16:ARG:HG2 | 51:D5:16:ARG:HH11 | 1.19 | 1.03 |
| 28:BE:48:GLN:O | 28:BE:49:LEU:HB2 | 1.57 | 1.02 |
| 25:DA:1070:A:H5' | 25:DA:1071:G:H5'' | 1.39 | 1.02 |
| 35:BO:61:ARG:HH21 | 35:BO:61:ARG:CB | 1.73 | 1.02 |
| 25:BA:2309:A:H2' | 25:BA:2310:A:H5' | 1.03 | 1.02 |
| 28:BE:81:ILE:HG21 | 28:BE:84:PHE:CG | 1.93 | 1.02 |
| 28:BE:51:PHE:CD1 | 28:BE:52:LEU:CD2 | 2.43 | 1.02 |
| 29:DF:89:VAL:CG1 | 29:DF:90:PHE:H | 1.65 | 1.02 |
| 35:DO:61:ARG:CB | 35:DO:61:ARG:HH21 | 1.73 | 1.02 |
| 2:CE:16:HIS:HD2 | 2:CE:209:ARG:HB3 | 1.21 | 1.02 |
| 25:DA:2580:U:H4' | 28:DE:130:GLY:HA3 | 1.38 | 1.02 |
| 1:AA:1004:A:H1' | 1:AA:1036:G:N1 | 1.75 | 1.02 |
| 25:BA:2309:A:C2' | 25:BA:2310:A:C5' | 2.35 | 1.02 |
| 52:D6:41:PRO:HD2 | 52:D6:45:LYS:O | 1.59 | 1.02 |
| 28:DE:48:GLN:C | 28:DE:49:LEU:HG | 1.76 | 1.02 |
| 41:D2:76:LYS:HB3 | 41:D2:79:VAL:HG21 | 1.38 | 1.02 |
| 25:DA:882:G:H1 | 25:DA:894:C:N4 | 1.57 | 1.02 |
| 2:AE:32:ILE:HD11 | 2:AE:40:HIS:HB3 | 1.39 | 1.02 |
| 23:AC:76:C:H5'' | 23:AC:77:A:OP2 | 1.60 | 1.02 |
| 39:BR:36:GLU:HG3 | 39:BR:41:ARG:HD2 | 1.42 | 1.02 |
| 51:D5:4:HIS:CB | 51:D5:5:PRO:CD | 2.30 | 1.01 |
| 1:AA:1182:G:H4' | 1:AA:1183:A:H5' | 1.39 | 1.01 |
| 28:BE:27:LEU:HD13 | 39:BR:1:MET:CE | 1.90 | 1.01 |
| 28:DE:46:ALA:HB1 | 28:DE:82:ARG:H | 1.18 | 1.01 |
| 36:DP:24:GLY:HA3 | 36:DP:25:ASP:HB3 | 1.37 | 1.01 |
| 52:D6:25:LYS:HB3 | 54:D8:34:TRP:CZ3 | 1.95 | 1.01 |
| 40:D1:91:ASP:OD2 | 40:D1:96:ALA:HB2 | 1.58 | 1.01 |
| 25:DA:672:C:C2' | 25:DA:673:C:H5'' | 1.89 | 1.01 |
| 39:DR:55:ASN:H | 39:DR:59:THR:HG22 | 1.23 | 1.01 |
| 31:BH:171:LEU:C | 31:BH:171:LEU:HD12 | 1.77 | 1.01 |
| 2:CE:74:LYS:NZ | 2:CE:205:ASP:O | 1.92 | 1.01 |
| 1:AA:1446:A:H4' | 1:AA:1446:A:OP1 | 1.58 | 1.01 |
| 36:DP:26:TYR:CD1 | 36:DP:139:GLU:HG2 | 1.90 | 1.01 |
| 28:BE:4:ILE:CD1 | 28:BE:28:ALA:HB1 | 1.90 | 1.01 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 28:DE:134:ILE:HD12 | 28:DE:134:ILE:O | 1.58 | 1.01 |
| 43:DT:8:ILE:HD11 | 43:DT:43:VAL:HG12 | 1.42 | 1.01 |
| 25:BA:993:G:OP1 | 40:B1:50:ARG:NH2 | 1.94 | 1.01 |
| 4:AG:65:ARG:NH1 | 4:AG:70:ILE:O | 1.94 | 1.01 |
| 47:BZ:86:SER:N | 47:BZ:87:PRO:HD2 | 1.69 | 1.01 |
| 25:BA:2467:C:H2' | 25:BA:2468:G:H5' | 1.07 | 1.01 |
| 25:BA:607:U:H3 | 25:BA:621:A:H2 | 1.07 | 1.00 |
| 29:BF:46:ARG:HH11 | 29:BF:46:ARG:HG2 | 1.26 | 1.00 |
| 1:AA:56:U:H4' | 32:DK:82:ARG:HH21 | 1.23 | 1.00 |
| 36:DP:75:THR:HB | 36:DP:88:GLY:HA3 | 1.41 | 1.00 |
| 25:BA:2404:C:H1' | 35:BO:67:MET:CE | 1.92 | 1.00 |
| 25:BA:2415:G:H4' | 35:BO:67:MET:H | 1.19 | 1.00 |
| 35:BO:64:LYS:CB | 54:B8:25:MET:HG3 | 1.90 | 1.00 |
| 25:DA:1012:U:N3 | 25:DA:1143:A:N1 | 2.09 | 1.00 |
| 27:DD:35:LYS:CE | 27:DD:104:TYR:HB2 | 1.90 | 1.00 |
| 28:BE:50:GLY:HA2 | 28:BE:77:ILE:HA | 1.42 | 1.00 |
| 1:CA:328:C:H2' | 1:CA:328:C:O2 | 1.61 | 1.00 |
| 48:BW:50:ILE:HD12 | 48:BW:51:ARG:H | 1.23 | 1.00 |
| 39:DR:26:ASP:HB2 | 39:DR:91:ARG:HA | 1.43 | 1.00 |
| 41:D2:85:LYS:HG3 | 41:D2:87:HIS:N | 1.75 | 1.00 |
| 51:D5:36:CYS:SG | 51:D5:49:CYS:HB3 | 2.00 | 1.00 |
| 25:BA:882:G:H2' | 25:BA:883:G:C8 | 1.97 | 1.00 |
| 28:BE:81:ILE:HG22 | 28:BE:84:PHE:CB | 1.92 | 1.00 |
| 35:DO:64:LYS:CD | 54:D8:25:MET:SD | 2.50 | 1.00 |
| 1:CA:1160:G:H1 | 1:CA:1177:G:N2 | 1.60 | 1.00 |
| 25:BA:1728:G:H3' | 25:BA:1729:A:C5' | 1.91 | 1.00 |
| 25:BA:1105:U:H2' | 25:BA:1106:G:H8 | 1.25 | 1.00 |
| 25:BA:2317:C:C2' | 25:BA:2318:G:H5' | 1.92 | 1.00 |
| 1:AA:820:U:H4' | 1:AA:821:G:OP2 | 1.60 | 1.00 |
| 31:DH:151:ILE:C | 31:DH:152:ARG:HG3 | 1.77 | 0.99 |
| 25:BA:1689:A:H62 | 25:BA:1698:A:H2 | 1.05 | 0.99 |
| 1:AA:1124:G:H3' | 1:AA:1145:C:H41 | 1.25 | 0.99 |
| 25:DA:1332:G:N2 | 25:DA:1609:A:O2' | 1.95 | 0.99 |
| 25:DA:2394:C:OP1 | 35:DO:62:LEU:HB2 | 1.62 | 0.99 |
| 41:D2:83:ARG:H | 41:D2:83:ARG:CD | 1.74 | 0.99 |
| 22:AB:7:G:H3' | 22:AB:8:U:H5' | 1.43 | 0.99 |
| 25:BA:885:C:C2 | 25:BA:890:A:N6 | 2.30 | 0.99 |
| 51:B5:4:HIS:HB3 | 51:B5:5:PRO:HD3 | 1.44 | 0.99 |
| 13:AP:65:LYS:HB3 | 50:B4:50:VAL:HG11 | 1.41 | 0.99 |
| 1:AA:1160:G:N1 | 1:AA:1177:G:N2 | 2.08 | 0.99 |
| 36:DP:66:ILE:HD12 | 36:DP:67:ARG:H | 0.86 | 0.99 |
| 16:AS:20:VAL:CG2 | 16:AS:32:TYR:CG | 2.44 | 0.99 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 33:DM:97:ARG:HH11 | 33:DM:97:ARG:HG2 | 1.24 | 0.99 |
| 29:DF:24:LEU:HD12 | 29:DF:25:PRO:HD3 | 1.43 | 0.99 |
| 36:DP:64:ILE:HA | 36:DP:106:VAL:HG12 | 1.42 | 0.99 |
| 38:DQ:78:LEU:HD11 | 38:DQ:107:GLU:HB3 | 1.44 | 0.99 |
| 27:BD:35:LYS:HD3 | 27:BD:63:ARG:CB | 1.92 | 0.99 |
| 27:DD:35:LYS:HB3 | 27:DD:63:ARG:HA | 1.41 | 0.99 |
| 28:BE:201:THR:HG22 | 28:BE:203:LYS:H | 1.25 | 0.99 |
| 28:BE:79:ARG:CD | 28:BE:197:ILE:CG2 | 2.41 | 0.98 |
| 25:BA:2577:A:H5'' | 25:BA:2578:G:H5' | 1.45 | 0.98 |
| 25:DA:273(C):C:H42 | 25:DA:363(C):G:H1 | 1.10 | 0.98 |
| 25:DA:1826:G:H4' | 27:DD:242:ARG:HH21 | 1.26 | 0.98 |
| 41:B2:47:VAL:CG2 | 41:B2:48:GLY:H | 1.75 | 0.98 |
| 45:BV:6:LYS:HA | 45:BV:60:GLU:HB2 | 1.43 | 0.98 |
| 22:CB:87:A:H8 | 25:DA:2583:G:H21 | 1.00 | 0.98 |
| 25:BA:2404:C:H1' | 35:BO:67:MET:HE1 | 0.98 | 0.98 |
| 4:CG:108:LEU:HD21 | 4:CG:183:GLY:HA3 | 1.44 | 0.98 |
| 48:DW:14:ARG:HG3 | 48:DW:15:LYS:HE3 | 1.42 | 0.98 |
| 25:DA:2422:A:H4' | 25:DA:2423:U:OP1 | 1.62 | 0.98 |
| 52:B6:47:THR:HG22 | 52:B6:48:VAL:N | 1.75 | 0.98 |
| 25:BA:1379:A:H1' | 25:BA:1380:G:OP1 | 1.64 | 0.98 |
| 12:AO:18:VAL:HG23 | 12:AO:19:ARG:H | 1.28 | 0.98 |
| 46:B3:40:GLN:NE2 | 46:B3:44:ARG:H | 1.60 | 0.98 |
| 1:AA:791:G:H2' | 1:AA:792:A:H5' | 1.43 | 0.98 |
| 25:DA:2275:C:O2' | 36:DP:84:GLY:HA3 | 1.61 | 0.98 |
| 11:AN:40:ILE:HG22 | 11:AN:75:TYR:HD2 | 1.27 | 0.98 |
| 35:BO:65:ARG:HH21 | 54:B8:15:LYS:HB2 | 1.29 | 0.98 |
| 45:DV:144:LEU:HD12 | 45:DV:144:LEU:O | 1.64 | 0.98 |
| 25:DA:2470:G:OP1 | 36:DP:56:ARG:NH2 | 1.96 | 0.98 |
| 29:BF:29:ASN:H | 29:BF:112:MET:CE | 1.77 | 0.98 |
| 2:AE:96:ARG:HD2 | 2:AE:96:ARG:H | 1.29 | 0.98 |
| 1:AA:975:A:H4' | 1:AA:976:G:H5'' | 1.43 | 0.98 |
| 20:AW:26:ASN:ND2 | 20:AW:26:ASN:H | 1.52 | 0.98 |
| 1:CA:992:U:H3 | 1:CA:1044:A:H62 | 1.08 | 0.98 |
| 35:DO:64:LYS:HB2 | 54:D8:25:MET:HG3 | 1.44 | 0.97 |
| 25:BA:883:G:H1 | 25:BA:893:C:N4 | 1.61 | 0.97 |
| 1:AA:838:G:H1 | 1:AA:848:C:H42 | 1.09 | 0.97 |
| 1:CA:1497:G:H2' | 1:CA:1498:U:H5' | 1.46 | 0.97 |
| 20:AW:10:LEU:CD2 | 20:AW:12:ALA:CB | 2.41 | 0.97 |
| 23:AC:17:C:C3' | 23:AC:18:C:H5'' | 1.94 | 0.97 |
| 25:DA:1012:U:C2 | 25:DA:1143:A:C2 | 2.52 | 0.97 |
| 44:DU:96:ILE:HG12 | 44:DU:101:LYS:HG3 | 1.41 | 0.97 |
| 31:BH:30:LYS:HD2 | 31:BH:81:GLU:H | 1.27 | 0.97 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|----------------------|--------------------|-------------|----------|
| 41:D2:35:LEU:HG | 41:D2:37:VAL:HG11 | 1.46 | 0.97 |
| 52:D6:43:CYS:O | 52:D6:44:ARG:HB2 | 1.63 | 0.97 |
| 47:DZ:87:PRO:HA | 47:DZ:90:ILE:HG23 | 1.47 | 0.97 |
| 35:DO:19:VAL:HG23 | 35:DO:27:HIS:HB3 | 0.97 | 0.97 |
| 33:BM:42:TRP:HA | 33:BM:48:MET:CE | 1.94 | 0.97 |
| 30:BG:73:ALA:HB2 | 30:BG:82:LEU:HD21 | 1.44 | 0.97 |
| 36:DP:66:ILE:O | 36:DP:67:ARG:HG3 | 1.65 | 0.97 |
| 29:DF:67:GLN:O | 29:DF:67:GLN:HG3 | 1.62 | 0.97 |
| 25:BA:654(M):C:H2' | 25:BA:654(N):G:C8 | 2.00 | 0.97 |
| 25:BA:67:U:H3 | 25:BA:74:A:H2 | 0.99 | 0.97 |
| 25:DA:2638:G:P | 28:DE:82:ARG:HH22 | 1.86 | 0.96 |
| 27:DD:35:LYS:HE3 | 27:DD:64:ILE:C | 1.85 | 0.96 |
| 36:BP:76:LYS:N | 36:BP:88:GLY:HA3 | 1.79 | 0.96 |
| 3:CF:119:ARG:HH22 | 3:CF:140:ARG:HG2 | 1.28 | 0.96 |
| 52:D6:41:PRO:CG | 52:D6:45:LYS:O | 2.14 | 0.96 |
| 1:CA:1330:U:H4' | 13:CP:23:TYR:CE2 | 2.00 | 0.96 |
| 1:AA:748:C:H4' | 1:AA:749:C:O5' | 1.62 | 0.96 |
| 30:DG:161:THR:HG22 | 30:DG:163:ALA:H | 1.30 | 0.96 |
| 27:DD:35:LYS:HD2 | 27:DD:104:TYR:HD1 | 1.27 | 0.96 |
| 26:DB:74:U:C2' | 26:DB:75:G:H5'' | 1.95 | 0.96 |
| 41:B2:47:VAL:HG22 | 41:B2:48:GLY:H | 1.29 | 0.96 |
| 34:DN:63:VAL:HG12 | 34:DN:106:LEU:HD11 | 1.47 | 0.96 |
| 52:B6:47:THR:CG2 | 52:B6:48:VAL:H | 1.78 | 0.96 |
| 4:AG:22:LYS:HB2 | 4:AG:26:CYS:HB2 | 1.48 | 0.96 |
| 52:D6:45:LYS:HE3 | 52:D6:45:LYS:HA | 1.48 | 0.96 |
| 36:BP:68:ILE:HD13 | 36:BP:103:MET:HG2 | 1.46 | 0.96 |
| 47:BZ:85:LEU:C | 47:BZ:87:PRO:CD | 2.33 | 0.96 |
| 25:DA:747:U:C5 | 51:D5:3:LYS:HB2 | 2.00 | 0.96 |
| 39:BR:52:ILE:HD13 | 39:BR:61:PHE:HB3 | 1.44 | 0.96 |
| 1:AA:1497:G:H2' | 1:AA:1498:U:H5' | 1.48 | 0.96 |
| 28:DE:48:GLN:O | 28:DE:49:LEU:HG | 1.65 | 0.95 |
| 44:DU:13:VAL:HG21 | 44:DU:72:VAL:HB | 1.48 | 0.95 |
| 35:DO:64:LYS:CB | 54:D8:25:MET:CG | 2.40 | 0.95 |
| 25:DA:2712(A):A:H5'' | 25:DA:2713:A:OP2 | 1.64 | 0.95 |
| 25:DA:2681:C:H5 | 25:DA:2725:A:N6 | 1.61 | 0.95 |
| 25:BA:2404:C:C1' | 35:BO:67:MET:HE1 | 1.95 | 0.95 |
| 54:B8:36:LYS:HB2 | 54:B8:40:GLU:HG2 | 1.48 | 0.95 |
| 23:CD:59:A:H1' | 23:CD:61:U:C5 | 2.02 | 0.95 |
| 25:DA:1012:U:O4 | 33:DM:25:ARG:HA | 1.67 | 0.95 |
| 35:BO:64:LYS:HD2 | 54:B8:25:MET:CE | 1.95 | 0.95 |
| 35:BO:64:LYS:HB3 | 54:B8:25:MET:HG3 | 1.43 | 0.95 |
| 31:DH:7:LEU:HD12 | 31:DH:8:PRO:HD3 | 1.45 | 0.95 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 30:BG:121:ASN:HD22 | 30:BG:123:ASN:H | 1.07 | 0.95 |
| 30:DG:104:GLU:HG2 | 50:D4:23:GLU:HG2 | 1.49 | 0.95 |
| 25:DA:1729:A:O2' | 25:DA:1731:G:N2 | 2.00 | 0.95 |
| 25:DA:2777:G:H5'' | 25:DA:2778:A:H5' | 1.46 | 0.95 |
| 26:DB:3:C:H42 | 26:DB:117:G:H1 | 1.09 | 0.95 |
| 27:DD:43:ARG:NH1 | 27:DD:44:ASN:ND2 | 2.15 | 0.95 |
| 52:D6:41:PRO:CD | 52:D6:45:LYS:O | 2.15 | 0.95 |
| 52:B6:41:PRO:HD2 | 52:B6:46:HIS:N | 1.81 | 0.95 |
| 1:CA:141:A:H1' | 1:CA:182:U:O2 | 1.66 | 0.95 |
| 25:DA:226:G:H21 | 25:DA:228:A:H62 | 1.15 | 0.95 |
| 1:AA:1160:G:H1 | 1:AA:1177:G:H22 | 1.05 | 0.95 |
| 41:D2:69:LYS:HG3 | 41:D2:86:GLY:HA3 | 1.44 | 0.95 |
| 25:BA:71:A:H2 | 43:BT:31:HIS:HE1 | 0.99 | 0.95 |
| 27:BD:35:LYS:HD2 | 27:BD:104:TYR:CE1 | 2.01 | 0.95 |
| 25:DA:1022:G:O2' | 25:DA:1023:U:OP2 | 1.85 | 0.94 |
| 27:DD:242:ARG:H | 27:DD:242:ARG:HD2 | 1.32 | 0.94 |
| 1:CA:804:U:H5'' | 1:CA:805:C:OP2 | 1.67 | 0.94 |
| 25:DA:1537:C:H2' | 25:DA:1538:G:C8 | 2.02 | 0.94 |
| 25:BA:1138:G:H21 | 33:BM:106:MET:HE3 | 1.32 | 0.94 |
| 25:DA:586:A:H5' | 29:DF:89:VAL:HG21 | 1.46 | 0.94 |
| 25:BA:1798:U:H5'' | 27:BD:259:THR:HG22 | 1.46 | 0.94 |
| 22:CB:49:C:H2' | 22:CB:50:A:O4' | 1.66 | 0.94 |
| 38:DQ:24:LEU:HD22 | 38:DQ:24:LEU:H | 1.31 | 0.94 |
| 28:BE:3:GLY:HA3 | 28:BE:81:ILE:HG13 | 1.47 | 0.94 |
| 31:BH:159:GLU:CG | 31:BH:170:ARG:NH1 | 2.30 | 0.94 |
| 25:DA:1062:G:H1 | 25:DA:1076:C:H42 | 1.05 | 0.94 |
| 25:DA:2392:A:H8 | 35:DO:60:MET:HB2 | 1.32 | 0.94 |
| 32:BK:92:VAL:HG13 | 32:BK:120:ILE:HG23 | 1.47 | 0.94 |
| 25:BA:2287:A:H62 | 25:BA:2344:U:H3 | 0.95 | 0.94 |
| 35:BO:64:LYS:HB3 | 54:B8:25:MET:CG | 1.97 | 0.94 |
| 1:CA:632:A:H1' | 1:CA:633:G:OP2 | 1.65 | 0.94 |
| 47:BZ:82:LEU:CD2 | 47:BZ:82:LEU:H | 1.79 | 0.94 |
| 35:DO:61:ARG:CB | 35:DO:61:ARG:NH2 | 2.30 | 0.94 |
| 27:BD:35:LYS:HG2 | 27:BD:64:ILE:H | 1.31 | 0.94 |
| 31:DH:153:LYS:N | 31:DH:154:PRO:CD | 2.30 | 0.94 |
| 1:CA:1176:A:N6 | 1:CA:1177:G:C6 | 2.35 | 0.94 |
| 31:BH:59:ARG:HG3 | 31:BH:59:ARG:HH11 | 1.29 | 0.94 |
| 28:BE:4:ILE:HD13 | 28:BE:28:ALA:CB | 1.97 | 0.94 |
| 25:BA:2210:G:H3' | 25:BA:2211:G:C8 | 2.02 | 0.94 |
| 25:DA:528:A:C2 | 25:DA:2043:C:H5' | 2.03 | 0.94 |
| 25:BA:1021:A:H3' | 25:BA:1022:G:H5'' | 1.48 | 0.94 |
| 25:BA:676:A:H8 | 25:BA:2069:G:H21 | 1.16 | 0.94 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 16:AS:16:HIS:O | 16:AS:39:TYR:O | 1.85 | 0.94 |
| 47:BZ:86:SER:N | 47:BZ:87:PRO:CD | 2.30 | 0.94 |
| 41:D2:82:ARG:HH11 | 41:D2:82:ARG:CG | 1.79 | 0.94 |
| 29:DF:89:VAL:HG12 | 29:DF:90:PHE:H | 0.79 | 0.94 |
| 23:AD:6:G:N2 | 23:AD:69:C:N3 | 2.15 | 0.94 |
| 1:CA:1139:G:H22 | 1:CA:1143:G:H1 | 1.03 | 0.94 |
| 25:DA:1689:A:H62 | 25:DA:1698:A:H2 | 1.09 | 0.94 |
| 35:DO:64:LYS:HD2 | 54:D8:25:MET:SD | 2.08 | 0.94 |
| 46:B3:40:GLN:HE22 | 46:B3:44:ARG:H | 1.00 | 0.94 |
| 25:DA:528:A:H2 | 25:DA:2043:C:H5' | 1.33 | 0.94 |
| 41:D2:83:ARG:N | 41:D2:83:ARG:CD | 2.30 | 0.94 |
| 25:DA:2420:C:H41 | 54:D8:31:HIS:HB3 | 1.31 | 0.94 |
| 1:AA:235:C:H5' | 17:AT:70:ARG:HG2 | 1.48 | 0.94 |
| 25:DA:545:G:H21 | 25:DA:548:A:H62 | 1.11 | 0.94 |
| 13:AP:15:VAL:O | 13:AP:19:LEU:HD23 | 1.66 | 0.94 |
| 38:DQ:88:ASP:O | 38:DQ:89:ARG:HB3 | 1.64 | 0.93 |
| 25:DA:1257:C:O2' | 29:DF:84:VAL:HG13 | 1.64 | 0.93 |
| 22:AB:37:G:H1 | 24:A1:19:U:H3 | 1.01 | 0.93 |
| 31:BH:83:TYR:HB3 | 31:BH:135:GLY:H | 1.31 | 0.93 |
| 25:DA:1434:A:H61 | 25:DA:1558:A:H62 | 1.14 | 0.93 |
| 27:BD:182:LEU:H | 27:BD:272:ALA:HB2 | 1.32 | 0.93 |
| 34:DN:47:ILE:HG13 | 34:DN:48:PRO:HD2 | 1.50 | 0.93 |
| 35:BO:61:ARG:O | 35:BO:62:LEU:HD23 | 1.68 | 0.93 |
| 1:AA:823:G:H21 | 8:AK:1:MET:HE1 | 1.34 | 0.93 |
| 3:AF:40:ARG:O | 3:AF:44:GLU:HG2 | 1.68 | 0.93 |
| 36:DP:79:LEU:O | 36:DP:79:LEU:HD12 | 1.69 | 0.93 |
| 11:CN:29:ILE:HG22 | 11:CN:44:SER:HB2 | 1.50 | 0.93 |
| 25:DA:2415:G:H4' | 35:DO:67:MET:N | 1.84 | 0.93 |
| 25:DA:2303:G:C2' | 25:DA:2304:G:H5' | 1.98 | 0.93 |
| 43:BT:49:VAL:HG11 | 43:BT:83:VAL:HG22 | 1.50 | 0.93 |
| 27:DD:166:GLN:HE21 | 27:DD:166:GLN:HA | 1.30 | 0.93 |
| 42:BS:95:ILE:O | 42:BS:95:ILE:HG13 | 1.68 | 0.93 |
| 28:BE:27:LEU:HD23 | 28:BE:27:LEU:O | 1.68 | 0.93 |
| 22:AB:7:G:H3' | 22:AB:8:U:C5' | 1.99 | 0.93 |
| 25:DA:2275:C:O2' | 36:DP:84:GLY:CA | 2.16 | 0.93 |
| 10:CM:79:ARG:O | 10:CM:83:GLU:HB2 | 1.67 | 0.93 |
| 25:BA:2439:A:H5' | 25:BA:2439:A:C8 | 2.04 | 0.93 |
| 20:AW:71:THR:HG22 | 20:AW:72:LEU:H | 1.28 | 0.93 |
| 33:BM:46:VAL:HG11 | 33:BM:48:MET:HG3 | 1.50 | 0.93 |
| 25:DA:90:U:HO2' | 25:DA:91:A:H8 | 1.16 | 0.93 |
| 30:BG:96:ARG:HH11 | 30:BG:96:ARG:HG2 | 1.30 | 0.93 |
| 25:BA:2373:G:H1 | 25:BA:2380:C:H42 | 1.16 | 0.93 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 54:D8:35:GLN:O | 54:D8:36:LYS:HG2 | 1.69 | 0.92 |
| 28:BE:78:LEU:HD12 | 28:BE:79:ARG:H | 1.32 | 0.92 |
| 27:DD:43:ARG:HH11 | 27:DD:44:ASN:HD21 | 1.13 | 0.92 |
| 41:D2:81:TYR:C | 41:D2:82:ARG:HG3 | 1.88 | 0.92 |
| 45:DV:146:ILE:HG13 | 45:DV:147:GLY:N | 1.84 | 0.92 |
| 38:BQ:88:ASP:O | 38:BQ:89:ARG:HB2 | 1.68 | 0.92 |
| 27:DD:49:ILE:HD11 | 27:DD:52:ARG:HA | 1.48 | 0.92 |
| 25:BA:71:A:H2 | 43:BT:31:HIS:CE1 | 1.87 | 0.92 |
| 36:DP:26:TYR:HD1 | 36:DP:139:GLU:HG3 | 1.30 | 0.92 |
| 32:DK:144:VAL:HG13 | 32:DK:145:VAL:HG23 | 1.50 | 0.92 |
| 54:D8:49:VAL:C | 54:D8:50:LEU:CD1 | 2.38 | 0.92 |
| 1:CA:1004:A:H8 | 1:CA:1036:G:H22 | 1.15 | 0.92 |
| 28:DE:47:VAL:HG12 | 28:DE:48:GLN:N | 1.85 | 0.92 |
| 1:CA:235:C:H5' | 17:CT:70:ARG:HG2 | 1.49 | 0.92 |
| 1:AA:201:C:H42 | 1:AA:216:G:H1 | 1.10 | 0.92 |
| 25:DA:1300:U:H4' | 25:DA:1301:A:C5' | 2.00 | 0.92 |
| 25:DA:2392:A:H2 | 25:DA:2424:C:H42 | 1.08 | 0.92 |
| 28:BE:23:VAL:HG11 | 28:BE:173:VAL:HG21 | 1.50 | 0.92 |
| 35:BO:15:ARG:NH1 | 35:BO:15:ARG:HG2 | 1.76 | 0.92 |
| 33:BM:46:VAL:CG1 | 33:BM:47:ALA:N | 2.33 | 0.92 |
| 31:DH:153:LYS:N | 31:DH:154:PRO:HD2 | 1.85 | 0.92 |
| 22:AB:87:A:H8 | 25:BA:2583:G:H21 | 0.99 | 0.92 |
| 35:DO:19:VAL:HG23 | 35:DO:27:HIS:CG | 2.04 | 0.92 |
| 28:DE:46:ALA:HB2 | 28:DE:82:ARG:CB | 1.99 | 0.92 |
| 25:BA:2467:C:H2' | 25:BA:2468:G:C5' | 1.98 | 0.92 |
| 38:DQ:24:LEU:O | 38:DQ:85:VAL:HG13 | 1.68 | 0.92 |
| 41:D2:71:LEU:N | 41:D2:86:GLY:HA2 | 1.85 | 0.92 |
| 1:CA:1160:G:O6 | 1:CA:1181:G:O6 | 1.87 | 0.92 |
| 25:DA:1678:G:H22 | 25:DA:1989:G:H22 | 1.16 | 0.92 |
| 28:BE:23:VAL:HG12 | 28:BE:185:LYS:HA | 1.50 | 0.91 |
| 35:DO:61:ARG:O | 35:DO:62:LEU:HD23 | 1.68 | 0.91 |
| 41:D2:82:ARG:NH1 | 41:D2:82:ARG:HG2 | 1.63 | 0.91 |
| 26:DB:39:A:N6 | 50:D4:1:MET:HB3 | 1.85 | 0.91 |
| 25:BA:1434:A:H61 | 25:BA:1558:A:N6 | 1.66 | 0.91 |
| 35:DO:15:ARG:NH1 | 35:DO:15:ARG:HG2 | 1.76 | 0.91 |
| 19:AV:41:VAL:HB | 19:AV:42:PRO:HA | 1.53 | 0.91 |
| 1:CA:1443:G:H3' | 1:CA:1446:A:H5'' | 1.50 | 0.91 |
| 25:DA:330:A:H2 | 25:DA:1210:A:HO2' | 1.09 | 0.91 |
| 4:AG:122:ARG:HG2 | 4:AG:122:ARG:HH11 | 1.35 | 0.91 |
| 27:DD:35:LYS:CD | 27:DD:104:TYR:CD1 | 2.54 | 0.91 |
| 1:CA:345:C:H1' | 1:CA:346:G:C2 | 2.05 | 0.91 |
| 30:BG:161:THR:HG22 | 30:BG:163:ALA:H | 1.35 | 0.91 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:1077:A:H3' | 25:BA:1078:U:C5' | 1.98 | 0.91 |
| 28:BE:81:ILE:HG21 | 28:BE:84:PHE:CB | 1.99 | 0.91 |
| 49:DX:7:LYS:HG3 | 49:DX:34:GLU:HG3 | 1.53 | 0.91 |
| 25:DA:259:G:H21 | 25:DA:621:A:H8 | 1.19 | 0.91 |
| 28:DE:45:THR:HG22 | 28:DE:45:THR:O | 1.70 | 0.91 |
| 1:AA:827:U:H5'' | 1:AA:828:A:OP2 | 1.70 | 0.91 |
| 5:CH:83:GLU:HB3 | 5:CH:88:LYS:HG3 | 1.52 | 0.91 |
| 35:BO:50:ARG:HD3 | 54:B8:7:HIS:HE2 | 1.35 | 0.91 |
| 44:BU:96:ILE:HG23 | 44:BU:101:LYS:HG2 | 1.52 | 0.91 |
| 25:DA:1005:C:C1' | 25:DA:1143:A:C2 | 2.54 | 0.91 |
| 33:BM:67:LEU:O | 33:BM:88:GLU:HG2 | 1.71 | 0.91 |
| 36:DP:26:TYR:HE1 | 36:DP:139:GLU:HB2 | 1.24 | 0.90 |
| 25:DA:2393:A:H5' | 35:DO:62:LEU:CB | 1.99 | 0.90 |
| 28:BE:79:ARG:HD2 | 28:BE:197:ILE:HG21 | 0.92 | 0.90 |
| 23:CD:15:G:H2' | 23:CD:60:A:H2 | 1.35 | 0.90 |
| 42:BS:94:ASP:O | 42:BS:95:ILE:HG22 | 1.71 | 0.90 |
| 25:BA:905:U:H2' | 25:BA:906:G:H5'' | 1.53 | 0.90 |
| 25:BA:483:A:H4' | 44:BU:49:VAL:HA | 1.51 | 0.90 |
| 32:BK:106:GLY:O | 32:BK:107:VAL:HG22 | 1.69 | 0.90 |
| 2:CE:42:ILE:HD11 | 2:CE:202:PRO:HB2 | 1.52 | 0.90 |
| 25:BA:2467:C:C2' | 25:BA:2468:G:C5' | 2.46 | 0.90 |
| 35:BO:61:ARG:CB | 35:BO:61:ARG:NH2 | 2.30 | 0.90 |
| 45:DV:175:VAL:HG22 | 45:DV:176:PRO:HD3 | 1.51 | 0.90 |
| 2:CE:111:ARG:HG2 | 2:CE:111:ARG:HH11 | 1.36 | 0.90 |
| 1:AA:992:U:H4' | 1:AA:993:G:O5' | 1.69 | 0.90 |
| 40:B1:92:ARG:O | 40:B1:94:ASN:N | 2.03 | 0.90 |
| 29:BF:9:ILE:HD11 | 29:BF:125:LEU:HG | 1.53 | 0.90 |
| 2:CE:137:ARG:HH12 | 2:CE:140:HIS:HB2 | 1.37 | 0.90 |
| 28:BE:35:GLN:HG3 | 28:BE:36:ARG:H | 1.33 | 0.90 |
| 1:CA:1321:C:H41 | 1:CA:1322:C:H41 | 1.09 | 0.90 |
| 9:CL:4:TYR:HB2 | 9:CL:19:LEU:HB2 | 1.50 | 0.90 |
| 30:DG:47:LYS:HG2 | 30:DG:48:GLU:N | 1.86 | 0.90 |
| 25:BA:1496:A:H8 | 25:BA:1577:C:HO2' | 0.92 | 0.90 |
| 2:CE:153:ARG:HG3 | 2:CE:154:LEU:H | 1.35 | 0.90 |
| 39:DR:54:ARG:CG | 39:DR:54:ARG:HH11 | 1.83 | 0.90 |
| 25:DA:885:C:C4 | 25:DA:890:A:N6 | 2.40 | 0.90 |
| 25:DA:1024:G:H3' | 25:DA:1025:G:H5'' | 1.51 | 0.90 |
| 4:CG:30:LYS:HB2 | 4:CG:35:ARG:HD2 | 1.53 | 0.90 |
| 36:DP:11:LYS:HD3 | 36:DP:87:LYS:HG2 | 1.51 | 0.90 |
| 30:DG:64:THR:HG23 | 30:DG:66:GLN:H | 1.35 | 0.90 |
| 37:D0:87:TYR:HE1 | 37:D0:117:VAL:HG12 | 1.37 | 0.90 |
| 25:DA:1652:A:H62 | 37:D0:11:ASN:HD21 | 1.11 | 0.90 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:1525:G:H2' | 25:BA:1526:G:H8 | 1.37 | 0.90 |
| 23:CC:17:C:H3' | 23:CC:18:C:C5' | 2.02 | 0.90 |
| 42:BS:13:SER:HB3 | 42:BS:16:LYS:HD3 | 1.53 | 0.90 |
| 25:BA:2402:C:O2' | 25:BA:2403:C:OP1 | 1.88 | 0.90 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:H62 | 1.18 | 0.90 |
| 52:D6:11:LEU:HD23 | 52:D6:26:ASN:HB3 | 1.54 | 0.90 |
| 1:CA:1004:A:H5'' | 1:CA:1025:U:O4 | 1.72 | 0.90 |
| 23:CC:21:U:O2 | 23:CC:21:U:H2' | 1.70 | 0.90 |
| 25:DA:1141:U:OP2 | 33:DM:63:THR:OG1 | 1.89 | 0.90 |
| 4:AG:108:LEU:HB3 | 4:AG:110:PHE:HE1 | 1.37 | 0.90 |
| 42:DS:9:TYR:H | 42:DS:102:HIS:HD2 | 1.20 | 0.90 |
| 25:DA:1496:A:H8 | 25:DA:1577:C:HO2' | 0.91 | 0.90 |
| 25:BA:2394:C:P | 35:BO:62:LEU:HB2 | 2.11 | 0.90 |
| 4:AG:19:LEU:H | 4:AG:19:LEU:HD22 | 1.37 | 0.90 |
| 2:AE:8:LYS:HE3 | 2:AE:11:LEU:HB2 | 1.52 | 0.90 |
| 28:BE:75:VAL:HG23 | 28:BE:76:ARG:H | 1.36 | 0.90 |
| 31:BH:4:ILE:HG21 | 31:BH:6:ARG:NH1 | 1.85 | 0.90 |
| 1:AA:686:U:H1' | 11:AN:42:TRP:HE1 | 1.34 | 0.90 |
| 1:CA:560:U:O2' | 1:CA:561:U:OP2 | 1.89 | 0.90 |
| 25:DA:2795:G:H3' | 25:DA:2797:U:H5'' | 1.54 | 0.90 |
| 1:CA:1129:C:H4' | 1:CA:1130:A:H5' | 1.54 | 0.89 |
| 9:CL:63:ILE:HD11 | 9:CL:81:ILE:HD11 | 1.50 | 0.89 |
| 26:DB:15:A:H5' | 26:DB:16:G:C8 | 2.07 | 0.89 |
| 20:AW:24:LEU:HD12 | 20:AW:24:LEU:O | 1.70 | 0.89 |
| 30:BG:83:ARG:CG | 30:BG:86:MET:CE | 2.48 | 0.89 |
| 28:BE:79:ARG:NE | 28:BE:197:ILE:CG2 | 2.35 | 0.89 |
| 25:DA:2394:C:P | 35:DO:62:LEU:HB2 | 2.12 | 0.89 |
| 45:DV:175:VAL:O | 45:DV:177:PRO:HD3 | 1.70 | 0.89 |
| 25:DA:71:A:H2 | 43:DT:31:HIS:CE1 | 1.89 | 0.89 |
| 23:CD:57:C:H42 | 25:DA:2112:G:H22 | 1.19 | 0.89 |
| 1:CA:1305:G:HO2' | 1:CA:1306:A:H8 | 0.90 | 0.89 |
| 38:DQ:24:LEU:O | 38:DQ:85:VAL:CG1 | 2.20 | 0.89 |
| 44:BU:97:ARG:HE | 44:BU:98:VAL:HG23 | 1.38 | 0.89 |
| 1:CA:64:G:H4' | 1:CA:65:U:O5' | 1.72 | 0.89 |
| 35:DO:65:ARG:HG3 | 35:DO:65:ARG:NH1 | 1.79 | 0.89 |
| 1:AA:1004:A:H8 | 1:AA:1036:G:H1 | 1.20 | 0.89 |
| 25:DA:1899:G:N2 | 25:DA:1902:C:H5 | 1.70 | 0.89 |
| 25:DA:1689:A:N6 | 25:DA:1698:A:H2 | 1.71 | 0.89 |
| 13:AP:108:ARG:HG3 | 13:AP:108:ARG:HH11 | 1.37 | 0.89 |
| 38:BQ:34:HIS:HB2 | 38:BQ:36:TYR:HE1 | 1.37 | 0.89 |
| 1:CA:1004:A:H1' | 1:CA:1036:G:H1 | 1.32 | 0.89 |
| 33:BM:46:VAL:HG12 | 33:BM:47:ALA:H | 1.35 | 0.89 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 30:BG:67:LYS:HE2 | 50:B4:6:HIS:HE1 | 1.34 | 0.89 |
| 35:DO:64:LYS:HB3 | 54:D8:25:MET:HG2 | 1.55 | 0.89 |
| 50:B4:16:CYS:SG | 50:B4:18:CYS:N | 2.45 | 0.89 |
| 23:CD:27:G:O6 | 23:CD:45:A:N6 | 2.06 | 0.89 |
| 13:CP:49:THR:HG22 | 13:CP:51:ALA:H | 1.36 | 0.89 |
| 45:BV:29:TYR:HE2 | 45:BV:87:ASP:HB2 | 1.38 | 0.89 |
| 39:DR:50:ILE:HD11 | 39:DR:102:ILE:HD11 | 1.53 | 0.89 |
| 44:BU:76:CYS:SG | 44:BU:77:PRO:HD3 | 2.12 | 0.89 |
| 1:AA:1004:A:H1' | 1:AA:1036:G:O6 | 1.71 | 0.89 |
| 27:BD:270:ILE:O | 27:BD:271:ILE:HG12 | 1.71 | 0.89 |
| 27:BD:35:LYS:HG2 | 27:BD:64:ILE:N | 1.88 | 0.89 |
| 52:D6:44:ARG:HG3 | 52:D6:44:ARG:HH11 | 1.35 | 0.89 |
| 36:DP:29:PHE:HB3 | 36:DP:65:PHE:CE1 | 2.08 | 0.88 |
| 28:BE:35:GLN:HB3 | 28:BE:48:GLN:CG | 2.02 | 0.88 |
| 1:AA:1145:C:H5'' | 1:AA:1146:A:OP1 | 1.72 | 0.88 |
| 28:DE:47:VAL:CG1 | 28:DE:48:GLN:N | 2.35 | 0.88 |
| 25:DA:1899:G:N2 | 25:DA:1902:C:C5 | 2.40 | 0.88 |
| 7:CJ:16:LEU:HD12 | 9:CL:42:ARG:HA | 1.54 | 0.88 |
| 2:AE:204:ASN:ND2 | 2:AE:206:ASP:H | 1.70 | 0.88 |
| 27:DD:35:LYS:CD | 27:DD:104:TYR:HD1 | 1.86 | 0.88 |
| 25:DA:1140:C:H1' | 25:DA:1143:A:H8 | 1.37 | 0.88 |
| 43:BT:84:ALA:HB1 | 43:BT:85:PRO:HD2 | 1.55 | 0.88 |
| 31:BH:4:ILE:HD13 | 31:BH:4:ILE:H | 1.37 | 0.88 |
| 28:DE:197:ILE:HD11 | 28:DE:199:ARG:HH21 | 1.38 | 0.88 |
| 25:BA:1250:G:N7 | 35:BO:18:ARG:NH2 | 2.21 | 0.88 |
| 25:BA:780:G:H21 | 25:BA:783:A:H62 | 0.97 | 0.88 |
| 28:DE:82:ARG:O | 28:DE:83:ASP:HB2 | 1.73 | 0.88 |
| 1:CA:963:G:H21 | 10:CM:55:LYS:CD | 1.85 | 0.88 |
| 25:DA:2255:G:N2 | 36:DP:85:LYS:HE2 | 1.87 | 0.88 |
| 33:BM:96:GLU:O | 33:BM:97:ARG:HB2 | 1.71 | 0.88 |
| 1:CA:1298:C:H41 | 7:CJ:114:ARG:HB3 | 1.34 | 0.88 |
| 54:B8:22:VAL:HB | 54:B8:53:PRO:HB3 | 1.55 | 0.88 |
| 23:AD:19:G:H1' | 23:AD:59:A:C2 | 2.08 | 0.88 |
| 25:DA:1464:C:O2' | 25:DA:1528:A:H8 | 1.55 | 0.88 |
| 1:AA:1321:C:H3' | 1:AA:1322:C:H5'' | 1.54 | 0.88 |
| 25:BA:1884:A:C2' | 25:BA:1885:A:H5'' | 2.01 | 0.88 |
| 25:BA:860:U:C5 | 25:BA:917:A:C2 | 2.60 | 0.88 |
| 1:CA:1330:U:H4' | 13:CP:23:TYR:HE2 | 1.38 | 0.88 |
| 47:BZ:82:LEU:CD2 | 47:BZ:82:LEU:N | 2.34 | 0.88 |
| 25:DA:2191:G:O2' | 25:DA:2192:G:OP1 | 1.92 | 0.88 |
| 25:DA:67:U:H3 | 25:DA:74:A:H2 | 1.21 | 0.88 |
| 26:DB:15:A:H5' | 26:DB:16:G:H8 | 1.38 | 0.88 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 42:BS:9:TYR:H | 42:BS:102:HIS:HD2 | 1.21 | 0.88 |
| 53:B7:8:ASN:HD21 | 53:B7:11:LYS:H | 0.95 | 0.88 |
| 36:DP:26:TYR:CD1 | 36:DP:139:GLU:HB2 | 2.09 | 0.88 |
| 25:BA:1056:G:H21 | 25:BA:1103:A:H62 | 1.16 | 0.88 |
| 41:D2:85:LYS:HG3 | 41:D2:86:GLY:H | 1.36 | 0.88 |
| 16:AS:22:THR:OG1 | 16:AS:32:TYR:HA | 1.74 | 0.88 |
| 25:DA:780:G:H21 | 25:DA:783:A:H62 | 1.16 | 0.88 |
| 5:CH:91:LEU:HD12 | 5:CH:120:THR:HG22 | 1.52 | 0.88 |
| 54:D8:34:TRP:CG | 54:D8:35:GLN:N | 2.40 | 0.88 |
| 27:BD:181:GLU:HA | 27:BD:272:ALA:HB1 | 1.54 | 0.88 |
| 38:DQ:88:ASP:OD2 | 38:DQ:90:GLY:N | 2.07 | 0.88 |
| 16:AS:19:ILE:O | 16:AS:19:ILE:HG22 | 1.73 | 0.88 |
| 23:CC:60:A:H2' | 23:CC:61:U:C5' | 2.04 | 0.88 |
| 1:CA:973:G:H1' | 10:CM:55:LYS:HE2 | 1.56 | 0.88 |
| 47:BZ:82:LEU:HD22 | 47:BZ:82:LEU:N | 1.87 | 0.88 |
| 1:CA:1139:G:N2 | 1:CA:1143:G:H1 | 1.72 | 0.88 |
| 41:B2:59:ALA:HB2 | 41:B2:96:ILE:HD13 | 1.53 | 0.88 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C6 | 2.09 | 0.88 |
| 20:AW:100:ILE:HG13 | 20:AW:102:GLY:H | 1.39 | 0.88 |
| 7:CJ:113:GLU:HB2 | 7:CJ:119:ARG:HG2 | 1.56 | 0.88 |
| 22:CB:39:U:H2' | 22:CB:40:G:H8 | 1.39 | 0.88 |
| 25:DA:882:G:H1 | 25:DA:894:C:H42 | 0.93 | 0.88 |
| 25:DA:2470:G:P | 36:DP:56:ARG:NH2 | 2.47 | 0.88 |
| 27:BD:186:HIS:HD2 | 27:BD:188:GLU:H | 1.20 | 0.88 |
| 31:DH:102:ALA:HB1 | 31:DH:115:VAL:O | 1.74 | 0.88 |
| 1:CA:1321:C:N4 | 1:CA:1322:C:H41 | 1.71 | 0.88 |
| 23:CD:15:G:N2 | 23:CD:49:C:O2 | 2.07 | 0.88 |
| 25:BA:443:A:N7 | 29:BF:45:ARG:HD2 | 1.89 | 0.88 |
| 5:CH:80:ILE:HD11 | 5:CH:138:ALA:HB1 | 1.54 | 0.88 |
| 38:BQ:23:ARG:CD | 38:BQ:85:VAL:O | 2.20 | 0.87 |
| 27:BD:35:LYS:CD | 27:BD:104:TYR:CD1 | 2.57 | 0.87 |
| 15:AR:39:LEU:HD13 | 15:AR:56:LEU:HB2 | 1.57 | 0.87 |
| 25:DA:1952:A:C5 | 34:DN:22:ILE:HD11 | 2.09 | 0.87 |
| 25:DA:1952:A:C6 | 34:DN:22:ILE:HD11 | 2.08 | 0.87 |
| 49:BX:7:LYS:HG3 | 49:BX:34:GLU:HG2 | 1.55 | 0.87 |
| 25:BA:2394:C:OP1 | 35:BO:62:LEU:HB2 | 1.74 | 0.87 |
| 28:BE:14:ILE:HG22 | 28:BE:15:PHE:H | 0.73 | 0.87 |
| 35:BO:65:ARG:HG3 | 35:BO:65:ARG:NH1 | 1.79 | 0.87 |
| 31:BH:4:ILE:HG13 | 31:BH:6:ARG:NE | 1.90 | 0.87 |
| 53:B7:8:ASN:HD22 | 53:B7:8:ASN:C | 1.78 | 0.87 |
| 25:DA:2571:C:H5' | 25:DA:2572:A:H5'' | 1.56 | 0.87 |
| 45:DV:108:PRO:CB | 45:DV:143:GLY:HA2 | 2.05 | 0.87 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:DD:35:LYS:HE2 | 27:DD:104:TYR:CB | 2.04 | 0.87 |
| 41:D2:70:ILE:HB | 41:D2:86:GLY:O | 1.74 | 0.87 |
| 1:AA:1128:C:HO2' | 1:AA:1130:A:H8 | 1.17 | 0.87 |
| 10:AM:61:GLU:OE1 | 14:AQ:58:LYS:HE2 | 1.74 | 0.87 |
| 41:D2:28:GLU:O | 41:D2:61:VAL:HG11 | 1.74 | 0.87 |
| 25:DA:676:A:H8 | 25:DA:2069:G:H21 | 1.18 | 0.87 |
| 25:BA:2309:A:O2' | 25:BA:2310:A:H5'' | 1.73 | 0.87 |
| 25:BA:1689:A:N6 | 25:BA:1698:A:H2 | 1.71 | 0.87 |
| 26:DB:3:C:N4 | 26:DB:117:G:H1 | 1.71 | 0.87 |
| 16:AS:21:VAL:CG2 | 16:AS:34:GLU:O | 2.22 | 0.87 |
| 27:DD:69:ARG:NH2 | 27:DD:128:GLY:O | 2.07 | 0.87 |
| 25:BA:2845:G:H5'' | 39:BR:54:ARG:O | 1.75 | 0.87 |
| 25:DA:1359:A:H62 | 25:DA:1372:U:H3 | 1.22 | 0.87 |
| 25:BA:1024:G:H3' | 25:BA:1025:G:H5'' | 1.56 | 0.87 |
| 27:DD:35:LYS:NZ | 27:DD:104:TYR:H | 1.72 | 0.87 |
| 2:CE:236:TYR:HA | 2:CE:239:VAL:HB | 1.57 | 0.87 |
| 46:D3:23:VAL:HG13 | 46:D3:38:VAL:HG22 | 1.55 | 0.87 |
| 30:BG:83:ARG:H | 30:BG:86:MET:HE2 | 1.40 | 0.87 |
| 28:BE:41:LYS:NZ | 28:BE:41:LYS:CB | 2.37 | 0.87 |
| 12:CO:46:LYS:HZ3 | 12:CO:47:LYS:HD3 | 1.40 | 0.87 |
| 25:BA:2444:G:OP2 | 29:BF:68:LYS:HE3 | 1.75 | 0.87 |
| 42:DS:65:LEU:HD13 | 42:DS:68:ARG:HD2 | 1.54 | 0.87 |
| 28:BE:51:PHE:O | 28:BE:74:PRO:HB2 | 1.75 | 0.87 |
| 52:D6:48:VAL:HG13 | 52:D6:49:HIS:H | 0.75 | 0.87 |
| 28:DE:38:THR:HG23 | 28:DE:40:GLU:H | 1.36 | 0.87 |
| 25:BA:620:G:H4' | 25:BA:621:A:C5' | 2.03 | 0.87 |
| 48:BW:18:PRO:HA | 48:BW:21:LEU:HB2 | 1.57 | 0.87 |
| 35:BO:75:ILE:H | 35:BO:75:ILE:HD13 | 1.38 | 0.87 |
| 25:BA:1803:A:O2' | 27:BD:259:THR:HG21 | 1.74 | 0.87 |
| 26:DB:40:U:O2 | 26:DB:45:A:N6 | 2.07 | 0.87 |
| 53:B7:8:ASN:ND2 | 53:B7:11:LYS:H | 1.72 | 0.87 |
| 16:CS:8:ARG:CG | 16:CS:8:ARG:HH11 | 1.88 | 0.87 |
| 4:CG:22:LYS:HB2 | 4:CG:26:CYS:HB2 | 1.57 | 0.87 |
| 28:DE:47:VAL:CG1 | 28:DE:48:GLN:H | 1.87 | 0.86 |
| 23:CC:18:C:O2 | 23:CC:18:C:H2' | 1.73 | 0.86 |
| 45:BV:19:ARG:NH1 | 45:BV:84:GLU:O | 2.08 | 0.86 |
| 5:CH:18:ARG:HD3 | 5:CH:25:ARG:HB3 | 1.57 | 0.86 |
| 3:CF:84:ILE:HD11 | 3:CF:88:ARG:HH21 | 1.40 | 0.86 |
| 25:DA:2032:G:H21 | 28:DE:146:THR:HG23 | 1.37 | 0.86 |
| 52:D6:44:ARG:O | 52:D6:45:LYS:HD2 | 1.74 | 0.86 |
| 28:BE:52:LEU:HB2 | 28:BE:75:VAL:HG21 | 1.55 | 0.86 |
| 28:DE:38:THR:OG1 | 28:DE:39:PRO:HD2 | 1.74 | 0.86 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 28:DE:47:VAL:O | 28:DE:80:GLU:CA | 2.22 | 0.86 |
| 25:DA:958:U:OP2 | 36:DP:14:ARG:NH1 | 2.08 | 0.86 |
| 43:BT:67:GLY:O | 43:BT:69:TYR:N | 2.07 | 0.86 |
| 1:AA:1028(B):C:H42 | 1:AA:1032(A):G:H1 | 1.24 | 0.86 |
| 25:DA:1057:A:H2 | 25:DA:1081:U:H3 | 1.23 | 0.86 |
| 45:DV:108:PRO:HB2 | 45:DV:143:GLY:HA2 | 1.54 | 0.86 |
| 25:DA:574:C:N3 | 28:DE:145:LYS:NZ | 2.22 | 0.86 |
| 36:DP:59:ARG:O | 36:DP:60:ARG:HB2 | 1.75 | 0.86 |
| 28:BE:38:THR:HG22 | 28:BE:45:THR:HG23 | 1.57 | 0.86 |
| 27:BD:30:GLU:HG3 | 27:BD:63:ARG:NH2 | 1.90 | 0.86 |
| 23:CC:60:A:C2' | 23:CC:61:U:H5' | 2.02 | 0.86 |
| 25:BA:1022:G:N2 | 25:BA:1023:U:O4 | 2.08 | 0.86 |
| 25:BA:855:G:O2' | 46:B3:27:GLU:OE2 | 1.93 | 0.86 |
| 7:CJ:16:LEU:HD11 | 9:CL:45:ALA:HB2 | 1.55 | 0.86 |
| 25:BA:2392:A:H8 | 35:BO:60:MET:HB2 | 1.38 | 0.86 |
| 54:D8:49:VAL:O | 54:D8:50:LEU:HG | 1.74 | 0.86 |
| 47:BZ:82:LEU:H | 47:BZ:82:LEU:HD23 | 1.40 | 0.86 |
| 1:AA:547:A:OP1 | 4:AG:73:ARG:NH2 | 2.08 | 0.86 |
| 25:DA:2467:C:H4' | 36:DP:123:HIS:CD2 | 2.10 | 0.86 |
| 35:DO:85:LEU:HA | 35:DO:88:LEU:HB3 | 1.56 | 0.86 |
| 2:CE:54:THR:HG23 | 2:CE:199:TYR:HB3 | 1.58 | 0.86 |
| 41:D2:85:LYS:CG | 41:D2:87:HIS:H | 1.88 | 0.86 |
| 44:DU:97:ARG:HH21 | 44:DU:98:VAL:HB | 1.39 | 0.86 |
| 25:DA:152:G:H1 | 25:DA:174:C:H42 | 1.15 | 0.86 |
| 25:DA:1459:G:H2' | 25:DA:1460:A:H5' | 1.56 | 0.86 |
| 31:BH:92:ILE:HD12 | 31:BH:92:ILE:H | 1.40 | 0.86 |
| 19:CV:67:VAL:HG12 | 19:CV:68:GLY:H | 1.38 | 0.86 |
| 25:BA:2790:A:H1' | 25:BA:2893:G:O2' | 1.76 | 0.86 |
| 43:DT:60:ARG:HG2 | 43:DT:60:ARG:HH11 | 1.40 | 0.86 |
| 52:D6:45:LYS:CE | 52:D6:45:LYS:HA | 2.00 | 0.86 |
| 16:AS:21:VAL:HG23 | 16:AS:34:GLU:O | 1.75 | 0.86 |
| 25:DA:141:A:H8 | 25:DA:1595:G:H21 | 1.23 | 0.86 |
| 31:BH:59:ARG:CG | 31:BH:59:ARG:HH11 | 1.88 | 0.85 |
| 25:DA:2720:U:N3 | 25:DA:2873:A:C2 | 2.44 | 0.85 |
| 33:BM:137:LYS:HG3 | 33:BM:138:LEU:H | 1.40 | 0.85 |
| 25:DA:1005:C:H1' | 25:DA:1143:A:C2 | 2.11 | 0.85 |
| 22:AB:22:G:N2 | 22:AB:59:U:O4' | 2.09 | 0.85 |
| 19:CV:22:LEU:O | 19:CV:27:GLU:HA | 1.77 | 0.85 |
| 24:C1:13:U:O2 | 24:C1:13:U:H2' | 1.74 | 0.85 |
| 36:DP:24:GLY:CA | 36:DP:25:ASP:HB2 | 1.97 | 0.85 |
| 45:BV:72:ARG:NH2 | 45:BV:97:GLU:O | 2.10 | 0.85 |
| 4:CG:3:ARG:HH21 | 4:CG:5:ILE:HG12 | 1.41 | 0.85 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:2137:C:H42 | 25:BA:2154:G:H1 | 1.22 | 0.85 |
| 25:DA:2875:C:H4' | 39:DR:5:ALA:HB2 | 1.58 | 0.85 |
| 36:DP:26:TYR:HD1 | 36:DP:139:GLU:HG2 | 1.28 | 0.85 |
| 25:DA:1899:G:H22 | 25:DA:1902:C:N4 | 1.74 | 0.85 |
| 1:AA:1453:G:O2' | 20:AW:39:LYS:HD2 | 1.76 | 0.85 |
| 25:BA:49:A:C8 | 25:BA:120:U:H5 | 1.94 | 0.85 |
| 1:CA:1223:C:H5'' | 1:CA:1224:G:C5' | 2.04 | 0.85 |
| 36:DP:79:LEU:HD12 | 36:DP:79:LEU:C | 1.97 | 0.85 |
| 25:DA:2303:G:H2' | 25:DA:2304:G:H5' | 1.58 | 0.85 |
| 25:BA:2438:U:O3' | 25:BA:2439:A:H3' | 1.76 | 0.85 |
| 16:AS:18:ARG:HD3 | 16:AS:35:LYS:HE3 | 1.55 | 0.85 |
| 28:DE:76:ARG:HG2 | 28:DE:195:LEU:HD22 | 1.58 | 0.85 |
| 28:BE:181:LEU:HD21 | 39:BR:7:ILE:HG23 | 1.58 | 0.85 |
| 1:AA:1305:G:N2 | 1:AA:1331:G:H2' | 1.91 | 0.85 |
| 25:DA:1420:U:O2' | 25:DA:1421:G:OP1 | 1.94 | 0.85 |
| 25:BA:2032:G:H21 | 28:BE:146:THR:HG23 | 1.40 | 0.85 |
| 2:CE:233:SER:HB3 | 2:CE:234:PRO:HD2 | 1.58 | 0.85 |
| 54:D8:33:ASN:O | 54:D8:34:TRP:CD1 | 2.30 | 0.85 |
| 25:DA:90:U:O2' | 25:DA:91:A:H8 | 1.57 | 0.85 |
| 54:B8:34:TRP:CE2 | 54:B8:35:GLN:OE1 | 2.30 | 0.85 |
| 27:DD:35:LYS:HA | 27:DD:64:ILE:HG23 | 1.58 | 0.85 |
| 27:BD:35:LYS:HZ1 | 27:BD:104:TYR:HB2 | 1.40 | 0.85 |
| 28:DE:25:VAL:HG12 | 28:DE:26:ILE:H | 1.41 | 0.85 |
| 28:DE:44:TYR:CD1 | 28:DE:44:TYR:N | 2.39 | 0.85 |
| 25:DA:1048:A:H2 | 25:DA:1112:G:H21 | 1.23 | 0.85 |
| 25:DA:2689:U:H4' | 25:DA:2690:C:OP2 | 1.76 | 0.85 |
| 35:DO:9:ASN:HB3 | 35:DO:10:PRO:HD2 | 1.57 | 0.85 |
| 28:BE:27:LEU:HD13 | 39:BR:1:MET:HE1 | 1.56 | 0.85 |
| 39:BR:56:GLY:O | 39:BR:59:THR:HG22 | 1.77 | 0.85 |
| 25:BA:2062:A:N3 | 25:BA:2062:A:H2' | 1.89 | 0.85 |
| 45:DV:128:VAL:HG22 | 45:DV:129:SER:H | 1.41 | 0.85 |
| 1:CA:812:C:H1' | 1:CA:813:U:OP2 | 1.76 | 0.85 |
| 36:DP:28:ALA:O | 36:DP:29:PHE:CD1 | 2.30 | 0.85 |
| 4:AG:9:CYS:O | 4:AG:13:ARG:CG | 2.24 | 0.85 |
| 1:AA:1004:A:N1 | 1:AA:1024:G:H2' | 1.91 | 0.85 |
| 25:DA:138:G:N2 | 43:DT:44:GLU:OE2 | 2.10 | 0.85 |
| 35:DO:49:ARG:O | 35:DO:49:ARG:HG2 | 1.75 | 0.85 |
| 27:BD:27:THR:O | 27:BD:28:GLU:HB2 | 1.75 | 0.85 |
| 1:AA:128:G:O2' | 17:AT:3:LYS:NZ | 2.09 | 0.85 |
| 17:AT:76:LEU:HD11 | 17:AT:79:SER:HB3 | 1.57 | 0.85 |
| 35:DO:36:LYS:CB | 35:DO:36:LYS:NZ | 2.39 | 0.85 |
| 34:BN:68:GLU:OE2 | 34:BN:78:ARG:NH1 | 2.09 | 0.85 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 41:D2:85:LYS:HG3 | 41:D2:86:GLY:N | 1.91 | 0.84 |
| 31:DH:125:VAL:CG2 | 31:DH:126:PRO:HD3 | 2.03 | 0.84 |
| 3:CF:111:LEU:HD21 | 3:CF:146:ALA:H | 1.42 | 0.84 |
| 36:DP:75:THR:HG21 | 36:DP:87:LYS:HE2 | 1.59 | 0.84 |
| 41:B2:47:VAL:CG2 | 41:B2:48:GLY:N | 2.39 | 0.84 |
| 25:BA:780:G:H21 | 25:BA:783:A:N6 | 1.73 | 0.84 |
| 25:DA:2298:A:H1' | 25:DA:2321:G:N2 | 1.92 | 0.84 |
| 2:AE:212:GLN:O | 2:AE:216:SER:HB2 | 1.75 | 0.84 |
| 25:BA:1332:G:N2 | 25:BA:1609:A:O2' | 2.10 | 0.84 |
| 27:DD:35:LYS:HZ1 | 27:DD:104:TYR:H | 1.22 | 0.84 |
| 28:DE:48:GLN:NE2 | 28:DE:78:LEU:HD13 | 1.91 | 0.84 |
| 23:CD:59:A:H1' | 23:CD:61:U:H5 | 1.37 | 0.84 |
| 15:AR:87:ILE:HG22 | 15:AR:88:ARG:H | 1.41 | 0.84 |
| 11:AN:121:PRO:HG2 | 11:AN:126:ARG:HG3 | 1.58 | 0.84 |
| 25:DA:2394:C:OP1 | 35:DO:63:PRO:HD2 | 1.76 | 0.84 |
| 25:BA:2310:A:O2' | 25:BA:2311:A:H5'' | 1.76 | 0.84 |
| 25:BA:1535:U:H3' | 25:BA:1536:A:H5'' | 1.60 | 0.84 |
| 25:BA:229:A:H1' | 25:BA:230:U:OP2 | 1.77 | 0.84 |
| 52:B6:40:CYS:HA | 52:B6:46:HIS:HA | 1.56 | 0.84 |
| 4:CG:15:GLU:HB3 | 4:CG:63:LYS:HE2 | 1.59 | 0.84 |
| 25:BA:780:G:N2 | 25:BA:783:A:H62 | 1.74 | 0.84 |
| 25:DA:2318:G:H1 | 38:DQ:2:ALA:HA | 1.40 | 0.84 |
| 50:D4:21:VAL:HG22 | 50:D4:22:ILE:HG12 | 1.57 | 0.84 |
| 25:BA:2712:U:O2 | 25:BA:2712:U:H5' | 1.78 | 0.84 |
| 48:DW:41:ILE:HD11 | 48:DW:44:LEU:HG | 1.59 | 0.84 |
| 25:DA:805:G:O4' | 35:DO:38:GLN:NE2 | 2.10 | 0.84 |
| 2:CE:164:VAL:HG23 | 2:CE:186:ALA:HB2 | 1.58 | 0.84 |
| 28:BE:16:ARG:HG3 | 28:BE:16:ARG:O | 1.75 | 0.84 |
| 1:CA:376:G:H5'' | 16:CS:5:ARG:HD3 | 1.57 | 0.84 |
| 1:CA:209:U:H4' | 1:CA:210:U:OP2 | 1.76 | 0.84 |
| 1:CA:686:U:H1' | 11:CN:42:TRP:HE1 | 1.42 | 0.84 |
| 1:AA:1160:G:O6 | 1:AA:1181:G:O6 | 1.95 | 0.84 |
| 28:BE:41:LYS:HB2 | 28:BE:41:LYS:HZ2 | 1.42 | 0.84 |
| 25:BA:2415:G:H4' | 35:BO:67:MET:N | 1.91 | 0.84 |
| 29:DF:25:PRO:HB3 | 29:DF:28:ILE:HG13 | 1.59 | 0.84 |
| 32:BK:104:GLN:O | 32:BK:105:HIS:CG | 2.31 | 0.84 |
| 54:B8:34:TRP:O | 54:B8:34:TRP:CG | 2.30 | 0.84 |
| 46:D3:36:ILE:HD13 | 46:D3:36:ILE:O | 1.77 | 0.84 |
| 4:CG:122:ARG:HH21 | 4:CG:134:ASP:HB3 | 1.42 | 0.84 |
| 25:DA:2287:A:H62 | 25:DA:2344:U:H3 | 1.22 | 0.84 |
| 29:DF:134:GLY:HA2 | 29:DF:166:ALA:HB2 | 1.60 | 0.84 |
| 2:CE:16:HIS:CD2 | 2:CE:209:ARG:HB3 | 2.12 | 0.84 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:560:U:O2' | 1:AA:561:U:OP2 | 1.95 | 0.84 |
| 5:AH:15:ARG:HD2 | 5:AH:26:PHE:CD2 | 2.13 | 0.84 |
| 31:BH:153:LYS:HG3 | 31:BH:162:ILE:H | 1.43 | 0.84 |
| 28:BE:78:LEU:CD1 | 28:BE:79:ARG:HG2 | 2.08 | 0.84 |
| 23:CC:20:G:C2 | 23:CC:58:A:N3 | 2.46 | 0.84 |
| 27:DD:242:ARG:N | 27:DD:242:ARG:HD2 | 1.90 | 0.84 |
| 45:BV:7:ALA:HB2 | 45:BV:59:LEU:HD13 | 1.59 | 0.84 |
| 33:DM:128:HIS:CE1 | 33:DM:134:ARG:HD2 | 2.13 | 0.84 |
| 35:DO:21:ARG:HA | 35:DO:21:ARG:HE | 1.40 | 0.84 |
| 1:CA:1002:G:H2' | 1:CA:1003:G:C8 | 2.13 | 0.84 |
| 28:DE:37:ARG:HD3 | 28:DE:44:TYR:CE2 | 2.13 | 0.84 |
| 10:AM:50:ILE:HD11 | 10:AM:57:LYS:HD2 | 1.60 | 0.84 |
| 46:D3:18:ALA:HB3 | 46:D3:20:ARG:HE | 1.42 | 0.83 |
| 25:BA:654(G):C:N3 | 25:BA:654(N):G:O6 | 2.11 | 0.83 |
| 30:BG:121:ASN:ND2 | 30:BG:123:ASN:H | 1.76 | 0.83 |
| 25:BA:34:C:O2' | 25:BA:35:G:OP2 | 1.96 | 0.83 |
| 1:AA:1285:A:H4' | 1:AA:1286:A:O5' | 1.78 | 0.83 |
| 28:BE:111:ARG:HD2 | 28:BE:160:TYR:CE1 | 2.13 | 0.83 |
| 28:BE:79:ARG:NE | 28:BE:197:ILE:HG21 | 1.93 | 0.83 |
| 28:BE:35:GLN:HB2 | 28:BE:48:GLN:HG3 | 1.57 | 0.83 |
| 28:BE:36:ARG:NH2 | 28:BE:88:GLY:HA2 | 1.93 | 0.83 |
| 10:AM:49:VAL:CG2 | 14:AQ:41:ARG:HB2 | 2.09 | 0.83 |
| 7:AJ:62:PHE:HD1 | 7:AJ:124:LEU:HD21 | 1.41 | 0.83 |
| 25:DA:660:G:N2 | 35:DO:12:ALA:HA | 1.93 | 0.83 |
| 25:DA:2404:C:H1' | 35:DO:67:MET:CE | 2.07 | 0.83 |
| 54:B8:36:LYS:CB | 54:B8:40:GLU:HG2 | 2.08 | 0.83 |
| 25:BA:652:C:H5' | 25:BA:653:A:OP2 | 1.77 | 0.83 |
| 25:BA:774:A:H2 | 25:BA:787:U:HO2' | 1.26 | 0.83 |
| 30:BG:83:ARG:CG | 30:BG:86:MET:HE2 | 2.08 | 0.83 |
| 53:D7:8:ASN:HD22 | 53:D7:11:LYS:H | 1.20 | 0.83 |
| 35:BO:64:LYS:CD | 54:B8:25:MET:SD | 2.66 | 0.83 |
| 39:BR:50:ILE:HD11 | 39:BR:102:ILE:CD1 | 2.08 | 0.83 |
| 13:AP:13:LYS:O | 13:AP:44:ARG:HD2 | 1.77 | 0.83 |
| 38:DQ:35:ILE:HD11 | 38:DQ:101:LEU:HD23 | 1.61 | 0.83 |
| 36:DP:29:PHE:HB3 | 36:DP:65:PHE:CD1 | 2.12 | 0.83 |
| 33:BM:130:HIS:HB3 | 33:BM:134:ARG:HH11 | 1.39 | 0.83 |
| 28:BE:3:GLY:CA | 28:BE:81:ILE:HG13 | 2.07 | 0.83 |
| 25:BA:2287:A:N6 | 25:BA:2344:U:H3 | 1.77 | 0.83 |
| 22:AB:87:A:H8 | 25:BA:2583:G:N2 | 1.77 | 0.83 |
| 51:B5:49:CYS:SG | 51:B5:60:VAL:HG23 | 2.18 | 0.83 |
| 1:CA:502:G:OP1 | 12:CO:118:SER:HB2 | 1.79 | 0.83 |
| 30:DG:117:PHE:HD1 | 30:DG:118:ARG:O | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:2522:U:H2' | 25:DA:2523:G:H5'' | 1.60 | 0.83 |
| 1:AA:1176:A:N6 | 1:AA:1177:G:C6 | 2.47 | 0.83 |
| 39:DR:26:ASP:CB | 39:DR:91:ARG:HA | 2.08 | 0.83 |
| 25:BA:1728:G:H3' | 25:BA:1729:A:H5' | 1.60 | 0.83 |
| 13:CP:33:ALA:O | 13:CP:37:THR:OG1 | 1.97 | 0.83 |
| 25:BA:1141:U:H6 | 33:BM:63:THR:HG1 | 1.24 | 0.83 |
| 22:AB:87:A:C8 | 25:BA:2583:G:N2 | 2.44 | 0.83 |
| 25:BA:2392:A:H8 | 35:BO:60:MET:CB | 1.91 | 0.83 |
| 27:DD:24:ILE:HD11 | 27:DD:91:ARG:HD3 | 1.59 | 0.83 |
| 28:BE:93:VAL:HG21 | 28:BE:180:ASN:HA | 1.61 | 0.83 |
| 8:AK:87:SER:HB2 | 8:AK:93:VAL:H | 1.41 | 0.83 |
| 38:BQ:89:ARG:HG2 | 38:BQ:92:TYR:O | 1.79 | 0.83 |
| 2:CE:47:THR:HA | 2:CE:202:PRO:HG2 | 1.61 | 0.83 |
| 17:CT:59:ILE:HG22 | 17:CT:71:PHE:HD1 | 1.42 | 0.83 |
| 25:DA:2404:C:H1' | 35:DO:67:MET:HE3 | 1.61 | 0.83 |
| 52:B6:15:GLU:HB2 | 52:B6:49:HIS:CE1 | 2.14 | 0.83 |
| 25:BA:889:C:H3' | 25:BA:890:A:H4' | 1.61 | 0.83 |
| 54:B8:34:TRP:CZ2 | 54:B8:35:GLN:OE1 | 2.32 | 0.83 |
| 9:CL:95:LYS:HD3 | 9:CL:96:LEU:N | 1.94 | 0.83 |
| 38:BQ:85:VAL:HG23 | 38:BQ:112:PHE:HE1 | 1.44 | 0.83 |
| 27:BD:35:LYS:NZ | 27:BD:64:ILE:O | 2.12 | 0.83 |
| 39:BR:74:ARG:HG2 | 39:BR:74:ARG:NH1 | 1.94 | 0.83 |
| 36:BP:65:PHE:O | 36:BP:66:ILE:HG12 | 1.79 | 0.83 |
| 25:BA:1105:U:H2' | 25:BA:1106:G:C8 | 2.12 | 0.83 |
| 25:DA:2275:C:HO2' | 36:DP:84:GLY:HA3 | 1.42 | 0.83 |
| 25:DA:1689:A:N6 | 25:DA:1698:A:C2 | 2.46 | 0.83 |
| 25:BA:2113:U:H5' | 25:BA:2114:A:H8 | 1.43 | 0.83 |
| 35:DO:38:GLN:HG2 | 35:DO:45:LEU:HD13 | 1.61 | 0.83 |
| 13:AP:14:ARG:HB2 | 13:AP:17:VAL:HG23 | 1.61 | 0.83 |
| 37:B0:100:LEU:HD11 | 37:B0:113:LEU:HD13 | 1.60 | 0.83 |
| 25:DA:2068:U:H3 | 25:DA:2430:A:H2 | 1.20 | 0.83 |
| 36:DP:26:TYR:CD1 | 36:DP:139:GLU:CB | 2.58 | 0.82 |
| 47:BZ:58:ILE:HD11 | 47:BZ:86:SER:HB2 | 1.59 | 0.82 |
| 33:BM:46:VAL:CG1 | 33:BM:48:MET:HG3 | 2.08 | 0.82 |
| 25:DA:2415:G:C4' | 35:DO:67:MET:H | 1.92 | 0.82 |
| 31:BH:171:LEU:CD1 | 31:BH:171:LEU:C | 2.46 | 0.82 |
| 25:BA:442:G:N3 | 29:BF:48:THR:HG21 | 1.93 | 0.82 |
| 25:DA:660:G:H21 | 35:DO:12:ALA:HA | 1.43 | 0.82 |
| 41:D2:44:LYS:O | 41:D2:46:VAL:N | 2.12 | 0.82 |
| 25:DA:1864:U:H2' | 25:DA:1869:G:H5'' | 1.60 | 0.82 |
| 40:B1:112:ARG:CG | 40:B1:112:ARG:HH11 | 1.91 | 0.82 |
| 11:AN:17:GLY:HA3 | 11:AN:77:MET:HE3 | 1.61 | 0.82 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 29:BF:29:ASN:H | 29:BF:112:MET:HE3 | 1.41 | 0.82 |
| 29:DF:31:HIS:CG | 35:DO:9:ASN:OD1 | 2.32 | 0.82 |
| 25:BA:2656:U:H3 | 25:BA:2665:A:H2 | 1.24 | 0.82 |
| 31:DH:152:ARG:NH2 | 31:DH:153:LYS:HG2 | 1.93 | 0.82 |
| 46:D3:38:VAL:HG12 | 46:D3:40:GLN:HG2 | 1.62 | 0.82 |
| 6:AI:4:TYR:HD1 | 6:AI:92:LYS:HA | 1.44 | 0.82 |
| 16:CS:11:SER:HB2 | 16:CS:14:ASN:HB3 | 1.61 | 0.82 |
| 35:DO:112:LEU:H | 35:DO:128:HIS:HD2 | 1.24 | 0.82 |
| 25:BA:1778:U:H2' | 25:BA:1784:A:N6 | 1.93 | 0.82 |
| 52:D6:41:PRO:HG2 | 52:D6:45:LYS:O | 1.77 | 0.82 |
| 23:CC:16:C:O2' | 23:CC:62:C:OP1 | 1.97 | 0.82 |
| 52:B6:44:ARG:O | 52:B6:45:LYS:HB2 | 1.78 | 0.82 |
| 25:DA:2392:A:C8 | 35:DO:60:MET:HB2 | 2.14 | 0.82 |
| 25:BA:1287:A:N7 | 37:B0:107:ASP:HB3 | 1.93 | 0.82 |
| 28:DE:116:VAL:O | 28:DE:117:MET:HB3 | 1.78 | 0.82 |
| 20:CW:82:SER:O | 20:CW:86:ARG:HB2 | 1.77 | 0.82 |
| 6:CI:61:LEU:HD23 | 6:CI:63:TYR:OH | 1.80 | 0.82 |
| 28:BE:47:VAL:CG2 | 28:BE:84:PHE:O | 2.28 | 0.82 |
| 25:DA:1062:G:H1 | 25:DA:1076:C:N4 | 1.77 | 0.82 |
| 25:DA:1057:A:N1 | 25:DA:1081:U:O4 | 2.11 | 0.82 |
| 26:DB:15:A:H1' | 26:DB:109:G:C8 | 2.14 | 0.82 |
| 2:CE:71:VAL:HG11 | 2:CE:97:TRP:CD1 | 2.13 | 0.82 |
| 25:BA:1864:U:H2' | 25:BA:1869:G:H5'' | 1.60 | 0.82 |
| 25:DA:654(C):G:H2' | 25:DA:654(D):G:O4' | 1.80 | 0.82 |
| 27:BD:35:LYS:CG | 27:BD:64:ILE:H | 1.92 | 0.82 |
| 23:CC:48:U:O2' | 23:CC:49:C:OP2 | 1.97 | 0.82 |
| 25:DA:2185:C:H2' | 25:DA:2186:G:H8 | 1.42 | 0.82 |
| 25:BA:919:G:N2 | 25:BA:2269:A:OP2 | 2.12 | 0.82 |
| 4:CG:13:ARG:C | 4:CG:15:GLU:H | 1.82 | 0.82 |
| 25:DA:1111:A:H4' | 31:DH:3:ARG:HD3 | 1.60 | 0.82 |
| 25:DA:2795:G:H3' | 25:DA:2797:U:C5' | 2.08 | 0.82 |
| 28:BE:111:ARG:HD2 | 28:BE:160:TYR:HE1 | 1.45 | 0.82 |
| 25:BA:674:G:H1' | 29:BF:74:ARG:HD3 | 1.59 | 0.82 |
| 2:AE:164:VAL:HG23 | 2:AE:186:ALA:HB2 | 1.60 | 0.82 |
| 49:DX:59:VAL:HG12 | 49:DX:60:GLU:H | 1.44 | 0.82 |
| 16:AS:22:THR:HG23 | 16:AS:23:ASP:N | 1.95 | 0.82 |
| 44:BU:78:ALA:HB3 | 44:BU:81:LYS:HZ1 | 1.44 | 0.82 |
| 51:B5:4:HIS:HB3 | 51:B5:5:PRO:CD | 2.09 | 0.82 |
| 25:DA:885:C:N4 | 25:DA:890:A:N6 | 2.26 | 0.82 |
| 23:CD:5:G:N2 | 23:CD:70:C:N3 | 2.27 | 0.82 |
| 25:DA:990:A:H5' | 25:DA:990:A:H8 | 1.44 | 0.82 |
| 54:D8:32:LEU:HB2 | 54:D8:36:LYS:HE3 | 1.62 | 0.82 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 28:DE:80:GLU:O | 28:DE:81:ILE:HG13 | 1.79 | 0.82 |
| 15:CR:17:ARG:HH11 | 15:CR:17:ARG:CG | 1.93 | 0.82 |
| 25:BA:885:C:O2 | 25:BA:890:A:N6 | 2.13 | 0.82 |
| 25:DA:71:A:H2 | 43:DT:31:HIS:HE1 | 1.24 | 0.82 |
| 52:B6:20:ASN:OD1 | 52:B6:22:ALA:N | 2.13 | 0.82 |
| 3:CF:117:ALA:HB2 | 3:CF:200:ALA:HB2 | 1.60 | 0.82 |
| 51:B5:40:LYS:HG2 | 51:B5:47:PRO:HD2 | 1.59 | 0.82 |
| 28:DE:46:ALA:HB2 | 28:DE:82:ARG:HA | 0.82 | 0.82 |
| 19:CV:20:LEU:O | 19:CV:23:ASN:HB3 | 1.79 | 0.82 |
| 25:BA:336:C:H5'' | 44:BU:6:HIS:CD2 | 2.15 | 0.82 |
| 31:DH:137:ASP:HB2 | 31:DH:140:LYS:HE2 | 1.62 | 0.82 |
| 1:AA:1080:A:H5'' | 1:AA:1081:G:OP2 | 1.80 | 0.82 |
| 25:DA:2137:C:H42 | 25:DA:2154:G:H1 | 1.27 | 0.82 |
| 51:D5:4:HIS:HB3 | 51:D5:5:PRO:HD3 | 0.83 | 0.81 |
| 25:DA:2327:A:H2' | 25:DA:2328:A:C8 | 2.15 | 0.81 |
| 1:CA:957:U:O2' | 1:CA:959:A:N7 | 2.13 | 0.81 |
| 29:DF:46:ARG:HG2 | 29:DF:46:ARG:HH11 | 1.45 | 0.81 |
| 25:BA:2610:C:H4' | 25:BA:2611:U:OP2 | 1.80 | 0.81 |
| 28:DE:46:ALA:CA | 28:DE:82:ARG:HA | 2.10 | 0.81 |
| 27:BD:181:GLU:HG3 | 27:BD:272:ALA:HB3 | 1.61 | 0.81 |
| 1:AA:1028(B):C:N4 | 1:AA:1032(A):G:H1 | 1.78 | 0.81 |
| 31:BH:151:ILE:O | 31:BH:153:LYS:CD | 2.28 | 0.81 |
| 33:BM:132:ALA:HB1 | 33:BM:133:GLN:HE21 | 1.44 | 0.81 |
| 5:AH:74:GLY:O | 5:AH:115:VAL:HA | 1.79 | 0.81 |
| 41:D2:85:LYS:CG | 41:D2:86:GLY:H | 1.92 | 0.81 |
| 1:CA:1004:A:H2 | 1:CA:1024:G:C8 | 1.98 | 0.81 |
| 25:DA:2276:G:OP1 | 36:DP:84:GLY:HA2 | 1.80 | 0.81 |
| 22:AB:87:A:O3' | 25:BA:2506:U:H1' | 1.80 | 0.81 |
| 35:BO:50:ARG:HD3 | 54:B8:7:HIS:NE2 | 1.95 | 0.81 |
| 2:AE:12:GLU:HA | 2:AE:16:HIS:CD2 | 2.16 | 0.81 |
| 50:D4:21:VAL:HG22 | 50:D4:22:ILE:H | 1.44 | 0.81 |
| 25:DA:1405:U:H2' | 25:DA:1406:U:C6 | 2.15 | 0.81 |
| 49:DX:29:ARG:H | 49:DX:33:GLN:HE22 | 1.25 | 0.81 |
| 28:BE:26:ILE:CD1 | 28:BE:198:VAL:HG21 | 2.09 | 0.81 |
| 45:BV:164:ALA:O | 45:BV:165:VAL:HG22 | 1.80 | 0.81 |
| 25:DA:9:U:C4 | 25:DA:2629:A:N1 | 2.49 | 0.81 |
| 28:BE:14:ILE:HB | 28:BE:21:VAL:CG2 | 2.10 | 0.81 |
| 4:AG:13:ARG:O | 4:AG:16:GLY:N | 2.13 | 0.81 |
| 39:BR:26:ASP:HB2 | 39:BR:91:ARG:HA | 1.62 | 0.81 |
| 34:DN:49:ARG:HD3 | 34:DN:49:ARG:H | 1.42 | 0.81 |
| 29:DF:9:ILE:HG12 | 29:DF:14:PRO:HA | 1.61 | 0.81 |
| 25:BA:297:C:H5'' | 44:BU:85:VAL:HG21 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 36:DP:24:GLY:CA | 36:DP:25:ASP:HB3 | 2.05 | 0.81 |
| 10:CM:49:VAL:HG23 | 10:CM:61:GLU:O | 1.80 | 0.81 |
| 25:DA:1434:A:H61 | 25:DA:1558:A:N6 | 1.77 | 0.81 |
| 7:CJ:20:ASP:HB3 | 7:CJ:23:VAL:HG23 | 1.62 | 0.81 |
| 11:AN:57:THR:HG22 | 11:AN:59:TYR:H | 1.44 | 0.81 |
| 26:BB:52:A:H62 | 38:BQ:33:LYS:HG3 | 1.44 | 0.81 |
| 20:AW:10:LEU:HD23 | 20:AW:12:ALA:H | 1.46 | 0.81 |
| 4:CG:13:ARG:O | 4:CG:15:GLU:HG2 | 1.79 | 0.81 |
| 48:BW:50:ILE:HD12 | 48:BW:51:ARG:N | 1.95 | 0.81 |
| 23:CD:15:G:H2' | 23:CD:60:A:C2 | 2.16 | 0.81 |
| 25:BA:1803:A:H4' | 27:BD:259:THR:CG2 | 2.10 | 0.81 |
| 1:CA:1191:A:P | 3:CF:3:ASN:HD21 | 2.03 | 0.81 |
| 25:BA:2310:A:N3 | 30:BG:77:ILE:CG1 | 2.43 | 0.81 |
| 28:BE:59:VAL:HG11 | 28:BE:63:LEU:HD13 | 1.63 | 0.81 |
| 13:CP:57:ARG:NH1 | 50:D4:34:GLU:O | 2.14 | 0.81 |
| 3:AF:130:VAL:O | 3:AF:134:ILE:HG12 | 1.79 | 0.81 |
| 32:BK:9:LEU:HB2 | 32:BK:11:ASN:O | 1.81 | 0.81 |
| 41:B2:44:LYS:CG | 41:B2:45:THR:H | 1.91 | 0.81 |
| 45:BV:113:ALA:N | 45:BV:114:GLY:HA2 | 1.95 | 0.81 |
| 25:DA:882:G:N2 | 25:DA:894:C:N3 | 2.26 | 0.81 |
| 23:CD:14:A:H8 | 23:CD:14:A:OP1 | 1.64 | 0.81 |
| 1:CA:537:G:H5'' | 12:CO:113:ARG:NH1 | 1.95 | 0.81 |
| 2:AE:18:GLY:H | 2:AE:42:ILE:HG22 | 1.45 | 0.81 |
| 27:BD:6:PHE:HE1 | 27:BD:18:VAL:HG23 | 1.44 | 0.81 |
| 46:B3:53:MET:HB2 | 46:B3:59:LEU:HD23 | 1.61 | 0.81 |
| 39:BR:16:ARG:HD3 | 39:BR:19:LEU:HD11 | 1.62 | 0.81 |
| 5:AH:67:VAL:HG21 | 5:AH:140:ARG:HA | 1.62 | 0.81 |
| 1:CA:452:A:O2' | 1:CA:453:A:O4' | 1.99 | 0.81 |
| 25:BA:1937:A:O2' | 25:BA:1938:A:OP1 | 1.99 | 0.81 |
| 34:BN:85:VAL:HG11 | 34:BN:114:ILE:HD13 | 1.63 | 0.81 |
| 25:DA:1252:G:N3 | 40:D1:33:ARG:HD2 | 1.96 | 0.81 |
| 38:BQ:106:ARG:NH2 | 38:BQ:107:GLU:HB2 | 1.96 | 0.81 |
| 37:D0:118:GLU:HA | 37:D0:118:GLU:OE1 | 1.81 | 0.81 |
| 29:BF:184:TYR:O | 29:BF:188:ARG:HG3 | 1.79 | 0.81 |
| 25:BA:2723:C:OP1 | 37:B0:3:HIS:HD2 | 1.63 | 0.81 |
| 1:AA:538:G:H5'' | 12:AO:114:LYS:HB2 | 1.63 | 0.81 |
| 54:D8:29:LYS:HA | 54:D8:32:LEU:HD23 | 1.62 | 0.80 |
| 25:BA:2310:A:H2' | 25:BA:2311:A:C5' | 2.11 | 0.80 |
| 27:DD:43:ARG:HH11 | 27:DD:44:ASN:HD22 | 1.24 | 0.80 |
| 1:AA:1306:A:N6 | 1:AA:1331:G:H1' | 1.96 | 0.80 |
| 4:AG:108:LEU:HB3 | 4:AG:110:PHE:CE1 | 2.15 | 0.80 |
| 33:BM:22:THR:HG22 | 33:BM:23:LEU:N | 1.96 | 0.80 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:762:U:H4' | 25:BA:763:G:O5' | 1.80 | 0.80 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:H5' | 1.62 | 0.80 |
| 28:DE:36:ARG:HH21 | 28:DE:88:GLY:HA3 | 1.42 | 0.80 |
| 5:AH:126:ARG:CG | 5:AH:126:ARG:HH11 | 1.94 | 0.80 |
| 36:DP:30:GLY:CA | 36:DP:107:ALA:HB2 | 2.11 | 0.80 |
| 25:BA:883:G:H1 | 25:BA:893:C:H42 | 0.85 | 0.80 |
| 25:DA:2392:A:H8 | 35:DO:60:MET:CB | 1.94 | 0.80 |
| 36:BP:35:VAL:HG13 | 36:BP:130:LYS:HB3 | 1.62 | 0.80 |
| 28:DE:8:LYS:O | 28:DE:9:VAL:HG22 | 1.80 | 0.80 |
| 26:BB:15:A:H5' | 26:BB:16:G:H8 | 1.40 | 0.80 |
| 2:AE:213:LEU:O | 2:AE:217:ARG:NH1 | 2.15 | 0.80 |
| 25:BA:2392:A:C8 | 35:BO:60:MET:HB2 | 2.16 | 0.80 |
| 25:BA:2473:U:H2' | 25:BA:2474:C:H5'' | 1.61 | 0.80 |
| 6:AI:101:ALA:HB2 | 18:AU:28:GLU:HG2 | 1.63 | 0.80 |
| 25:BA:1597:A:H5'' | 25:BA:1598:C:OP1 | 1.82 | 0.80 |
| 27:DD:186:HIS:HD2 | 27:DD:188:GLU:H | 1.28 | 0.80 |
| 29:BF:32:LEU:HD13 | 29:BF:105:VAL:HG13 | 1.63 | 0.80 |
| 31:BH:159:GLU:HG3 | 31:BH:170:ARG:NH1 | 1.95 | 0.80 |
| 1:CA:1256:A:OP2 | 3:CF:26:LYS:NZ | 2.15 | 0.80 |
| 12:CO:62:SER:HB2 | 12:CO:64:TYR:HD1 | 1.45 | 0.80 |
| 25:DA:2371:G:H4' | 52:D6:45:LYS:HG3 | 1.62 | 0.80 |
| 28:DE:44:TYR:O | 28:DE:45:THR:HB | 1.81 | 0.80 |
| 25:BA:2371:G:C4' | 52:B6:45:LYS:HG3 | 2.11 | 0.80 |
| 25:BA:1019:U:HO2' | 25:BA:1021:A:H2 | 1.28 | 0.80 |
| 43:BT:49:VAL:HG12 | 43:BT:50:LYS:N | 1.97 | 0.80 |
| 36:DP:59:ARG:HG2 | 36:DP:59:ARG:HH21 | 1.46 | 0.80 |
| 49:BX:4:LEU:HG | 49:BX:39:ASP:HB2 | 1.64 | 0.80 |
| 38:DQ:87:PHE:CE1 | 38:DQ:102:ALA:CB | 2.53 | 0.80 |
| 33:BM:56:ASN:N | 33:BM:125:GLY:O | 2.14 | 0.80 |
| 8:AK:87:SER:HB2 | 8:AK:93:VAL:N | 1.96 | 0.80 |
| 27:DD:206:LEU:HD22 | 27:DD:211:ARG:HG2 | 1.64 | 0.80 |
| 25:DA:2557:G:H2' | 25:DA:2558:C:H6 | 1.45 | 0.80 |
| 1:CA:1095:U:H5'' | 1:CA:1109:C:O2 | 1.79 | 0.80 |
| 44:DU:40:GLU:OE2 | 44:DU:40:GLU:HA | 1.82 | 0.80 |
| 1:CA:975:A:C4' | 1:CA:976:G:H5'' | 2.09 | 0.80 |
| 25:BA:879:G:H1 | 25:BA:898:C:H42 | 1.26 | 0.80 |
| 25:DA:1899:G:H22 | 25:DA:1902:C:H41 | 1.27 | 0.80 |
| 25:DA:2872:G:C5 | 25:DA:2873:A:N1 | 2.49 | 0.80 |
| 21:CX:8:THR:HG22 | 21:CX:11:GLY:H | 1.43 | 0.80 |
| 5:CH:148:VAL:HG21 | 8:CK:107:LEU:HD23 | 1.64 | 0.80 |
| 25:BA:1470:G:H5'' | 25:BA:1471:A:OP1 | 1.82 | 0.80 |
| 19:AV:65:ASN:H | 19:AV:65:ASN:HD22 | 1.28 | 0.80 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 44:DU:17:SER:HB2 | 44:DU:71:LYS:HD2 | 1.61 | 0.80 |
| 54:B8:34:TRP:CH2 | 54:B8:35:GLN:OE1 | 2.35 | 0.80 |
| 54:B8:34:TRP:O | 54:B8:35:GLN:CG | 2.30 | 0.80 |
| 2:AE:18:GLY:N | 2:AE:42:ILE:HG22 | 1.96 | 0.80 |
| 25:DA:468:G:N7 | 53:D7:39:ARG:NH2 | 2.29 | 0.80 |
| 4:AG:5:ILE:HG22 | 4:AG:6:GLY:H | 1.45 | 0.80 |
| 43:DT:80:ILE:HG13 | 43:DT:80:ILE:O | 1.79 | 0.80 |
| 25:BA:1179:C:H2' | 25:BA:1180:C:H5'' | 1.61 | 0.80 |
| 29:DF:83:PHE:O | 29:DF:84:VAL:CG1 | 2.30 | 0.80 |
| 36:DP:63:LYS:O | 36:DP:63:LYS:CD | 2.30 | 0.80 |
| 2:AE:7:VAL:HB | 2:AE:217:ARG:HH21 | 1.46 | 0.80 |
| 41:B2:38:LEU:HD12 | 41:B2:57:VAL:HG12 | 1.62 | 0.80 |
| 54:D8:49:VAL:O | 54:D8:50:LEU:CG | 2.30 | 0.80 |
| 28:BE:52:LEU:N | 28:BE:52:LEU:HD23 | 1.93 | 0.80 |
| 31:BH:171:LEU:O | 31:BH:171:LEU:CD1 | 2.30 | 0.80 |
| 20:AW:26:ASN:ND2 | 20:AW:26:ASN:N | 2.30 | 0.80 |
| 23:AD:19:G:H1' | 23:AD:59:A:H2 | 1.46 | 0.80 |
| 25:DA:486:C:H4' | 42:DS:60:ASN:HD21 | 1.47 | 0.80 |
| 15:CR:26:GLU:OE2 | 15:CR:77:ARG:NH1 | 2.15 | 0.80 |
| 2:CE:231:GLU:HB3 | 2:CE:232:PRO:CD | 2.11 | 0.80 |
| 3:CF:134:ILE:HG22 | 3:CF:168:ALA:HB3 | 1.63 | 0.80 |
| 45:DV:76:LEU:HD23 | 45:DV:76:LEU:H | 1.45 | 0.79 |
| 27:DD:30:GLU:HG3 | 27:DD:63:ARG:NH2 | 1.97 | 0.79 |
| 28:BE:52:LEU:CD2 | 28:BE:52:LEU:H | 1.93 | 0.79 |
| 28:DE:134:ILE:CD1 | 28:DE:134:ILE:O | 2.30 | 0.79 |
| 1:CA:1160:G:H1 | 1:CA:1177:G:H22 | 0.82 | 0.79 |
| 33:DM:97:ARG:HH11 | 33:DM:97:ARG:CG | 1.93 | 0.79 |
| 25:BA:74:A:H4' | 25:BA:75:G:O5' | 1.82 | 0.79 |
| 42:BS:95:ILE:O | 42:BS:95:ILE:CG1 | 2.30 | 0.79 |
| 42:BS:9:TYR:H | 42:BS:102:HIS:CD2 | 1.99 | 0.79 |
| 25:DA:2154:G:H2' | 25:DA:2155:G:H8 | 1.47 | 0.79 |
| 34:BN:71:ARG:HH11 | 34:BN:71:ARG:HG3 | 1.48 | 0.79 |
| 28:DE:55:ASN:O | 28:DE:57:LYS:N | 2.15 | 0.79 |
| 1:AA:977:A:H8 | 1:AA:1223:C:C4 | 1.98 | 0.79 |
| 1:CA:1183:A:O2' | 1:CA:1184:G:OP1 | 1.98 | 0.79 |
| 25:DA:864:G:N7 | 36:DP:22:LYS:NZ | 2.26 | 0.79 |
| 25:DA:2307:G:O2' | 25:DA:2308:G:N7 | 2.15 | 0.79 |
| 54:B8:52:LYS:N | 54:B8:53:PRO:HD2 | 1.97 | 0.79 |
| 35:DO:36:LYS:HB3 | 35:DO:36:LYS:HZ3 | 1.45 | 0.79 |
| 25:BA:1533:C:H2' | 25:BA:1534:G:C8 | 2.18 | 0.79 |
| 25:DA:2557:G:H2' | 25:DA:2558:C:C6 | 2.16 | 0.79 |
| 12:CO:41:ARG:HB3 | 12:CO:41:ARG:HH11 | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 6:CI:87:ARG:HH11 | 6:CI:87:ARG:CG | 1.96 | 0.79 |
| 25:BA:2261:C:C2' | 25:BA:2262:U:H5' | 2.12 | 0.79 |
| 20:AW:89:ARG:HH21 | 20:AW:104:LEU:HD11 | 1.47 | 0.79 |
| 1:AA:1386:G:O2' | 1:AA:1387:G:H5' | 1.82 | 0.79 |
| 47:BZ:78:LYS:HD2 | 47:BZ:78:LYS:O | 1.82 | 0.79 |
| 36:DP:90:VAL:CG1 | 36:DP:90:VAL:O | 2.30 | 0.79 |
| 9:AL:53:VAL:HG23 | 9:AL:95:LYS:HD2 | 1.64 | 0.79 |
| 35:DO:61:ARG:HB2 | 35:DO:61:ARG:HH21 | 0.77 | 0.79 |
| 40:D1:100:VAL:O | 40:D1:101:ARG:HG2 | 1.82 | 0.79 |
| 16:AS:19:ILE:CG2 | 16:AS:19:ILE:O | 2.30 | 0.79 |
| 1:CA:976:G:P | 14:CQ:32:SER:H | 2.04 | 0.79 |
| 27:DD:27:THR:HG21 | 27:DD:83:GLU:CG | 2.10 | 0.79 |
| 25:DA:1678:G:N2 | 25:DA:1989:G:H22 | 1.79 | 0.79 |
| 40:B1:92:ARG:NH1 | 41:B2:11:GLN:O | 2.15 | 0.79 |
| 13:CP:3:ARG:HG3 | 13:CP:9:ILE:HG12 | 1.62 | 0.79 |
| 19:CV:31:ILE:HG21 | 19:CV:49:ILE:HG23 | 1.64 | 0.79 |
| 41:B2:1:MET:HG3 | 41:B2:43:GLU:HG2 | 1.63 | 0.79 |
| 25:BA:2257:U:O2' | 25:BA:2258:C:H5' | 1.83 | 0.79 |
| 1:AA:1182:G:H4' | 1:AA:1183:A:C5' | 2.12 | 0.79 |
| 1:AA:542:G:OP1 | 4:AG:10:ARG:NH2 | 2.16 | 0.79 |
| 11:AN:40:ILE:HG22 | 11:AN:75:TYR:CD2 | 2.16 | 0.79 |
| 2:AE:204:ASN:HD22 | 2:AE:206:ASP:H | 1.31 | 0.79 |
| 14:AQ:43:CYS:HA | 14:AQ:46:GLU:HG3 | 1.65 | 0.79 |
| 4:AG:114:ARG:HH11 | 4:AG:114:ARG:CG | 1.95 | 0.79 |
| 27:DD:43:ARG:NH1 | 27:DD:44:ASN:HD21 | 1.77 | 0.79 |
| 27:BD:30:GLU:HG3 | 27:BD:63:ARG:CZ | 2.12 | 0.79 |
| 33:BM:115:ARG:O | 33:BM:118:LYS:N | 2.15 | 0.79 |
| 36:DP:78:PRO:O | 36:DP:79:LEU:HD12 | 1.82 | 0.79 |
| 25:DA:90:U:C2' | 25:DA:91:A:H5'' | 2.12 | 0.79 |
| 50:D4:56:VAL:HA | 50:D4:60:GLN:HE21 | 1.47 | 0.79 |
| 41:B2:15:GLU:HG3 | 41:B2:16:PRO:HD2 | 1.62 | 0.79 |
| 52:D6:52:VAL:HG22 | 52:D6:53:LYS:H | 1.46 | 0.79 |
| 22:AB:74:C:H5' | 22:AB:75:G:OP2 | 1.83 | 0.79 |
| 25:BA:594:U:H5' | 54:B8:61:LEU:HD13 | 1.65 | 0.79 |
| 25:BA:524:U:H4' | 25:BA:554:U:H4' | 1.64 | 0.79 |
| 54:D8:49:VAL:O | 54:D8:50:LEU:CD1 | 2.30 | 0.79 |
| 30:BG:77:ILE:CG2 | 30:BG:77:ILE:O | 2.31 | 0.79 |
| 1:AA:1004:A:H1' | 1:AA:1036:G:H1 | 1.44 | 0.79 |
| 15:AR:87:ILE:HG22 | 15:AR:88:ARG:N | 1.97 | 0.79 |
| 25:BA:2327:A:H2' | 25:BA:2328:A:C8 | 2.16 | 0.79 |
| 7:CJ:26:PHE:O | 7:CJ:30:ILE:HG13 | 1.82 | 0.79 |
| 39:BR:136:GLN:HG3 | 39:BR:137:LYS:H | 1.45 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 3:AF:126:ARG:HH11 | 3:AF:126:ARG:CG | 1.96 | 0.79 |
| 25:DA:2331:G:O3' | 46:D3:43:THR:HG22 | 1.82 | 0.79 |
| 35:DO:19:VAL:HG22 | 35:DO:20:GLY:H | 1.47 | 0.79 |
| 3:CF:150:LYS:HG3 | 3:CF:169:ALA:HB2 | 1.62 | 0.79 |
| 28:DE:48:GLN:O | 28:DE:49:LEU:CG | 2.30 | 0.79 |
| 35:BO:9:ASN:HB3 | 35:BO:10:PRO:CD | 2.11 | 0.79 |
| 48:DW:70:GLN:HG2 | 48:DW:71:ASN:H | 1.47 | 0.79 |
| 25:BA:2210:G:H3' | 25:BA:2211:G:N7 | 1.98 | 0.79 |
| 12:CO:47:LYS:HB3 | 12:CO:48:PRO:HD2 | 1.63 | 0.79 |
| 17:AT:81:ARG:NH2 | 17:AT:83:ASP:OD2 | 2.16 | 0.79 |
| 25:BA:140:A:C8 | 25:BA:1408:C:O2' | 2.35 | 0.79 |
| 25:BA:330:A:O2' | 25:BA:331:A:H8 | 1.65 | 0.79 |
| 3:AF:50:ALA:HB1 | 3:AF:70:VAL:HG11 | 1.64 | 0.79 |
| 28:BE:27:LEU:CD2 | 28:BE:27:LEU:O | 2.30 | 0.79 |
| 4:AG:13:ARG:NH1 | 4:AG:38:TYR:O | 2.15 | 0.79 |
| 11:AN:79:SER:O | 11:AN:80:VAL:CG1 | 2.30 | 0.79 |
| 38:BQ:34:HIS:HB2 | 38:BQ:36:TYR:CE1 | 2.18 | 0.79 |
| 25:BA:1864:U:C2' | 25:BA:1869:G:H5'' | 2.13 | 0.79 |
| 39:DR:47:GLY:HA3 | 39:DR:63:VAL:HG12 | 1.64 | 0.79 |
| 47:BZ:92:LYS:HA | 47:BZ:95:LEU:HB2 | 1.64 | 0.79 |
| 27:BD:166:GLN:HA | 27:BD:166:GLN:HE21 | 1.45 | 0.79 |
| 40:D1:90:VAL:HG22 | 41:D2:39:LEU:HB3 | 1.64 | 0.79 |
| 28:DE:80:GLU:O | 28:DE:81:ILE:CG1 | 2.30 | 0.79 |
| 25:DA:2747:G:H2' | 25:DA:2748:A:H8 | 1.46 | 0.79 |
| 29:BF:29:ASN:H | 29:BF:112:MET:HE1 | 1.48 | 0.79 |
| 25:BA:654(G):C:O2 | 25:BA:654(N):G:N1 | 2.15 | 0.79 |
| 42:BS:94:ASP:O | 42:BS:95:ILE:CG2 | 2.30 | 0.79 |
| 26:DB:15:A:H3' | 26:DB:16:G:H5' | 1.65 | 0.79 |
| 25:DA:848:G:H2' | 25:DA:849:A:C8 | 2.17 | 0.78 |
| 36:DP:66:ILE:O | 36:DP:67:ARG:CB | 2.31 | 0.78 |
| 28:BE:51:PHE:HD1 | 28:BE:52:LEU:CD2 | 1.92 | 0.78 |
| 1:AA:1128:C:O2' | 1:AA:1130:A:H8 | 1.65 | 0.78 |
| 25:DA:1342:A:C2 | 25:DA:1397:U:C2 | 2.71 | 0.78 |
| 54:B8:34:TRP:O | 54:B8:34:TRP:CD2 | 2.36 | 0.78 |
| 1:CA:1090:U:H2' | 1:CA:1091:U:H6 | 1.48 | 0.78 |
| 25:DA:1270:C:H5'' | 25:DA:1271:G:O5' | 1.83 | 0.78 |
| 36:DP:26:TYR:CD1 | 36:DP:139:GLU:HG3 | 2.08 | 0.78 |
| 4:CG:13:ARG:HG2 | 4:CG:14:ARG:N | 1.98 | 0.78 |
| 36:BP:86:GLY:C | 36:BP:88:GLY:H | 1.83 | 0.78 |
| 47:DZ:91:LYS:HZ3 | 47:DZ:91:LYS:HB2 | 1.45 | 0.78 |
| 11:AN:17:GLY:HA3 | 11:AN:77:MET:CE | 2.12 | 0.78 |
| 38:BQ:88:ASP:O | 38:BQ:89:ARG:CB | 2.31 | 0.78 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|---------------------|-------------|----------|
| 1:AA:201:C:N4 | 1:AA:216:G:H1 | 1.81 | 0.78 |
| 1:CA:503:C:OP2 | 12:CO:116:SER:HB3 | 1.83 | 0.78 |
| 51:B5:56:LYS:H | 51:B5:56:LYS:HD2 | 1.47 | 0.78 |
| 31:BH:11:VAL:HB | 31:BH:12:PRO:HD2 | 1.64 | 0.78 |
| 54:D8:35:GLN:O | 54:D8:36:LYS:CG | 2.30 | 0.78 |
| 41:D2:71:LEU:H | 41:D2:86:GLY:HA2 | 1.43 | 0.78 |
| 27:BD:71:ASP:OD2 | 27:BD:103:ARG:NH2 | 2.16 | 0.78 |
| 25:DA:1012:U:N3 | 25:DA:1143:A:C2 | 2.51 | 0.78 |
| 25:DA:531:C:OP1 | 25:DA:561:G:N2 | 2.17 | 0.78 |
| 1:AA:827:U:H5 | 1:AA:872:A:N1 | 1.81 | 0.78 |
| 25:DA:1496:A:H8 | 25:DA:1577:C:O2' | 1.67 | 0.78 |
| 25:DA:654(D):G:H1 | 25:DA:654(Q):C:H42 | 1.32 | 0.78 |
| 1:AA:119:A:H4' | 1:AA:120:A:O5' | 1.83 | 0.78 |
| 25:BA:1404:C:O2' | 25:BA:1405:U:H5' | 1.84 | 0.78 |
| 36:BP:14:ARG:HG2 | 36:BP:41:TRP:HH2 | 1.46 | 0.78 |
| 1:AA:630:G:H2' | 1:AA:631:G:O4' | 1.84 | 0.78 |
| 25:DA:84:A:N6 | 25:DA:102:G:O2' | 2.10 | 0.78 |
| 30:BG:83:ARG:H | 30:BG:86:MET:HE3 | 1.41 | 0.78 |
| 27:BD:273:ARG:CG | 27:BD:273:ARG:O | 2.32 | 0.78 |
| 27:DD:35:LYS:HE3 | 27:DD:64:ILE:O | 1.82 | 0.78 |
| 36:DP:66:ILE:O | 36:DP:67:ARG:CG | 2.30 | 0.78 |
| 27:BD:35:LYS:CD | 27:BD:63:ARG:HB3 | 2.12 | 0.78 |
| 39:DR:52:ILE:CG2 | 39:DR:52:ILE:O | 2.30 | 0.78 |
| 25:BA:1021:A:H61 | 25:BA:1142(A):A:H61 | 1.32 | 0.78 |
| 1:CA:1131:G:H2' | 1:CA:1132:C:H6 | 1.49 | 0.78 |
| 30:BG:96:ARG:CG | 30:BG:96:ARG:HH11 | 1.96 | 0.78 |
| 25:DA:329:G:O6 | 44:DU:19:LYS:HG2 | 1.83 | 0.78 |
| 1:CA:168:G:H2' | 1:CA:169:C:H5'' | 1.64 | 0.78 |
| 7:AJ:78:ARG:HD2 | 7:AJ:80:VAL:HG22 | 1.65 | 0.78 |
| 52:B6:25:LYS:HZ1 | 52:B6:27:LYS:HD3 | 1.48 | 0.78 |
| 28:BE:47:VAL:O | 28:BE:48:GLN:O | 2.01 | 0.78 |
| 51:D5:16:ARG:CG | 51:D5:16:ARG:HH11 | 1.95 | 0.78 |
| 39:DR:26:ASP:O | 39:DR:49:VAL:HG12 | 1.83 | 0.78 |
| 35:BO:50:ARG:HG3 | 35:BO:50:ARG:HH21 | 1.47 | 0.78 |
| 2:CE:50:GLU:O | 2:CE:54:THR:OG1 | 2.01 | 0.78 |
| 35:DO:37:GLY:O | 35:DO:40:SER:N | 2.16 | 0.78 |
| 35:DO:101:VAL:HA | 35:DO:105:LEU:O | 1.84 | 0.78 |
| 25:BA:2292:C:P | 38:BQ:17:ARG:HH22 | 2.05 | 0.78 |
| 1:AA:804:U:H5'' | 1:AA:805:C:OP2 | 1.84 | 0.78 |
| 51:D5:16:ARG:NH1 | 51:D5:16:ARG:HG2 | 1.94 | 0.78 |
| 1:AA:838:G:H1 | 1:AA:848:C:N4 | 1.81 | 0.78 |
| 25:BA:67:U:N3 | 25:BA:74:A:H2 | 1.79 | 0.78 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 28:DE:1:MET:HB2 | 28:DE:200:GLU:OE2 | 1.84 | 0.78 |
| 25:BA:2113:U:H5' | 25:BA:2114:A:C8 | 2.17 | 0.78 |
| 25:BA:671:C:OP1 | 35:BO:42:SER:O | 2.02 | 0.78 |
| 1:AA:501:C:H2' | 1:AA:502:G:H8 | 1.48 | 0.78 |
| 52:D6:48:VAL:O | 52:D6:49:HIS:CB | 2.31 | 0.78 |
| 28:BE:3:GLY:HA3 | 28:BE:81:ILE:CG1 | 2.12 | 0.78 |
| 41:D2:76:LYS:O | 41:D2:79:VAL:CG2 | 2.30 | 0.78 |
| 1:AA:791:G:C2' | 1:AA:792:A:H5' | 2.13 | 0.78 |
| 8:AK:87:SER:HB2 | 8:AK:93:VAL:HB | 1.66 | 0.78 |
| 45:DV:27:VAL:HG12 | 45:DV:87:ASP:HB3 | 1.64 | 0.78 |
| 25:DA:2854:G:N2 | 25:DA:2864:G:C4 | 2.52 | 0.78 |
| 26:DB:75:G:H5' | 26:DB:75:G:H8 | 1.47 | 0.78 |
| 2:AE:76:GLN:HB3 | 2:AE:211:ILE:HD11 | 1.65 | 0.78 |
| 25:BA:2701:C:H3' | 25:BA:2702:U:H5'' | 1.66 | 0.78 |
| 23:AD:6:G:C2 | 23:AD:7:G:N7 | 2.52 | 0.78 |
| 30:DG:36:LYS:HE3 | 30:DG:38:VAL:HG21 | 1.66 | 0.78 |
| 25:BA:1496:A:H5' | 25:BA:1497:U:OP1 | 1.84 | 0.78 |
| 3:AF:126:ARG:HH11 | 3:AF:126:ARG:HG3 | 1.49 | 0.78 |
| 5:AH:100:VAL:HG22 | 5:AH:118:ILE:HG22 | 1.66 | 0.78 |
| 2:AE:77:ALA:HB1 | 2:AE:165:VAL:HG11 | 1.65 | 0.78 |
| 25:DA:459:U:H5'' | 53:D7:40:TRP:CD2 | 2.18 | 0.78 |
| 6:AI:89:MET:CE | 18:AU:76:LEU:HD23 | 2.14 | 0.78 |
| 41:D2:35:LEU:O | 41:D2:37:VAL:HG22 | 1.84 | 0.78 |
| 1:CA:1003:G:C2' | 1:CA:1004:A:H5' | 2.13 | 0.78 |
| 25:DA:1257:C:O2' | 29:DF:84:VAL:HG12 | 1.83 | 0.78 |
| 25:DA:2638:G:OP1 | 28:DE:82:ARG:NH2 | 2.13 | 0.77 |
| 52:D6:43:CYS:O | 52:D6:44:ARG:CB | 2.32 | 0.77 |
| 47:DZ:91:LYS:HZ2 | 47:DZ:91:LYS:HB2 | 1.49 | 0.77 |
| 27:DD:166:GLN:HE21 | 27:DD:166:GLN:CA | 1.96 | 0.77 |
| 25:DA:2689:U:H5'' | 25:DA:2690:C:H5' | 1.66 | 0.77 |
| 25:DA:2438:U:O3' | 25:DA:2439:A:H3' | 1.85 | 0.77 |
| 2:CE:82:ARG:HD2 | 2:CE:92:TYR:OH | 1.84 | 0.77 |
| 27:DD:35:LYS:HE3 | 27:DD:65:ILE:HA | 1.66 | 0.77 |
| 44:BU:76:CYS:O | 44:BU:78:ALA:N | 2.16 | 0.77 |
| 25:BA:2346:A:H4' | 25:BA:2347:C:OP2 | 1.81 | 0.77 |
| 25:BA:882:G:H3' | 25:BA:883:G:H5'' | 1.66 | 0.77 |
| 25:BA:1525:G:H2' | 25:BA:1526:G:C8 | 2.18 | 0.77 |
| 41:B2:44:LYS:O | 41:B2:46:VAL:HG12 | 1.83 | 0.77 |
| 31:BH:10:PRO:HD2 | 31:BH:50:VAL:O | 1.83 | 0.77 |
| 5:AH:110:LEU:HD13 | 5:AH:118:ILE:HD13 | 1.64 | 0.77 |
| 15:CR:87:ILE:HG22 | 15:CR:88:ARG:N | 1.99 | 0.77 |
| 50:D4:58:ARG:O | 50:D4:61:ARG:HB3 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 40:B1:79:PHE:O | 40:B1:79:PHE:HD2 | 1.68 | 0.77 |
| 6:AI:36:ARG:NH2 | 6:AI:38:GLU:HG2 | 1.97 | 0.77 |
| 28:BE:41:LYS:HB3 | 28:BE:41:LYS:HZ3 | 1.49 | 0.77 |
| 29:DF:67:GLN:O | 29:DF:67:GLN:CG | 2.30 | 0.77 |
| 28:DE:48:GLN:HA | 28:DE:80:GLU:HA | 1.65 | 0.77 |
| 25:DA:2415:G:O3' | 35:DO:66:GLY:HA3 | 1.85 | 0.77 |
| 36:DP:59:ARG:O | 36:DP:60:ARG:CB | 2.33 | 0.77 |
| 10:CM:15:THR:HG21 | 10:CM:92:THR:HG21 | 1.65 | 0.77 |
| 54:D8:52:LYS:HB2 | 54:D8:53:PRO:HD3 | 1.67 | 0.77 |
| 25:BA:1614:A:N6 | 42:BS:92:ARG:O | 2.16 | 0.77 |
| 1:CA:673:G:H2' | 1:CA:674:G:C8 | 2.19 | 0.77 |
| 25:DA:2439:A:H5' | 25:DA:2439:A:C8 | 2.18 | 0.77 |
| 22:AB:18:G:H1' | 22:AB:19:G:OP1 | 1.85 | 0.77 |
| 27:DD:35:LYS:CA | 27:DD:64:ILE:HG23 | 2.14 | 0.77 |
| 1:CA:1004:A:C2 | 1:CA:1024:G:C8 | 2.73 | 0.77 |
| 36:BP:66:ILE:HG13 | 36:BP:67:ARG:N | 1.98 | 0.77 |
| 1:AA:819:A:H4' | 1:AA:820:U:OP2 | 1.84 | 0.77 |
| 25:DA:885:C:N4 | 25:DA:890:A:H62 | 1.83 | 0.77 |
| 42:DS:9:TYR:H | 42:DS:102:HIS:CD2 | 2.03 | 0.77 |
| 20:CW:25:ARG:HG3 | 20:CW:25:ARG:HH11 | 1.50 | 0.77 |
| 28:DE:182:LEU:HD12 | 28:DE:183:LEU:H | 1.49 | 0.77 |
| 1:CA:1002:G:H2' | 1:CA:1003:G:H8 | 1.47 | 0.77 |
| 1:CA:1061:G:H2' | 1:CA:1062:U:H5' | 1.66 | 0.77 |
| 1:AA:1034:G:H2' | 1:AA:1035:A:C8 | 2.19 | 0.77 |
| 25:BA:1434:A:H61 | 25:BA:1558:A:H62 | 1.29 | 0.77 |
| 1:CA:1443:G:H3' | 1:CA:1446:A:C5' | 2.14 | 0.77 |
| 25:BA:2162:G:H2' | 25:BA:2163:C:C6 | 2.19 | 0.77 |
| 31:DH:117:PRO:HB3 | 31:DH:123:PHE:CE1 | 2.20 | 0.77 |
| 41:B2:4:ILE:HG22 | 41:B2:39:LEU:HD23 | 1.66 | 0.77 |
| 6:CI:87:ARG:HG2 | 6:CI:87:ARG:HH11 | 1.49 | 0.77 |
| 25:BA:847:U:C4 | 25:BA:933:A:N1 | 2.53 | 0.77 |
| 25:BA:534:U:H5' | 40:B1:42:ALA:HB1 | 1.66 | 0.77 |
| 12:AO:6:THR:H | 12:AO:9:GLN:HE21 | 1.30 | 0.77 |
| 44:BU:40:GLU:OE1 | 44:BU:40:GLU:HA | 1.83 | 0.77 |
| 35:BO:61:ARG:HH21 | 35:BO:61:ARG:HB2 | 0.77 | 0.77 |
| 20:AW:10:LEU:HD23 | 20:AW:12:ALA:N | 1.98 | 0.77 |
| 40:D1:65:ILE:HD11 | 40:D1:96:ALA:HB3 | 1.67 | 0.77 |
| 35:DO:16:ARG:HH11 | 35:DO:16:ARG:HG3 | 1.49 | 0.77 |
| 22:CB:21:A:H1' | 22:CB:22:G:O5' | 1.85 | 0.77 |
| 25:BA:860:U:C5 | 25:BA:917:A:H2 | 2.01 | 0.77 |
| 48:DW:9:GLN:HE22 | 48:DW:56:GLN:HG2 | 1.49 | 0.77 |
| 2:AE:67:THR:HG21 | 2:AE:155:LEU:HG | 1.65 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 29:DF:118:ALA:HB2 | 29:DF:123:LEU:HD23 | 1.65 | 0.77 |
| 1:CA:1497:G:C2' | 1:CA:1498:U:H5' | 2.14 | 0.77 |
| 2:AE:80:ILE:HG21 | 2:AE:212:GLN:HA | 1.67 | 0.77 |
| 8:AK:87:SER:CB | 8:AK:93:VAL:H | 1.98 | 0.77 |
| 35:DO:112:LEU:H | 35:DO:128:HIS:CD2 | 2.02 | 0.77 |
| 25:BA:900:A:H5' | 25:BA:901:A:OP2 | 1.85 | 0.77 |
| 25:BA:2334:G:H5' | 38:BQ:9:ARG:HG2 | 1.67 | 0.77 |
| 33:DM:103:VAL:HG11 | 33:DM:120:LEU:HD13 | 1.67 | 0.77 |
| 27:DD:65:ILE:HD11 | 27:DD:67:PHE:CE2 | 2.20 | 0.77 |
| 28:BE:27:LEU:CD2 | 28:BE:27:LEU:C | 2.53 | 0.77 |
| 23:CC:20:G:C2 | 23:CC:58:A:C2 | 2.72 | 0.77 |
| 36:DP:63:LYS:CD | 36:DP:63:LYS:C | 2.52 | 0.77 |
| 46:B3:38:VAL:CG1 | 46:B3:40:GLN:HG2 | 2.13 | 0.77 |
| 4:AG:110:PHE:H | 4:AG:110:PHE:HD1 | 1.33 | 0.77 |
| 26:BB:30:C:H2' | 26:BB:31:C:O5' | 1.85 | 0.77 |
| 9:CL:78:LYS:NZ | 9:CL:78:LYS:HB2 | 2.00 | 0.77 |
| 25:DA:2355:C:H5' | 46:D3:36:ILE:HD11 | 1.67 | 0.77 |
| 51:B5:33:CYS:HB2 | 51:B5:40:LYS:HD3 | 1.66 | 0.77 |
| 12:CO:27:LEU:HD23 | 12:CO:33:ARG:HG2 | 1.67 | 0.77 |
| 16:CS:36:ILE:HG13 | 16:CS:36:ILE:O | 1.84 | 0.77 |
| 1:AA:5:U:H2' | 1:AA:5:U:O2 | 1.84 | 0.77 |
| 5:AH:31:LEU:HD23 | 5:AH:45:PHE:HD1 | 1.50 | 0.77 |
| 54:D8:29:LYS:HG2 | 54:D8:29:LYS:O | 1.85 | 0.77 |
| 25:DA:2394:C:OP1 | 35:DO:62:LEU:CB | 2.33 | 0.77 |
| 25:BA:2415:G:O3' | 35:BO:66:GLY:HA3 | 1.84 | 0.77 |
| 25:DA:2306:C:H3' | 25:DA:2307:G:C5' | 2.13 | 0.77 |
| 25:DA:259:G:O2' | 25:DA:621:A:O2' | 2.03 | 0.77 |
| 38:BQ:37:ALA:HB2 | 38:BQ:101:LEU:HD21 | 1.67 | 0.77 |
| 25:DA:2872:G:C4 | 25:DA:2873:A:N1 | 2.54 | 0.77 |
| 33:BM:22:THR:HG22 | 33:BM:23:LEU:H | 1.49 | 0.77 |
| 25:DA:654(B):C:H2' | 25:DA:654(C):G:C8 | 2.20 | 0.77 |
| 2:AE:97:TRP:CH2 | 2:AE:176:GLU:HG3 | 2.19 | 0.77 |
| 27:DD:35:LYS:CG | 27:DD:64:ILE:H | 1.96 | 0.76 |
| 28:BE:14:ILE:O | 28:BE:15:PHE:CG | 2.39 | 0.76 |
| 1:AA:1037:C:H2' | 1:AA:1038:C:C6 | 2.19 | 0.76 |
| 46:B3:40:GLN:HE22 | 46:B3:44:ARG:N | 1.80 | 0.76 |
| 41:B2:44:LYS:HD2 | 41:B2:45:THR:H | 1.48 | 0.76 |
| 1:CA:382:A:H2' | 1:CA:383:A:C8 | 2.20 | 0.76 |
| 1:AA:953:G:H5' | 1:AA:965:A:H61 | 1.50 | 0.76 |
| 30:BG:77:ILE:HG23 | 30:BG:77:ILE:O | 1.85 | 0.76 |
| 25:BA:2346:A:H5'' | 25:BA:2383:G:O4' | 1.85 | 0.76 |
| 54:B8:38:GLY:H | 54:B8:41:ILE:HG23 | 1.51 | 0.76 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|---------------------|-------------|----------|
| 25:DA:2392:A:H2 | 25:DA:2424:C:N4 | 1.82 | 0.76 |
| 36:DP:79:LEU:CD1 | 36:DP:79:LEU:C | 2.54 | 0.76 |
| 1:CA:345:C:O2' | 1:CA:346:G:O5' | 2.03 | 0.76 |
| 25:BA:1359:A:C2 | 25:BA:1372:U:O4 | 2.38 | 0.76 |
| 25:DA:140:A:C8 | 25:DA:1408:C:O2' | 2.37 | 0.76 |
| 41:D2:44:LYS:C | 41:D2:46:VAL:H | 1.89 | 0.76 |
| 29:BF:66:PRO:O | 29:BF:67:GLN:HB3 | 1.83 | 0.76 |
| 12:CO:79:GLU:HG3 | 12:CO:80:HIS:CD2 | 2.19 | 0.76 |
| 26:BB:40:U:H1' | 26:BB:45:A:H61 | 1.47 | 0.76 |
| 37:D0:37:THR:CG2 | 37:D0:39:PRO:HD2 | 2.15 | 0.76 |
| 32:BK:78:THR:HG23 | 32:BK:141:LYS:NZ | 2.00 | 0.76 |
| 25:BA:2310:A:C2' | 25:BA:2311:A:H5'' | 2.15 | 0.76 |
| 28:DE:50:GLY:O | 28:DE:51:PHE:CB | 2.33 | 0.76 |
| 39:DR:54:ARG:NH1 | 39:DR:54:ARG:HG2 | 1.89 | 0.76 |
| 19:AV:40:ILE:HG12 | 19:AV:41:VAL:HG13 | 1.68 | 0.76 |
| 54:B8:34:TRP:CD2 | 54:B8:35:GLN:OE1 | 2.38 | 0.76 |
| 22:AB:18:G:H4' | 22:AB:19:G:OP2 | 1.84 | 0.76 |
| 25:DA:1138:G:H21 | 33:DM:106:MET:HE3 | 1.49 | 0.76 |
| 50:B4:37:SER:HB3 | 50:B4:42:PHE:HB3 | 1.67 | 0.76 |
| 25:BA:1188:U:H4' | 41:B2:79:VAL:HG22 | 1.67 | 0.76 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:H22 | 1.27 | 0.76 |
| 37:B0:79:LEU:HA | 37:B0:83:ILE:HG13 | 1.66 | 0.76 |
| 2:AE:120:ALA:O | 2:AE:121:LEU:HB2 | 1.84 | 0.76 |
| 25:BA:1899:G:N2 | 25:BA:1902:C:C5 | 2.54 | 0.76 |
| 25:BA:2317:C:H2' | 25:BA:2318:G:C5' | 2.13 | 0.76 |
| 39:DR:55:ASN:N | 39:DR:59:THR:HG22 | 1.98 | 0.76 |
| 1:CA:1322:C:O2' | 1:CA:1323:G:H5' | 1.85 | 0.76 |
| 26:DB:103:U:O2' | 45:DV:72:ARG:HG2 | 1.86 | 0.76 |
| 25:BA:607:U:OP1 | 29:BF:102:PRO:HA | 1.85 | 0.76 |
| 25:DA:1019:U:H3 | 25:DA:1142(A):A:H62 | 1.30 | 0.76 |
| 1:CA:1277:C:HO2' | 1:CA:1279:A:H8 | 1.34 | 0.76 |
| 39:BR:3:ARG:HB3 | 39:BR:7:ILE:HG13 | 1.68 | 0.76 |
| 35:BO:83:VAL:HG12 | 35:BO:112:LEU:HD21 | 1.67 | 0.76 |
| 6:AI:67:MET:HB2 | 6:AI:68:PRO:HD2 | 1.66 | 0.76 |
| 23:AC:1:C:C2' | 23:AC:2:G:OP2 | 2.34 | 0.76 |
| 39:BR:64:ARG:HB2 | 39:BR:73:GLU:HG2 | 1.65 | 0.76 |
| 2:AE:22:LYS:NZ | 2:AE:22:LYS:HA | 2.01 | 0.76 |
| 36:DP:7:MET:HB3 | 36:DP:10:ARG:NH2 | 2.00 | 0.76 |
| 25:DA:1864:U:OP1 | 25:DA:2410:G:O2' | 2.04 | 0.76 |
| 37:D0:37:THR:HG23 | 37:D0:39:PRO:HD2 | 1.67 | 0.76 |
| 13:AP:39:ILE:HD13 | 13:AP:52:GLU:HB3 | 1.68 | 0.76 |
| 23:AC:62:C:H2' | 23:AC:63:C:H6 | 1.51 | 0.76 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 23:CC:24:C:H2' | 23:CC:25:U:C6 | 2.19 | 0.76 |
| 23:CC:24:C:H2' | 23:CC:25:U:H6 | 1.50 | 0.76 |
| 1:CA:1320:C:H2' | 1:CA:1321:C:C6 | 2.21 | 0.76 |
| 25:DA:2872:G:C5 | 25:DA:2873:A:C2 | 2.74 | 0.76 |
| 37:D0:24:GLN:NE2 | 37:D0:36:THR:HG21 | 2.01 | 0.76 |
| 6:CI:33:TYR:CE1 | 6:CI:78:GLU:HG3 | 2.20 | 0.76 |
| 22:AB:16:U:OP1 | 22:AB:17:U:N3 | 2.19 | 0.76 |
| 25:DA:861:A:C2 | 25:DA:917:A:C4 | 2.74 | 0.76 |
| 25:DA:2880:C:H1' | 37:D0:92:GLY:HA3 | 1.65 | 0.76 |
| 25:DA:2893:G:H4' | 25:DA:2894:G:O5' | 1.85 | 0.76 |
| 25:DA:2638:G:P | 28:DE:82:ARG:NH2 | 2.58 | 0.76 |
| 25:BA:2467:C:C3' | 25:BA:2468:G:H5' | 2.14 | 0.76 |
| 35:BO:63:PRO:HB3 | 54:B8:12:LYS:O | 1.86 | 0.76 |
| 25:DA:2420:C:N4 | 54:D8:31:HIS:HB3 | 2.00 | 0.76 |
| 27:BD:181:GLU:CA | 27:BD:272:ALA:CB | 2.62 | 0.76 |
| 28:BE:34:VAL:CG1 | 28:BE:49:LEU:O | 2.34 | 0.76 |
| 1:CA:1319:A:H5' | 1:CA:1320:C:OP1 | 1.85 | 0.76 |
| 25:DA:1005:C:H1' | 25:DA:1143:A:N1 | 1.99 | 0.76 |
| 1:CA:802:A:H5' | 1:CA:803:G:OP2 | 1.85 | 0.76 |
| 25:DA:330:A:H2 | 25:DA:1210:A:O2' | 1.68 | 0.76 |
| 28:BE:26:ILE:HD11 | 28:BE:198:VAL:HG21 | 1.67 | 0.76 |
| 45:BV:164:ALA:C | 45:BV:165:VAL:HG13 | 2.05 | 0.76 |
| 25:DA:2553:G:H5'' | 25:DA:2554:U:OP2 | 1.85 | 0.76 |
| 3:AF:150:LYS:HG3 | 3:AF:169:ALA:HB2 | 1.66 | 0.76 |
| 1:AA:1329:A:H5' | 13:AP:29:ARG:HD2 | 1.68 | 0.76 |
| 25:BA:2432:A:C4 | 47:BZ:33:LYS:HG2 | 2.20 | 0.76 |
| 29:DF:178:PRO:HB2 | 29:DF:201:VAL:HG11 | 1.66 | 0.76 |
| 25:BA:528:A:O2' | 25:BA:529:A:H5'' | 1.85 | 0.76 |
| 25:BA:2466:C:C2' | 25:BA:2467:C:H5' | 2.16 | 0.76 |
| 28:BE:46:ALA:O | 28:BE:47:VAL:HG22 | 1.85 | 0.76 |
| 1:AA:1053:G:C5' | 1:AA:1054:C:H5' | 2.12 | 0.76 |
| 29:BF:178:PRO:HB2 | 29:BF:201:VAL:CG1 | 2.16 | 0.76 |
| 36:BP:68:ILE:HD13 | 36:BP:103:MET:CG | 2.15 | 0.76 |
| 25:DA:1140:C:H1' | 25:DA:1143:A:C8 | 2.20 | 0.76 |
| 35:DO:47:ASP:OD2 | 35:DO:49:ARG:HD3 | 1.86 | 0.76 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.21 | 0.76 |
| 4:CG:175:SER:HB3 | 4:CG:186:LEU:HD11 | 1.68 | 0.76 |
| 2:AE:178:ARG:HH22 | 2:AE:196:LEU:HA | 1.51 | 0.76 |
| 27:DD:148:GLU:HB2 | 27:DD:151:LYS:HD2 | 1.68 | 0.76 |
| 40:B1:66:ASN:HB2 | 40:B1:76:TYR:HB2 | 1.68 | 0.76 |
| 1:CA:1025:U:O2' | 1:CA:1026:G:O4' | 2.04 | 0.76 |
| 31:DH:151:ILE:O | 31:DH:152:ARG:CG | 2.30 | 0.76 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:1023:G:H3' | 1:AA:1024:G:H5'' | 1.68 | 0.76 |
| 2:CE:16:HIS:CE1 | 2:CE:213:LEU:HD13 | 2.20 | 0.76 |
| 39:DR:90:GLN:HE21 | 39:DR:90:GLN:HA | 1.49 | 0.76 |
| 26:DB:38:C:H42 | 26:DB:44:G:H1 | 1.34 | 0.76 |
| 20:AW:53:LEU:HB3 | 20:AW:102:GLY:HA3 | 1.67 | 0.76 |
| 25:DA:2688:U:H5 | 25:DA:2720:U:OP2 | 1.68 | 0.76 |
| 25:BA:2134:A:N6 | 25:BA:2157:G:H1' | 2.01 | 0.76 |
| 1:AA:1286:A:H5'' | 21:AX:26:LYS:HD2 | 1.68 | 0.76 |
| 1:AA:365:U:H5'' | 1:AA:366:C:OP1 | 1.86 | 0.76 |
| 25:BA:2309:A:C2' | 25:BA:2310:A:H5'' | 2.14 | 0.76 |
| 45:DV:115:GLY:HA3 | 45:DV:174:VAL:HG12 | 1.68 | 0.76 |
| 35:BO:64:LYS:HB2 | 54:B8:25:MET:HG3 | 1.66 | 0.76 |
| 25:BA:1728:G:H8 | 25:BA:1732:A:H62 | 1.32 | 0.76 |
| 32:DK:72:LEU:HD21 | 32:DK:107:VAL:HG11 | 1.67 | 0.76 |
| 1:AA:474:G:H2' | 1:AA:475:G:H8 | 1.51 | 0.76 |
| 25:DA:1427:A:H4' | 25:DA:1428:C:O5' | 1.85 | 0.76 |
| 37:B0:33:ARG:HG3 | 37:B0:115:GLU:HB3 | 1.67 | 0.76 |
| 25:BA:138:G:N2 | 43:BT:44:GLU:OE2 | 2.16 | 0.76 |
| 2:CE:178:ARG:HB2 | 2:CE:178:ARG:HH11 | 1.50 | 0.76 |
| 1:CA:1187:G:OP1 | 9:CL:113:LYS:NZ | 2.18 | 0.76 |
| 25:DA:774:A:H2 | 25:DA:787:U:HO2' | 1.33 | 0.76 |
| 28:DE:48:GLN:HG2 | 28:DE:78:LEU:CB | 2.15 | 0.75 |
| 45:DV:146:ILE:CG1 | 45:DV:147:GLY:H | 1.89 | 0.75 |
| 25:DA:273(C):C:N4 | 25:DA:363(C):G:H1 | 1.82 | 0.75 |
| 48:BW:17:SER:HB3 | 48:BW:67:LYS:HD3 | 1.67 | 0.75 |
| 35:DO:36:LYS:HB2 | 35:DO:36:LYS:HZ2 | 1.50 | 0.75 |
| 28:BE:16:ARG:O | 28:BE:17:ASP:HB2 | 1.85 | 0.75 |
| 8:AK:86:ILE:HG22 | 8:AK:87:SER:H | 1.50 | 0.75 |
| 3:AF:70:VAL:HG12 | 3:AF:72:LYS:H | 1.52 | 0.75 |
| 1:AA:1126:U:H5 | 1:AA:1127:G:C4 | 2.04 | 0.75 |
| 52:D6:29:ASN:H | 52:D6:29:ASN:ND2 | 1.85 | 0.75 |
| 24:C1:14:U:H4' | 24:C1:14:U:OP1 | 1.78 | 0.75 |
| 25:BA:2780:G:OP2 | 33:BM:118:LYS:HD3 | 1.86 | 0.75 |
| 29:DF:89:VAL:CG1 | 29:DF:90:PHE:N | 2.30 | 0.75 |
| 28:DE:80:GLU:O | 28:DE:81:ILE:CB | 2.34 | 0.75 |
| 25:DA:1188:U:C2' | 25:DA:1189:A:H5' | 2.16 | 0.75 |
| 44:BU:81:LYS:NZ | 44:BU:96:ILE:HD12 | 2.01 | 0.75 |
| 10:CM:49:VAL:HG12 | 14:CQ:41:ARG:HB2 | 1.66 | 0.75 |
| 25:BA:1885:A:H8 | 25:BA:1885:A:H5' | 1.51 | 0.75 |
| 25:BA:881:G:H3' | 25:BA:882:G:O4' | 1.86 | 0.75 |
| 25:BA:1509:C:H3' | 25:BA:1510:A:H5'' | 1.67 | 0.75 |
| 25:DA:1460:A:H4' | 25:DA:1461:G:OP2 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:1422:G:H5' | 34:BN:48:PRO:HB3 | 1.68 | 0.75 |
| 2:AE:14:GLY:HA3 | 2:AE:209:ARG:HH21 | 1.51 | 0.75 |
| 1:CA:365:U:H5'' | 1:CA:366:C:OP1 | 1.86 | 0.75 |
| 15:CR:39:LEU:HD12 | 15:CR:56:LEU:HB2 | 1.68 | 0.75 |
| 31:BH:86:GLU:H | 31:BH:86:GLU:CD | 1.88 | 0.75 |
| 54:D8:39:LYS:HG2 | 54:D8:40:GLU:N | 1.99 | 0.75 |
| 38:DQ:86:ALA:O | 38:DQ:87:PHE:CB | 2.34 | 0.75 |
| 30:BG:67:LYS:O | 30:BG:67:LYS:HD2 | 1.85 | 0.75 |
| 25:DA:2128:C:H2' | 25:DA:2129:C:C6 | 2.21 | 0.75 |
| 31:BH:153:LYS:CG | 31:BH:162:ILE:H | 1.99 | 0.75 |
| 36:DP:90:VAL:HG12 | 36:DP:90:VAL:O | 1.84 | 0.75 |
| 5:AH:45:PHE:CE2 | 5:AH:47:LYS:HD2 | 2.21 | 0.75 |
| 9:AL:63:ILE:HD11 | 9:AL:81:ILE:HD11 | 1.67 | 0.75 |
| 17:AT:22:LEU:HD11 | 17:AT:39:SER:HB3 | 1.68 | 0.75 |
| 8:CK:20:TYR:HE2 | 8:CK:75:ARG:HD2 | 1.49 | 0.75 |
| 25:DA:1485:G:O2' | 25:DA:1486:A:H5' | 1.86 | 0.75 |
| 23:AD:64:G:H2' | 23:AD:65:G:C8 | 2.21 | 0.75 |
| 28:BE:59:VAL:HG21 | 28:BE:73:GLU:HB3 | 1.69 | 0.75 |
| 28:BE:59:VAL:HG11 | 28:BE:63:LEU:CD1 | 2.15 | 0.75 |
| 35:BO:16:ARG:HH11 | 35:BO:16:ARG:HG3 | 1.49 | 0.75 |
| 25:BA:1053:C:H42 | 25:BA:1106:G:H1 | 1.31 | 0.75 |
| 9:CL:47:LEU:HD23 | 9:CL:50:LEU:HD12 | 1.69 | 0.75 |
| 50:D4:32:TYR:O | 50:D4:33:VAL:HG22 | 1.86 | 0.75 |
| 35:BO:112:LEU:H | 35:BO:128:HIS:CD2 | 2.05 | 0.75 |
| 28:BE:23:VAL:CG1 | 28:BE:185:LYS:HA | 2.17 | 0.75 |
| 28:BE:35:GLN:O | 28:BE:36:ARG:HG2 | 1.85 | 0.75 |
| 1:AA:1132:C:H2' | 1:AA:1133:G:C8 | 2.22 | 0.75 |
| 1:AA:1025:U:O2' | 1:AA:1026:G:O5' | 2.04 | 0.75 |
| 25:BA:2373:G:H1 | 25:BA:2380:C:N4 | 1.84 | 0.75 |
| 31:BH:4:ILE:HG13 | 31:BH:6:ARG:CZ | 2.16 | 0.75 |
| 1:AA:686:U:O2' | 1:AA:687:A:O5' | 2.04 | 0.75 |
| 3:CF:43:LEU:O | 3:CF:47:LEU:HB2 | 1.87 | 0.75 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:H6 | 1.50 | 0.75 |
| 1:CA:164:U:H2' | 1:CA:165:C:H6 | 1.50 | 0.75 |
| 25:DA:851:U:OP1 | 49:DX:49:LYS:HE2 | 1.87 | 0.75 |
| 25:DA:587:C:O2 | 35:DO:33:ARG:NH1 | 2.20 | 0.75 |
| 1:AA:1450:U:O2' | 1:AA:1451:A:H8 | 1.69 | 0.75 |
| 38:BQ:85:VAL:HG23 | 38:BQ:112:PHE:CE1 | 2.22 | 0.75 |
| 40:D1:92:ARG:HD2 | 40:D1:95:LEU:HD12 | 1.68 | 0.75 |
| 22:CB:17:U:H5'' | 22:CB:18:G:C8 | 2.21 | 0.75 |
| 25:BA:1728:G:H3' | 25:BA:1729:A:H5'' | 1.67 | 0.75 |
| 43:DT:23:GLU:HG3 | 43:DT:24:GLY:H | 1.52 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 29:BF:127:GLU:OE2 | 29:BF:127:GLU:HA | 1.84 | 0.75 |
| 25:BA:2306:C:H3' | 25:BA:2307:G:C5' | 2.17 | 0.75 |
| 26:BB:37:C:H2' | 26:BB:38:C:H5' | 1.69 | 0.75 |
| 25:DA:2015:A:C2 | 51:D5:6:VAL:HG23 | 2.22 | 0.75 |
| 10:AM:8:LEU:HD12 | 10:AM:20:ALA:HB2 | 1.68 | 0.75 |
| 25:DA:2602:A:H4' | 25:DA:2603:G:O5' | 1.87 | 0.75 |
| 36:DP:29:PHE:CG | 36:DP:65:PHE:CE1 | 2.75 | 0.75 |
| 52:D6:15:GLU:HG2 | 52:D6:16:CYS:H | 1.52 | 0.75 |
| 1:CA:1036:G:H2' | 1:CA:1037:C:C2 | 2.21 | 0.75 |
| 25:BA:654(M):C:H2' | 25:BA:654(N):G:N7 | 2.01 | 0.75 |
| 1:CA:1274:G:O2' | 1:CA:1275:A:H5' | 1.86 | 0.75 |
| 25:BA:2116:G:P | 25:BA:2165:G:H22 | 2.09 | 0.75 |
| 25:BA:273(F):C:H3' | 25:BA:274:G:H5'' | 1.68 | 0.75 |
| 36:BP:20:ALA:HB2 | 36:BP:99:PRO:HD2 | 1.67 | 0.75 |
| 1:AA:1318:A:H1' | 19:AV:37:ARG:HH21 | 1.49 | 0.75 |
| 25:BA:2422:A:H4' | 25:BA:2423:U:OP1 | 1.87 | 0.75 |
| 38:BQ:106:ARG:HA | 38:BQ:110:LEU:HD11 | 1.68 | 0.75 |
| 41:D2:76:LYS:CB | 41:D2:79:VAL:HG21 | 2.17 | 0.75 |
| 36:BP:66:ILE:O | 36:BP:67:ARG:HB2 | 1.86 | 0.75 |
| 25:DA:90:U:O2' | 25:DA:91:A:C8 | 2.37 | 0.75 |
| 1:AA:437:U:H5'' | 4:AG:155:LEU:HD22 | 1.68 | 0.75 |
| 1:AA:977:A:H8 | 1:AA:1223:C:N3 | 1.85 | 0.75 |
| 25:BA:330:A:HO2' | 25:BA:331:A:H8 | 1.30 | 0.75 |
| 42:BS:29:LEU:HD21 | 42:BS:33:ARG:CZ | 2.17 | 0.75 |
| 1:AA:624:C:O3' | 16:AS:10:GLY:HA2 | 1.87 | 0.75 |
| 35:BO:39:LYS:HG3 | 35:BO:45:LEU:HD22 | 1.69 | 0.75 |
| 25:BA:1427:A:H4' | 25:BA:1428:C:O5' | 1.84 | 0.75 |
| 25:DA:2340:G:O2' | 25:DA:2341:G:H5' | 1.86 | 0.75 |
| 25:BA:1060:U:H1' | 25:BA:1061:U:OP2 | 1.87 | 0.75 |
| 33:BM:46:VAL:CG1 | 33:BM:47:ALA:H | 1.98 | 0.75 |
| 1:CA:983:A:N1 | 1:CA:1222:G:N2 | 2.33 | 0.75 |
| 25:DA:1070:A:H8 | 25:DA:1096:A:HO2' | 1.34 | 0.75 |
| 25:BA:879:G:H1 | 25:BA:898:C:N4 | 1.85 | 0.75 |
| 1:CA:1129:C:C4 | 1:CA:1139:G:C2 | 2.75 | 0.75 |
| 1:CA:1298:C:OP2 | 7:CJ:114:ARG:NH2 | 2.18 | 0.75 |
| 50:D4:20:ASN:CG | 50:D4:21:VAL:H | 1.89 | 0.75 |
| 30:DG:111:LEU:HB2 | 30:DG:112:PRO:HD3 | 1.69 | 0.75 |
| 14:CQ:45:ARG:HG3 | 14:CQ:45:ARG:HH11 | 1.52 | 0.75 |
| 7:CJ:78:ARG:CZ | 7:CJ:80:VAL:HB | 2.17 | 0.75 |
| 1:CA:1286:A:C8 | 1:CA:1287:A:H4' | 2.21 | 0.75 |
| 29:DF:132:VAL:HG22 | 29:DF:133:ASN:H | 1.50 | 0.75 |
| 35:DO:135:LEU:O | 35:DO:139:LYS:HB2 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 38:BQ:85:VAL:HG21 | 38:BQ:112:PHE:HZ | 1.52 | 0.74 |
| 36:DP:66:ILE:CG1 | 36:DP:67:ARG:N | 2.49 | 0.74 |
| 41:D2:83:ARG:HD3 | 41:D2:83:ARG:H | 1.49 | 0.74 |
| 1:CA:179:A:H2' | 1:CA:180:U:H6 | 1.51 | 0.74 |
| 25:BA:1403:C:H5'' | 25:BA:1471:A:H1' | 1.66 | 0.74 |
| 25:BA:330:A:O2' | 25:BA:331:A:C8 | 2.40 | 0.74 |
| 34:DN:115:VAL:HG13 | 34:DN:121:VAL:HG21 | 1.68 | 0.74 |
| 33:DM:29:LYS:HA | 33:DM:29:LYS:HE2 | 1.68 | 0.74 |
| 25:BA:1607:C:H4' | 25:BA:1608:A:O5' | 1.86 | 0.74 |
| 45:DV:28:MET:HG3 | 45:DV:37:VAL:HG11 | 1.69 | 0.74 |
| 54:D8:49:VAL:O | 54:D8:50:LEU:HD12 | 1.86 | 0.74 |
| 28:BE:51:PHE:CD1 | 28:BE:52:LEU:HD21 | 2.22 | 0.74 |
| 25:BA:1026:U:H4' | 25:BA:1027:A:OP1 | 1.85 | 0.74 |
| 25:DA:1142:U:H2' | 25:DA:1142:U:O2 | 1.87 | 0.74 |
| 25:DA:1012:U:C4 | 25:DA:1143:A:N1 | 2.55 | 0.74 |
| 1:CA:1305:G:O2' | 1:CA:1306:A:H8 | 1.68 | 0.74 |
| 33:DM:128:HIS:NE2 | 33:DM:134:ARG:HD2 | 2.02 | 0.74 |
| 13:AP:3:ARG:HG2 | 13:AP:9:ILE:CG1 | 2.17 | 0.74 |
| 25:BA:654(A):A:C2 | 25:BA:654(T):A:N1 | 2.54 | 0.74 |
| 1:AA:1348:U:H4' | 9:AL:120:ARG:HD2 | 1.68 | 0.74 |
| 25:BA:2298:A:H62 | 25:BA:2318:G:H8 | 1.31 | 0.74 |
| 35:BO:64:LYS:CB | 54:B8:25:MET:CG | 2.60 | 0.74 |
| 1:AA:975:A:C4' | 1:AA:976:G:H5'' | 2.17 | 0.74 |
| 3:AF:166:GLU:HG3 | 3:AF:167:TRP:H | 1.51 | 0.74 |
| 27:DD:246:PRO:HD2 | 27:DD:255:LYS:HE2 | 1.68 | 0.74 |
| 1:CA:1325:C:H4' | 21:CX:17:THR:HG21 | 1.68 | 0.74 |
| 28:BE:23:VAL:HA | 28:BE:185:LYS:HA | 1.70 | 0.74 |
| 45:DV:175:VAL:HG22 | 45:DV:176:PRO:CD | 2.17 | 0.74 |
| 25:DA:2580:U:H4' | 28:DE:130:GLY:CA | 2.17 | 0.74 |
| 54:B8:34:TRP:CZ3 | 54:B8:35:GLN:OE1 | 2.41 | 0.74 |
| 54:B8:34:TRP:O | 54:B8:35:GLN:HG3 | 1.88 | 0.74 |
| 28:BE:116:VAL:O | 28:BE:117:MET:HB3 | 1.88 | 0.74 |
| 29:DF:181:LEU:HD21 | 29:DF:186:ILE:HD11 | 1.69 | 0.74 |
| 38:DQ:19:LYS:O | 38:DQ:20:ARG:HD3 | 1.86 | 0.74 |
| 47:BZ:8:SER:OG | 47:BZ:10:LYS:HG3 | 1.88 | 0.74 |
| 25:BA:2467:C:H4' | 36:BP:123:HIS:ND1 | 2.02 | 0.74 |
| 35:DO:64:LYS:HB3 | 54:D8:25:MET:HG3 | 1.49 | 0.74 |
| 4:CG:15:GLU:OE1 | 4:CG:66:ARG:NH1 | 2.21 | 0.74 |
| 1:AA:1347:G:N2 | 1:AA:1373:G:H2' | 2.03 | 0.74 |
| 1:CA:913:A:H4' | 1:CA:914:A:O5' | 1.87 | 0.74 |
| 25:BA:2690:C:H5'' | 25:BA:2872:G:H21 | 1.51 | 0.74 |
| 25:BA:314:A:C2' | 25:BA:315:G:H5' | 2.18 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 10:AM:55:LYS:HZ3 | 10:AM:55:LYS:HB3 | 1.51 | 0.74 |
| 10:AM:48:THR:HG23 | 10:AM:62:HIS:HB3 | 1.69 | 0.74 |
| 4:CG:24:GLU:N | 4:CG:24:GLU:OE2 | 2.21 | 0.74 |
| 25:BA:1264:G:H5' | 51:B5:11:THR:CG2 | 2.18 | 0.74 |
| 5:AH:10:MET:HB3 | 5:AH:32:VAL:HG22 | 1.69 | 0.74 |
| 25:DA:2531:A:H4' | 31:DH:157:TYR:CD2 | 2.22 | 0.74 |
| 27:BD:182:LEU:N | 27:BD:272:ALA:HB2 | 2.02 | 0.74 |
| 54:D8:50:LEU:O | 54:D8:51:ALA:HB3 | 1.87 | 0.74 |
| 25:DA:674:G:H1' | 29:DF:74:ARG:HD3 | 1.68 | 0.74 |
| 35:DO:15:ARG:CB | 35:DO:15:ARG:HH11 | 2.01 | 0.74 |
| 35:DO:38:GLN:HG2 | 35:DO:45:LEU:CD1 | 2.18 | 0.74 |
| 49:DX:19:GLN:HE22 | 49:DX:52:HIS:HE1 | 1.35 | 0.74 |
| 25:BA:1049:C:H2' | 25:BA:1050:A:H5' | 1.68 | 0.74 |
| 1:AA:27:G:H4' | 4:AG:209:ARG:HG3 | 1.69 | 0.74 |
| 45:BV:54:HIS:NE2 | 45:BV:123:ASP:OD2 | 2.20 | 0.74 |
| 1:AA:1004:A:H8 | 1:AA:1036:G:N1 | 1.85 | 0.74 |
| 10:AM:48:THR:HA | 10:AM:62:HIS:HB3 | 1.70 | 0.74 |
| 2:CE:91:PRO:HG3 | 2:CE:154:LEU:HB3 | 1.69 | 0.74 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:H6 | 1.52 | 0.74 |
| 45:DV:60:GLU:HA | 45:DV:66:SER:HA | 1.69 | 0.74 |
| 1:CA:407:G:H1 | 1:CA:435:C:H42 | 1.34 | 0.74 |
| 1:AA:1096:C:H2' | 1:AA:1097:C:H6 | 1.53 | 0.74 |
| 39:BR:39:ARG:HG2 | 39:BR:40:THR:H | 1.53 | 0.74 |
| 35:DO:122:PRO:HB3 | 35:DO:141:ALA:HB1 | 1.68 | 0.74 |
| 28:BE:66:HIS:HD1 | 28:BE:66:HIS:C | 1.91 | 0.74 |
| 36:DP:66:ILE:CG1 | 36:DP:67:ARG:H | 1.99 | 0.74 |
| 28:DE:44:TYR:O | 28:DE:45:THR:CB | 2.36 | 0.74 |
| 1:CA:972:C:O3' | 10:CM:57:LYS:HG3 | 1.87 | 0.74 |
| 2:CE:19:HIS:NE2 | 2:CE:206:ASP:HB2 | 2.03 | 0.74 |
| 26:DB:42:C:O2 | 30:DG:93:THR:N | 2.18 | 0.74 |
| 4:CG:3:ARG:NH2 | 4:CG:5:ILE:HG12 | 2.01 | 0.74 |
| 27:DD:68:LYS:HD3 | 27:DD:70:TRP:CZ2 | 2.23 | 0.74 |
| 2:AE:60:ASP:HB3 | 2:AE:64:ARG:HH12 | 1.52 | 0.74 |
| 41:B2:35:LEU:H | 41:B2:35:LEU:HD22 | 1.53 | 0.74 |
| 2:CE:7:VAL:HG22 | 2:CE:8:LYS:H | 1.52 | 0.74 |
| 25:DA:2210:G:H3' | 25:DA:2211:G:C5 | 2.21 | 0.74 |
| 22:CB:44:G:C2' | 22:CB:45:U:H5' | 2.18 | 0.74 |
| 43:DT:63:LYS:O | 43:DT:63:LYS:HD2 | 1.88 | 0.74 |
| 25:DA:2057:A:O2' | 25:DA:2058:A:H5' | 1.88 | 0.74 |
| 30:BG:70:VAL:HG21 | 30:BG:87:PRO:HB3 | 1.69 | 0.74 |
| 47:BZ:58:ILE:CD1 | 47:BZ:86:SER:HB2 | 2.18 | 0.74 |
| 33:DM:47:ALA:HB2 | 33:DM:112:LEU:CD1 | 2.13 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 21:AX:15:ARG:HH11 | 21:AX:15:ARG:CG | 1.98 | 0.74 |
| 25:BA:1139:G:O2' | 25:BA:1143:A:N1 | 2.20 | 0.74 |
| 1:AA:687:A:H4' | 1:AA:688:G:O5' | 1.86 | 0.74 |
| 53:B7:8:ASN:C | 53:B7:8:ASN:ND2 | 2.38 | 0.74 |
| 7:AJ:26:PHE:CE2 | 7:AJ:30:ILE:HD11 | 2.22 | 0.74 |
| 25:BA:336:C:H5'' | 44:BU:6:HIS:HD2 | 1.53 | 0.74 |
| 1:AA:438:G:H4' | 4:AG:123:HIS:CG | 2.23 | 0.74 |
| 30:BG:112:PRO:HB3 | 50:B4:37:SER:CB | 2.17 | 0.74 |
| 52:D6:23:THR:O | 52:D6:24:GLU:HB2 | 1.88 | 0.74 |
| 12:CO:70:ILE:HD13 | 12:CO:77:LEU:HD12 | 1.67 | 0.74 |
| 3:AF:19:GLU:HA | 3:AF:54:ARG:HH12 | 1.52 | 0.74 |
| 25:BA:102:G:OP1 | 48:BW:7:ARG:NH2 | 2.20 | 0.74 |
| 25:DA:2656:U:H3 | 25:DA:2665:A:H2 | 1.35 | 0.74 |
| 5:CH:101:ILE:HD11 | 5:CH:119:LEU:HD23 | 1.70 | 0.74 |
| 23:CC:32:G:C5 | 23:CC:33:C:C5 | 2.76 | 0.73 |
| 14:AQ:23:ARG:HH11 | 14:AQ:23:ARG:HG3 | 1.53 | 0.73 |
| 44:DU:76:CYS:O | 44:DU:78:ALA:N | 2.21 | 0.73 |
| 1:AA:254:G:OP1 | 17:AT:67:LYS:O | 2.06 | 0.73 |
| 30:BG:96:ARG:NH1 | 30:BG:96:ARG:HG2 | 1.97 | 0.73 |
| 38:BQ:36:TYR:HD1 | 38:BQ:36:TYR:N | 1.85 | 0.73 |
| 15:AR:56:LEU:O | 15:AR:60:VAL:HG23 | 1.88 | 0.73 |
| 4:CG:3:ARG:HH11 | 4:CG:115:ARG:HB3 | 1.53 | 0.73 |
| 30:DG:111:LEU:HB3 | 30:DG:117:PHE:HE2 | 1.51 | 0.73 |
| 30:BG:110:ALA:HA | 30:BG:140:ILE:O | 1.87 | 0.73 |
| 1:AA:244:U:H4' | 1:AA:245:C:O5' | 1.86 | 0.73 |
| 2:AE:141:GLU:O | 2:AE:145:LEU:HB2 | 1.88 | 0.73 |
| 1:AA:382:A:H2' | 1:AA:383:A:C8 | 2.22 | 0.73 |
| 25:BA:566:U:OP1 | 35:BO:29:LYS:HE3 | 1.88 | 0.73 |
| 24:A1:13:U:H2' | 24:A1:13:U:O2 | 1.87 | 0.73 |
| 15:AR:70:LEU:HD11 | 15:AR:77:ARG:HG3 | 1.70 | 0.73 |
| 25:BA:2733:A:H2' | 25:BA:2734:A:H5'' | 1.70 | 0.73 |
| 25:DA:2420:C:H41 | 54:D8:31:HIS:CB | 2.01 | 0.73 |
| 28:BE:78:LEU:CD1 | 28:BE:79:ARG:H | 2.00 | 0.73 |
| 38:BQ:85:VAL:HG21 | 38:BQ:112:PHE:CZ | 2.23 | 0.73 |
| 36:DP:66:ILE:HD12 | 36:DP:67:ARG:CA | 2.17 | 0.73 |
| 25:BA:2310:A:C2 | 30:BG:77:ILE:HG13 | 2.21 | 0.73 |
| 41:D2:71:LEU:CA | 41:D2:86:GLY:HA2 | 2.17 | 0.73 |
| 28:BE:38:THR:CB | 28:BE:39:PRO:HD2 | 2.18 | 0.73 |
| 31:DH:125:VAL:HG22 | 31:DH:126:PRO:CD | 2.06 | 0.73 |
| 25:DA:1300:U:H4' | 25:DA:1301:A:H5'' | 1.70 | 0.73 |
| 35:BO:50:ARG:HH21 | 35:BO:50:ARG:CG | 2.01 | 0.73 |
| 25:DA:1952:A:C6 | 34:DN:22:ILE:CD1 | 2.71 | 0.73 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 29:BF:67:GLN:HG3 | 29:BF:67:GLN:O | 1.86 | 0.73 |
| 25:DA:1597:A:H5'' | 25:DA:1598:C:OP1 | 1.88 | 0.73 |
| 17:AT:45:HIS:O | 17:AT:73:VAL:HG23 | 1.87 | 0.73 |
| 52:D6:35:GLU:O | 52:D6:36:LEU:HB2 | 1.89 | 0.73 |
| 25:DA:287:C:H2' | 25:DA:288:C:H6 | 1.51 | 0.73 |
| 32:DK:101:LEU:H | 32:DK:101:LEU:HD23 | 1.53 | 0.73 |
| 25:BA:1165:U:H2' | 25:BA:1166:C:H6 | 1.53 | 0.73 |
| 28:BE:41:LYS:NZ | 28:BE:41:LYS:HB2 | 2.03 | 0.73 |
| 36:DP:75:THR:CB | 36:DP:88:GLY:HA3 | 2.16 | 0.73 |
| 26:BB:37:C:C2' | 26:BB:38:C:H5' | 2.18 | 0.73 |
| 25:BA:2690:C:H5'' | 25:BA:2872:G:N2 | 2.03 | 0.73 |
| 45:BV:152:ALA:HB3 | 45:BV:167:PRO:O | 1.88 | 0.73 |
| 25:DA:1126:A:H4' | 25:DA:1127:A:O5' | 1.88 | 0.73 |
| 29:DF:82:ILE:HD12 | 29:DF:82:ILE:C | 2.09 | 0.73 |
| 1:AA:250:A:H4' | 1:AA:251:G:C5' | 2.18 | 0.73 |
| 9:CL:79:LEU:HD13 | 9:CL:83:ARG:HD2 | 1.68 | 0.73 |
| 52:D6:31:PRO:HB2 | 52:D6:33:LYS:HB2 | 1.70 | 0.73 |
| 25:BA:2310:A:H2' | 25:BA:2311:A:H5'' | 1.70 | 0.73 |
| 1:CA:1028:C:H42 | 1:CA:1033:G:H1 | 1.35 | 0.73 |
| 35:BO:15:ARG:CB | 35:BO:15:ARG:HH11 | 2.01 | 0.73 |
| 26:DB:39:A:C6 | 50:D4:1:MET:HB3 | 2.22 | 0.73 |
| 20:AW:100:ILE:HG13 | 20:AW:101:GLY:N | 2.03 | 0.73 |
| 16:CS:5:ARG:NH1 | 16:CS:22:THR:HG21 | 2.03 | 0.73 |
| 41:B2:44:LYS:CD | 41:B2:45:THR:H | 1.99 | 0.73 |
| 29:BF:32:LEU:O | 29:BF:32:LEU:HD12 | 1.88 | 0.73 |
| 25:BA:1298:C:H5'' | 25:BA:1299:G:OP2 | 1.88 | 0.73 |
| 25:BA:654(A):A:H2 | 25:BA:654(T):A:N1 | 1.87 | 0.73 |
| 54:D8:60:LEU:C | 54:D8:61:LEU:HG | 2.08 | 0.73 |
| 2:CE:132:LYS:HA | 2:CE:135:GLN:HB2 | 1.69 | 0.73 |
| 10:AM:55:LYS:HB3 | 10:AM:55:LYS:NZ | 2.03 | 0.73 |
| 42:DS:65:LEU:HD13 | 42:DS:68:ARG:CD | 2.17 | 0.73 |
| 1:AA:1251:A:H4' | 9:AL:12:GLU:OE1 | 1.88 | 0.73 |
| 25:DA:598:G:H1' | 35:DO:12:ALA:HB2 | 1.70 | 0.73 |
| 30:DG:112:PRO:HB2 | 50:D4:37:SER:HA | 1.71 | 0.73 |
| 25:BA:1210:A:H8 | 25:BA:1210:A:H5' | 1.52 | 0.73 |
| 33:BM:58:ASP:H | 33:BM:60:ILE:HD11 | 1.54 | 0.73 |
| 1:AA:280:C:H3' | 1:AA:281:G:H5' | 1.70 | 0.73 |
| 1:CA:1346:A:H1' | 1:CA:1347:G:OP2 | 1.88 | 0.73 |
| 25:DA:205:G:H1' | 25:DA:206:U:OP2 | 1.88 | 0.73 |
| 50:B4:52:THR:OG1 | 50:B4:53:GLU:N | 2.21 | 0.73 |
| 40:D1:65:ILE:HD11 | 40:D1:96:ALA:CB | 2.18 | 0.73 |
| 29:DF:68:LYS:HZ3 | 29:DF:68:LYS:HA | 1.53 | 0.73 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 28:DE:47:VAL:HG11 | 28:DE:49:LEU:HD23 | 1.71 | 0.73 |
| 26:BB:15:A:OP1 | 26:BB:15:A:H4' | 1.88 | 0.73 |
| 25:DA:1070:A:H5' | 25:DA:1071:G:C5' | 2.18 | 0.73 |
| 33:DM:97:ARG:NH1 | 33:DM:97:ARG:HG2 | 1.95 | 0.73 |
| 15:AR:55:GLY:HA2 | 15:AR:58:MET:HE2 | 1.70 | 0.73 |
| 36:DP:3:MET:HB2 | 36:DP:93:TYR:CD1 | 2.24 | 0.73 |
| 47:DZ:78:LYS:HD2 | 47:DZ:78:LYS:O | 1.89 | 0.73 |
| 25:BA:1063:G:H1 | 25:BA:1075:C:H42 | 1.36 | 0.73 |
| 33:DM:47:ALA:CB | 33:DM:112:LEU:HD11 | 2.12 | 0.73 |
| 29:DF:83:PHE:C | 29:DF:84:VAL:CG1 | 2.57 | 0.73 |
| 9:AL:5:TYR:HE2 | 9:AL:16:ARG:HG2 | 1.54 | 0.73 |
| 1:CA:972:C:H4' | 10:CM:57:LYS:HG3 | 1.71 | 0.73 |
| 52:D6:52:VAL:HG22 | 52:D6:53:LYS:HG3 | 1.71 | 0.73 |
| 1:AA:606:G:H22 | 1:AA:631:G:H8 | 1.36 | 0.73 |
| 25:DA:2343:C:O2' | 25:DA:2373:G:O2' | 2.05 | 0.73 |
| 25:BA:2562:U:H1' | 34:BN:23:ARG:HH11 | 1.51 | 0.73 |
| 1:AA:530:G:H4' | 1:AA:531:U:OP2 | 1.87 | 0.73 |
| 25:BA:2393:A:H5' | 35:BO:62:LEU:CB | 2.19 | 0.73 |
| 25:DA:1826:G:H4' | 27:DD:242:ARG:NH2 | 2.01 | 0.73 |
| 25:DA:2127:G:H21 | 25:DA:2173:A:H8 | 1.37 | 0.73 |
| 35:DO:88:LEU:HD11 | 35:DO:95:VAL:HG21 | 1.71 | 0.73 |
| 43:DT:60:ARG:HH11 | 43:DT:60:ARG:CG | 2.01 | 0.73 |
| 4:AG:5:ILE:HG22 | 4:AG:6:GLY:N | 2.01 | 0.73 |
| 25:DA:2531:A:H5' | 31:DH:157:TYR:HE2 | 1.52 | 0.73 |
| 1:CA:353:A:H5' | 1:CA:353:A:H8 | 1.52 | 0.73 |
| 41:B2:66:ARG:NH1 | 41:B2:88:ARG:HD3 | 2.04 | 0.73 |
| 36:BP:30:GLY:CA | 36:BP:107:ALA:HB2 | 2.18 | 0.73 |
| 25:DA:228:A:H3' | 25:DA:228:A:H8 | 1.53 | 0.73 |
| 27:BD:35:LYS:HA | 27:BD:64:ILE:HG22 | 1.71 | 0.73 |
| 28:DE:47:VAL:HG13 | 28:DE:48:GLN:H | 1.53 | 0.73 |
| 1:CA:1199:U:H4' | 10:CM:54:PHE:CE1 | 2.23 | 0.73 |
| 10:CM:54:PHE:CD2 | 10:CM:55:LYS:HD2 | 2.24 | 0.73 |
| 33:BM:133:GLN:NE2 | 33:BM:133:GLN:H | 1.87 | 0.73 |
| 5:AH:10:MET:SD | 5:AH:13:ILE:HD13 | 2.29 | 0.73 |
| 1:AA:200:G:N2 | 1:AA:218:C:O2 | 2.22 | 0.73 |
| 3:CF:35:GLU:HG3 | 3:CF:38:ARG:HH21 | 1.54 | 0.73 |
| 1:CA:1392:G:H21 | 1:CA:1502:A:H8 | 1.36 | 0.73 |
| 25:BA:49:A:C8 | 25:BA:120:U:C5 | 2.74 | 0.73 |
| 36:DP:33:GLY:HA2 | 36:DP:105:GLU:HB2 | 1.70 | 0.73 |
| 41:D2:70:ILE:O | 41:D2:71:LEU:HB2 | 1.88 | 0.73 |
| 28:DE:5:LEU:HD21 | 28:DE:79:ARG:HB2 | 1.70 | 0.73 |
| 39:BR:74:ARG:HD3 | 39:BR:76:PHE:CZ | 2.24 | 0.73 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:527:C:OP2 | 25:DA:2779:U:H5 | 1.71 | 0.73 |
| 16:CS:8:ARG:HH11 | 16:CS:8:ARG:HG2 | 1.53 | 0.73 |
| 25:DA:864:G:C6 | 25:DA:865:C:N4 | 2.56 | 0.73 |
| 32:BK:125:GLU:OE1 | 32:BK:141:LYS:HB3 | 1.89 | 0.73 |
| 2:AE:60:ASP:HB3 | 2:AE:64:ARG:NH1 | 2.03 | 0.73 |
| 22:CB:55:G:H2' | 22:CB:56:G:H8 | 1.53 | 0.73 |
| 46:B3:83:PRO:O | 46:B3:84:LEU:HB2 | 1.87 | 0.73 |
| 5:CH:143:ARG:NH1 | 8:CK:77:GLU:OE1 | 2.22 | 0.73 |
| 23:AD:21:U:H3' | 23:AD:22:A:C5' | 2.19 | 0.73 |
| 27:BD:69:ARG:NH2 | 27:BD:128:GLY:O | 2.22 | 0.73 |
| 1:AA:156:G:H1 | 1:AA:165:C:H42 | 1.37 | 0.73 |
| 1:CA:498:A:H4' | 1:CA:500:G:OP1 | 1.87 | 0.73 |
| 36:DP:64:ILE:HD13 | 36:DP:64:ILE:N | 2.01 | 0.72 |
| 28:BE:27:LEU:HD13 | 39:BR:1:MET:HE2 | 1.69 | 0.72 |
| 23:CD:7:G:H3' | 23:CD:8:U:H5' | 1.71 | 0.72 |
| 1:CA:250:A:H4' | 1:CA:251:G:O5' | 1.88 | 0.72 |
| 25:BA:559:G:H22 | 40:B1:49:HIS:CD2 | 2.06 | 0.72 |
| 25:BA:2068:U:N3 | 25:BA:2430:A:C2 | 2.53 | 0.72 |
| 12:CO:8:ASN:HD22 | 17:CT:34:LYS:HE2 | 1.54 | 0.72 |
| 25:BA:1204:A:C2 | 25:BA:1241:A:N1 | 2.57 | 0.72 |
| 25:BA:1062:G:H2' | 25:BA:1063:G:C8 | 2.23 | 0.72 |
| 27:DD:35:LYS:CE | 27:DD:64:ILE:O | 2.37 | 0.72 |
| 27:BD:64:ILE:O | 27:BD:64:ILE:HG12 | 1.87 | 0.72 |
| 25:DA:2681:C:H2' | 25:DA:2681:C:O2 | 1.88 | 0.72 |
| 28:DE:52:LEU:O | 28:DE:74:PRO:CA | 2.36 | 0.72 |
| 1:AA:1036:G:H3' | 1:AA:1037:C:C6 | 2.24 | 0.72 |
| 25:DA:1012:U:C5 | 33:DM:28:THR:HG21 | 2.23 | 0.72 |
| 25:DA:2128:C:H4' | 25:DA:2173:A:N6 | 2.04 | 0.72 |
| 1:AA:523:A:H61 | 12:AO:92:ASP:HB2 | 1.54 | 0.72 |
| 25:BA:1903:G:OP1 | 27:BD:241:PRO:HB2 | 1.89 | 0.72 |
| 25:DA:1839:G:C8 | 25:DA:1927:A:H1' | 2.24 | 0.72 |
| 41:D2:70:ILE:O | 41:D2:71:LEU:CB | 2.36 | 0.72 |
| 27:BD:34:VAL:O | 27:BD:34:VAL:HG13 | 1.89 | 0.72 |
| 25:DA:1188:U:O2' | 25:DA:1189:A:H5' | 1.88 | 0.72 |
| 1:CA:1321:C:H3' | 1:CA:1322:C:H5'' | 1.71 | 0.72 |
| 43:DT:50:LYS:H | 43:DT:87:GLN:HE22 | 1.35 | 0.72 |
| 29:DF:31:HIS:CB | 35:DO:9:ASN:OD1 | 2.37 | 0.72 |
| 25:DA:1278:A:O2' | 37:D0:34:ILE:HD11 | 1.89 | 0.72 |
| 25:DA:2219:G:H2' | 25:DA:2224:G:H5' | 1.71 | 0.72 |
| 38:DQ:58:LEU:HD12 | 38:DQ:65:VAL:HG22 | 1.72 | 0.72 |
| 31:DH:154:PRO:O | 31:DH:155:SER:HB3 | 1.89 | 0.72 |
| 1:AA:57:G:H2' | 1:AA:58:C:C6 | 2.23 | 0.72 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 36:DP:75:THR:HG21 | 36:DP:87:LYS:CE | 2.18 | 0.72 |
| 22:CB:87:A:H8 | 25:DA:2583:G:N2 | 1.83 | 0.72 |
| 25:DA:545:G:H21 | 25:DA:548:A:N6 | 1.86 | 0.72 |
| 1:CA:235:C:C5' | 17:CT:70:ARG:HG2 | 2.18 | 0.72 |
| 35:DO:36:LYS:HB2 | 35:DO:36:LYS:NZ | 2.02 | 0.72 |
| 25:DA:832:G:H5' | 35:DO:45:LEU:HD11 | 1.71 | 0.72 |
| 33:BM:133:GLN:HE21 | 33:BM:133:GLN:H | 1.37 | 0.72 |
| 25:DA:1864:U:C2' | 25:DA:1869:G:H5'' | 2.20 | 0.72 |
| 31:BH:86:GLU:HG3 | 31:BH:165:ALA:HB2 | 1.72 | 0.72 |
| 45:DV:105:VAL:HG22 | 45:DV:106:GLY:H | 1.52 | 0.72 |
| 25:DA:195:A:OP1 | 35:DO:46:LYS:CE | 2.36 | 0.72 |
| 1:CA:1005:A:C2 | 1:CA:1006:C:H1' | 2.24 | 0.72 |
| 45:BV:76:LEU:HD23 | 45:BV:76:LEU:H | 1.54 | 0.72 |
| 25:DA:1156:A:OP1 | 40:D1:55:ARG:NH1 | 2.22 | 0.72 |
| 30:BG:72:ARG:HH21 | 30:BG:87:PRO:HD3 | 1.54 | 0.72 |
| 27:BD:34:VAL:HG22 | 27:BD:35:LYS:HG3 | 1.72 | 0.72 |
| 25:DA:1342:A:C2 | 25:DA:1602:U:N3 | 2.57 | 0.72 |
| 40:B1:92:ARG:HD3 | 40:B1:94:ASN:HB3 | 1.72 | 0.72 |
| 25:DA:71:A:OP2 | 25:DA:71:A:H3' | 1.89 | 0.72 |
| 25:DA:2131:G:OP1 | 25:DA:2132:U:H3' | 1.89 | 0.72 |
| 23:AD:57:C:N3 | 25:BA:2112:G:N2 | 2.36 | 0.72 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:H1 | 1.38 | 0.72 |
| 25:DA:511:U:H3' | 25:DA:512:G:H5'' | 1.72 | 0.72 |
| 1:CA:748:C:H4' | 1:CA:749:C:O5' | 1.87 | 0.72 |
| 19:AV:50:ALA:HB1 | 19:AV:57:HIS:HB3 | 1.70 | 0.72 |
| 25:BA:518:G:H4' | 42:BS:18:ARG:HH11 | 1.53 | 0.72 |
| 1:AA:625:G:C5' | 16:AS:16:HIS:HD2 | 2.03 | 0.72 |
| 47:BZ:85:LEU:CA | 47:BZ:87:PRO:HD2 | 2.19 | 0.72 |
| 25:DA:2287:A:N1 | 25:DA:2346:A:C2 | 2.58 | 0.72 |
| 33:BM:46:VAL:O | 33:BM:47:ALA:HB3 | 1.89 | 0.72 |
| 52:B6:15:GLU:HG2 | 52:B6:16:CYS:N | 2.05 | 0.72 |
| 4:CG:13:ARG:CG | 4:CG:14:ARG:H | 1.93 | 0.72 |
| 25:DA:888:C:H4' | 25:DA:889:C:C5' | 2.20 | 0.72 |
| 34:BN:67:LYS:HE3 | 34:BN:68:GLU:OE1 | 1.88 | 0.72 |
| 1:AA:731:G:OP1 | 1:AA:766:A:H1' | 1.90 | 0.72 |
| 33:BM:46:VAL:HG13 | 33:BM:47:ALA:N | 2.05 | 0.72 |
| 44:BU:78:ALA:HB3 | 44:BU:81:LYS:NZ | 2.03 | 0.72 |
| 25:BA:2402:C:HO2' | 25:BA:2403:C:P | 2.12 | 0.72 |
| 25:DA:2185:C:H2' | 25:DA:2186:G:C8 | 2.24 | 0.72 |
| 49:DX:19:GLN:HE22 | 49:DX:52:HIS:CE1 | 2.07 | 0.72 |
| 36:BP:30:GLY:HA2 | 36:BP:107:ALA:HB2 | 1.72 | 0.72 |
| 1:AA:143:A:H2 | 1:AA:220:G:H1 | 1.37 | 0.72 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 4:AG:81:GLU:OE1 | 4:AG:139:ARG:NH2 | 2.22 | 0.72 |
| 25:DA:1416:G:O2' | 25:DA:1417:C:O5' | 2.06 | 0.72 |
| 30:BG:104:GLU:CD | 50:B4:23:GLU:HG3 | 2.10 | 0.72 |
| 1:AA:977:A:C8 | 1:AA:1223:C:C4 | 2.78 | 0.72 |
| 25:BA:847:U:C5 | 25:BA:933:A:N1 | 2.57 | 0.72 |
| 1:AA:1423:G:OP1 | 34:BN:49:ARG:NH2 | 2.21 | 0.72 |
| 19:CV:78:ARG:HD3 | 19:CV:79:THR:H | 1.53 | 0.72 |
| 25:BA:1991:U:H2' | 25:BA:1992:G:H5'' | 1.71 | 0.72 |
| 40:D1:92:ARG:HD3 | 40:D1:94:ASN:HB3 | 1.71 | 0.72 |
| 52:B6:30:THR:HA | 52:B6:31:PRO:C | 2.10 | 0.72 |
| 1:CA:973:G:OP1 | 10:CM:57:LYS:NZ | 2.23 | 0.72 |
| 31:BH:159:GLU:HG2 | 31:BH:170:ARG:NH1 | 2.05 | 0.72 |
| 1:AA:1497:G:C2' | 1:AA:1498:U:H5' | 2.20 | 0.72 |
| 54:B8:37:SER:HA | 54:B8:41:ILE:HG21 | 1.72 | 0.72 |
| 25:BA:1141:U:H6 | 33:BM:63:THR:OG1 | 1.71 | 0.72 |
| 25:BA:2157:G:O2' | 25:BA:2158:A:O5' | 2.07 | 0.72 |
| 3:CF:130:VAL:O | 3:CF:134:ILE:HG12 | 1.89 | 0.72 |
| 30:BG:112:PRO:HB3 | 50:B4:37:SER:HB2 | 1.72 | 0.72 |
| 1:CA:421:U:H5'' | 1:CA:422:C:OP2 | 1.89 | 0.72 |
| 30:BG:109:VAL:HG13 | 50:B4:33:VAL:HG21 | 1.71 | 0.72 |
| 25:DA:239:U:H5'' | 25:DA:239:U:H6 | 1.55 | 0.72 |
| 1:AA:503:C:OP1 | 12:AO:119:LYS:HE2 | 1.90 | 0.72 |
| 30:BG:73:ALA:CB | 30:BG:82:LEU:HD21 | 2.18 | 0.72 |
| 28:DE:79:ARG:O | 28:DE:80:GLU:CB | 2.37 | 0.72 |
| 25:DA:1342:A:N1 | 25:DA:1602:U:C2 | 2.57 | 0.72 |
| 35:BO:64:LYS:HD2 | 54:B8:25:MET:SD | 2.27 | 0.72 |
| 23:CD:54:G:H2' | 23:CD:55:U:C6 | 2.24 | 0.72 |
| 30:DG:37:VAL:O | 30:DG:94:LEU:HD23 | 1.90 | 0.72 |
| 25:BA:1473:G:C2' | 25:BA:1474:C:H5' | 2.20 | 0.72 |
| 1:AA:501:C:H2' | 1:AA:502:G:C8 | 2.25 | 0.72 |
| 1:CA:191:G:O2' | 20:CW:103:GLY:HA2 | 1.90 | 0.72 |
| 6:AI:14:LEU:HD22 | 6:AI:18:GLN:NE2 | 2.05 | 0.72 |
| 25:DA:148:C:C5' | 25:DA:148:C:H6 | 2.02 | 0.72 |
| 1:AA:376:G:H5'' | 16:AS:5:ARG:HD2 | 1.69 | 0.72 |
| 45:DV:138:GLU:O | 45:DV:156:LYS:HG3 | 1.89 | 0.72 |
| 7:CJ:97:GLN:HE21 | 7:CJ:101:LEU:HD11 | 1.55 | 0.72 |
| 28:BE:19:ARG:NH1 | 34:BN:72:PRO:CG | 2.53 | 0.71 |
| 25:BA:2439:A:C5' | 25:BA:2439:A:C8 | 2.73 | 0.71 |
| 1:CA:560:U:HO2' | 1:CA:561:U:P | 2.11 | 0.71 |
| 25:BA:2119:A:H61 | 25:BA:2170:A:N6 | 1.88 | 0.71 |
| 33:BM:131:GLN:NE2 | 33:BM:132:ALA:H | 1.88 | 0.71 |
| 8:CK:20:TYR:CE2 | 8:CK:75:ARG:HD2 | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 9:CL:125:TYR:HD2 | 9:CL:126:SER:N | 1.87 | 0.71 |
| 12:CO:32:PHE:HB3 | 12:CO:84:LEU:CD2 | 2.20 | 0.71 |
| 18:CU:22:VAL:HG13 | 18:CU:56:THR:HA | 1.71 | 0.71 |
| 25:DA:323:G:HO2' | 25:DA:1205:U:H3 | 1.35 | 0.71 |
| 23:CD:64:G:H2' | 23:CD:65:G:C8 | 2.25 | 0.71 |
| 25:BA:2467:C:O2' | 25:BA:2468:G:H5' | 1.90 | 0.71 |
| 27:BD:35:LYS:HZ1 | 27:BD:65:ILE:HA | 1.55 | 0.71 |
| 1:CA:973:G:N3 | 10:CM:55:LYS:HE2 | 2.05 | 0.71 |
| 39:DR:93:ARG:HG2 | 39:DR:117:ASP:CB | 2.19 | 0.71 |
| 25:BA:654:A:H2' | 25:BA:654:A:N3 | 2.04 | 0.71 |
| 25:BA:314:A:H2' | 25:BA:315:G:H5' | 1.72 | 0.71 |
| 44:DU:61:ILE:HG22 | 44:DU:62:GLU:H | 1.55 | 0.71 |
| 36:DP:83:MET:SD | 36:DP:83:MET:N | 2.63 | 0.71 |
| 25:DA:2748:A:C8 | 25:DA:2754:U:O4 | 2.42 | 0.71 |
| 4:AG:122:ARG:HG2 | 4:AG:122:ARG:NH1 | 1.98 | 0.71 |
| 2:CE:71:VAL:HG11 | 2:CE:97:TRP:HD1 | 1.54 | 0.71 |
| 25:DA:598:G:C1' | 35:DO:12:ALA:HB2 | 2.21 | 0.71 |
| 45:DV:87:ASP:OD2 | 45:DV:87:ASP:N | 2.22 | 0.71 |
| 50:B4:37:SER:HB3 | 50:B4:42:PHE:CD1 | 2.25 | 0.71 |
| 23:AC:1:C:H2' | 23:AC:2:G:OP2 | 1.90 | 0.71 |
| 25:BA:2689:U:H4' | 25:BA:2690:C:H5' | 1.71 | 0.71 |
| 49:BX:31:LEU:O | 49:BX:32:GLN:HB2 | 1.88 | 0.71 |
| 8:AK:25:ASP:OD2 | 8:AK:60:ARG:HG2 | 1.91 | 0.71 |
| 25:DA:2839:G:H5' | 37:D0:46:GLY:HA2 | 1.72 | 0.71 |
| 23:CC:43:G:H2' | 23:CC:44:A:H8 | 1.56 | 0.71 |
| 25:DA:2611:U:H5' | 25:DA:2611:U:H6 | 1.55 | 0.71 |
| 26:BB:43:C:OP1 | 30:BG:67:LYS:NZ | 2.24 | 0.71 |
| 25:BA:905:U:C2' | 25:BA:906:G:H5'' | 2.21 | 0.71 |
| 1:CA:1300:G:O2' | 1:CA:1301:U:O5' | 2.07 | 0.71 |
| 51:B5:33:CYS:SG | 51:B5:40:LYS:NZ | 2.61 | 0.71 |
| 15:CR:87:ILE:CG2 | 15:CR:88:ARG:H | 2.03 | 0.71 |
| 47:DZ:4:VAL:HG12 | 47:DZ:11:ARG:HB3 | 1.72 | 0.71 |
| 29:DF:34:TRP:CZ3 | 35:DO:8:PRO:HB3 | 2.24 | 0.71 |
| 31:BH:115:VAL:O | 31:BH:115:VAL:HG12 | 1.90 | 0.71 |
| 25:DA:12:U:O2 | 25:DA:12:U:H2' | 1.90 | 0.71 |
| 22:AB:56:G:H2' | 22:AB:57:C:H6 | 1.55 | 0.71 |
| 25:BA:2682:U:O2' | 39:BR:58:ASN:OD1 | 2.07 | 0.71 |
| 3:AF:58:GLU:HB2 | 3:AF:65:ALA:CB | 2.20 | 0.71 |
| 13:CP:110:ARG:CG | 13:CP:110:ARG:HH11 | 2.04 | 0.71 |
| 1:AA:353:A:H8 | 1:AA:353:A:H5' | 1.55 | 0.71 |
| 28:DE:79:ARG:O | 28:DE:80:GLU:HB2 | 1.89 | 0.71 |
| 3:CF:180:ALA:HB1 | 3:CF:203:PHE:HE1 | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 47:DZ:92:LYS:HE2 | 47:DZ:93:GLU:H | 1.54 | 0.71 |
| 9:AL:112:LYS:HA | 9:AL:119:ALA:HB2 | 1.71 | 0.71 |
| 25:DA:531:C:H4' | 25:DA:532:A:H5'' | 1.71 | 0.71 |
| 13:AP:15:VAL:HG23 | 13:AP:43:THR:O | 1.90 | 0.71 |
| 17:CT:67:LYS:HA | 17:CT:70:ARG:HH12 | 1.55 | 0.71 |
| 23:AD:57:C:N4 | 25:BA:2112:G:H1 | 1.88 | 0.71 |
| 45:DV:108:PRO:HA | 45:DV:143:GLY:N | 2.04 | 0.71 |
| 25:DA:2321:G:H2' | 25:DA:2321:G:N3 | 2.04 | 0.71 |
| 2:AE:84:GLU:HB3 | 2:AE:219:VAL:HG21 | 1.72 | 0.71 |
| 25:DA:654(R):C:N4 | 25:DA:654(S):G:O6 | 2.24 | 0.71 |
| 1:AA:1450:U:HO2' | 1:AA:1451:A:H8 | 1.37 | 0.71 |
| 1:CA:1285:A:H4' | 1:CA:1286:A:O5' | 1.91 | 0.71 |
| 1:AA:1346:A:H5'' | 9:AL:120:ARG:NH1 | 2.04 | 0.71 |
| 25:BA:873:G:H1 | 25:BA:904:C:H42 | 1.38 | 0.71 |
| 38:DQ:14:VAL:HG21 | 38:DQ:89:ARG:CG | 2.21 | 0.71 |
| 38:DQ:11:LYS:O | 38:DQ:15:ARG:HB2 | 1.90 | 0.71 |
| 27:BD:35:LYS:HE3 | 27:BD:64:ILE:C | 2.11 | 0.71 |
| 41:D2:76:LYS:HB3 | 41:D2:79:VAL:CG2 | 2.16 | 0.71 |
| 27:DD:25:THR:O | 27:DD:27:THR:N | 2.23 | 0.71 |
| 10:CM:54:PHE:CE2 | 10:CM:55:LYS:HD2 | 2.26 | 0.71 |
| 1:CA:509:A:O2' | 1:CA:510:A:OP1 | 2.09 | 0.71 |
| 30:DG:60:LEU:O | 30:DG:64:THR:HG22 | 1.91 | 0.71 |
| 26:DB:111:U:H2' | 26:DB:112:G:C8 | 2.26 | 0.71 |
| 13:AP:108:ARG:HG3 | 13:AP:108:ARG:NH1 | 2.01 | 0.71 |
| 26:BB:28:C:OP1 | 38:BQ:36:TYR:OH | 2.06 | 0.71 |
| 30:DG:117:PHE:CD1 | 30:DG:118:ARG:O | 2.43 | 0.71 |
| 26:DB:83:G:H1 | 26:DB:93:C:H42 | 1.36 | 0.71 |
| 3:CF:63:ASN:HB3 | 3:CF:98:ASN:HB3 | 1.73 | 0.71 |
| 28:BE:51:PHE:O | 28:BE:74:PRO:CB | 2.39 | 0.71 |
| 1:AA:1004:A:H5'' | 1:AA:1025:U:C4 | 2.26 | 0.71 |
| 25:BA:2211:G:H4' | 25:BA:2212:A:OP2 | 1.90 | 0.71 |
| 25:DA:152:G:H1 | 25:DA:174:C:N4 | 1.88 | 0.71 |
| 25:BA:2032:G:H21 | 28:BE:146:THR:CG2 | 2.04 | 0.71 |
| 28:BE:119:ARG:HD3 | 28:BE:160:TYR:HB2 | 1.73 | 0.71 |
| 1:CA:1372:U:OP1 | 9:CL:72:GLY:N | 2.24 | 0.71 |
| 47:BZ:65:SER:OG | 47:BZ:66:HIS:HD2 | 1.73 | 0.71 |
| 1:CA:1451:A:OP2 | 1:CA:1452:C:N4 | 2.23 | 0.71 |
| 26:BB:3:C:H2' | 26:BB:4:C:H6 | 1.54 | 0.71 |
| 1:CA:828:A:H5'' | 1:CA:859:A:C2 | 2.26 | 0.71 |
| 1:CA:827:U:H3 | 1:CA:872:A:H62 | 1.36 | 0.71 |
| 25:DA:2446:G:H2' | 25:DA:2447:G:H5'' | 1.72 | 0.71 |
| 27:DD:43:ARG:HD2 | 27:DD:44:ASN:ND2 | 2.06 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 16:AS:23:ASP:OD1 | 16:AS:25:ARG:HG2 | 1.91 | 0.71 |
| 28:BE:35:GLN:CG | 28:BE:36:ARG:H | 2.02 | 0.71 |
| 45:BV:6:LYS:CA | 45:BV:60:GLU:HB2 | 2.20 | 0.71 |
| 31:DH:4:ILE:HB | 31:DH:6:ARG:NH1 | 2.06 | 0.71 |
| 25:DA:528:A:H8 | 25:DA:528:A:H3' | 1.56 | 0.71 |
| 31:BH:151:ILE:O | 31:BH:153:LYS:HD2 | 1.88 | 0.71 |
| 25:DA:2068:U:N3 | 25:DA:2430:A:H2 | 1.87 | 0.71 |
| 19:CV:28:LYS:HE3 | 19:CV:29:ARG:H | 1.55 | 0.71 |
| 28:BE:2:LYS:HD3 | 28:BE:95:ILE:HG22 | 1.72 | 0.71 |
| 10:AM:24:VAL:HG21 | 10:AM:37:PRO:HD3 | 1.73 | 0.71 |
| 23:CD:42:C:H2' | 23:CD:43:G:H8 | 1.55 | 0.71 |
| 36:DP:23:GLY:HA2 | 36:DP:25:ASP:HB2 | 1.73 | 0.71 |
| 33:DM:45:ASN:O | 33:DM:46:VAL:CG2 | 2.36 | 0.71 |
| 28:BE:35:GLN:NE2 | 28:BE:37:ARG:NH1 | 2.38 | 0.71 |
| 31:BH:83:TYR:HB3 | 31:BH:135:GLY:N | 2.03 | 0.71 |
| 30:DG:67:LYS:HD2 | 50:D4:6:HIS:HE2 | 1.55 | 0.71 |
| 25:DA:887:A:H3' | 25:DA:888:C:H5' | 1.73 | 0.71 |
| 1:AA:686:U:O4 | 1:AA:703:G:H1' | 1.91 | 0.71 |
| 2:CE:92:TYR:CE2 | 2:CE:151:GLY:HA3 | 2.26 | 0.71 |
| 23:AD:15:G:N2 | 23:AD:49:C:O2 | 2.21 | 0.71 |
| 10:CM:22:LYS:HD2 | 10:CM:26:ALA:HB2 | 1.73 | 0.71 |
| 36:DP:21:THR:CG2 | 36:DP:21:THR:O | 2.38 | 0.71 |
| 31:BH:138:LYS:HA | 31:BH:141:VAL:HB | 1.73 | 0.71 |
| 25:BA:270(L):U:H2' | 25:BA:270(L):U:O2 | 1.90 | 0.71 |
| 4:AG:170:VAL:HG22 | 4:AG:171:GLY:H | 1.56 | 0.71 |
| 36:DP:27:VAL:CG1 | 36:DP:105:GLU:OE2 | 2.35 | 0.71 |
| 25:DA:517:C:OP1 | 51:D5:16:ARG:NH2 | 2.22 | 0.71 |
| 25:DA:1899:G:N2 | 25:DA:1902:C:H41 | 1.88 | 0.71 |
| 13:CP:39:ILE:HD13 | 13:CP:52:GLU:HB3 | 1.73 | 0.71 |
| 25:DA:885:C:C4 | 25:DA:890:A:C6 | 2.79 | 0.71 |
| 25:DA:71:A:C2 | 43:DT:31:HIS:HE1 | 2.09 | 0.71 |
| 25:DA:2119:A:N6 | 25:DA:2170:A:N7 | 2.38 | 0.71 |
| 25:BA:1359:A:H2 | 25:BA:1372:U:O4 | 1.73 | 0.71 |
| 8:AK:87:SER:HB2 | 8:AK:93:VAL:CB | 2.20 | 0.71 |
| 25:DA:2337:G:H5'' | 25:DA:2338:G:OP2 | 1.89 | 0.71 |
| 43:DT:63:LYS:HE3 | 43:DT:63:LYS:H | 1.55 | 0.71 |
| 23:AD:8:U:H3 | 23:AD:14:A:H62 | 1.38 | 0.71 |
| 23:CC:1:C:C2' | 23:CC:2:G:OP2 | 2.39 | 0.71 |
| 23:CD:21:U:H2' | 23:CD:22:A:H5'' | 1.73 | 0.71 |
| 45:BV:45:ASP:O | 45:BV:49:ARG:HG2 | 1.89 | 0.71 |
| 13:CP:55:ARG:HG3 | 13:CP:55:ARG:HH11 | 1.56 | 0.71 |
| 1:AA:484:G:O2' | 1:AA:485:G:OP2 | 2.05 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 44:BU:87:LYS:HD2 | 44:BU:92:ASN:HB3 | 1.73 | 0.71 |
| 35:DO:19:VAL:HG22 | 35:DO:27:HIS:HB3 | 1.68 | 0.70 |
| 25:DA:2371:G:O4' | 52:D6:45:LYS:CE | 2.31 | 0.70 |
| 28:BE:48:GLN:O | 28:BE:49:LEU:CB | 2.34 | 0.70 |
| 28:BE:14:ILE:HB | 28:BE:21:VAL:HG23 | 1.71 | 0.70 |
| 45:DV:175:VAL:CG2 | 45:DV:176:PRO:HD3 | 2.21 | 0.70 |
| 1:CA:963:G:HO2' | 10:CM:54:PHE:HZ | 1.39 | 0.70 |
| 29:BF:103:LYS:HA | 29:BF:106:ARG:HG3 | 1.71 | 0.70 |
| 36:BP:104:PHE:HE1 | 36:BP:125:LEU:HD11 | 1.54 | 0.70 |
| 32:DK:82:ARG:HB3 | 32:DK:89:TYR:HD2 | 1.55 | 0.70 |
| 9:CL:20:ARG:O | 9:CL:60:ASP:HB2 | 1.91 | 0.70 |
| 25:BA:2402:C:H2' | 25:BA:2403:C:H5' | 1.73 | 0.70 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:N6 | 1.89 | 0.70 |
| 33:DM:15:LEU:HB2 | 33:DM:134:ARG:HG2 | 1.71 | 0.70 |
| 44:DU:39:VAL:HG23 | 44:DU:40:GLU:H | 1.55 | 0.70 |
| 29:DF:123:LEU:HA | 29:DF:192:LEU:O | 1.91 | 0.70 |
| 27:DD:255:LYS:HD2 | 27:DD:255:LYS:O | 1.90 | 0.70 |
| 3:AF:19:GLU:HA | 3:AF:54:ARG:NH1 | 2.06 | 0.70 |
| 1:AA:217:C:O2' | 1:AA:466:C:N4 | 2.23 | 0.70 |
| 48:DW:17:SER:HB2 | 48:DW:18:PRO:C | 2.11 | 0.70 |
| 32:DK:7:GLU:HA | 32:DK:15:VAL:HG22 | 1.73 | 0.70 |
| 25:BA:76:C:O2' | 48:BW:62:THR:HG21 | 1.91 | 0.70 |
| 26:DB:5:C:H42 | 26:DB:115:G:H1 | 1.37 | 0.70 |
| 1:AA:1175:G:H2' | 1:AA:1176:A:C8 | 2.26 | 0.70 |
| 23:CC:62:C:H2' | 23:CC:63:C:H6 | 1.56 | 0.70 |
| 1:CA:328:C:C2' | 1:CA:328:C:O2 | 2.39 | 0.70 |
| 54:B8:34:TRP:CE3 | 54:B8:35:GLN:OE1 | 2.44 | 0.70 |
| 27:BD:25:THR:HB | 27:BD:82:ILE:H | 1.55 | 0.70 |
| 25:DA:2154:G:H2' | 25:DA:2155:G:C8 | 2.26 | 0.70 |
| 45:BV:121:HIS:HB3 | 45:BV:123:ASP:O | 1.91 | 0.70 |
| 15:AR:74:ASP:CG | 15:AR:77:ARG:HG2 | 2.10 | 0.70 |
| 25:BA:1799:G:H5' | 25:BA:1819:A:H61 | 1.56 | 0.70 |
| 25:BA:32:C:C2' | 25:BA:33:U:H5' | 2.21 | 0.70 |
| 14:AQ:44:LEU:O | 14:AQ:44:LEU:HD12 | 1.91 | 0.70 |
| 25:BA:1329:U:H5'' | 25:BA:1330:C:H5 | 1.56 | 0.70 |
| 43:DT:5:TYR:CZ | 48:DW:30:ARG:HG3 | 2.25 | 0.70 |
| 1:CA:1004:A:C5' | 1:CA:1025:U:O4 | 2.39 | 0.70 |
| 1:CA:1004:A:H1' | 1:CA:1036:G:C2 | 2.26 | 0.70 |
| 23:CC:18:C:O2 | 23:CC:18:C:C2' | 2.39 | 0.70 |
| 7:CJ:113:GLU:O | 7:CJ:119:ARG:HD3 | 1.91 | 0.70 |
| 25:BA:2392:A:H2 | 25:BA:2424:C:H42 | 1.37 | 0.70 |
| 25:DA:2531:A:H4' | 31:DH:157:TYR:HD2 | 1.54 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:1430:C:H2' | 25:DA:1431:U:H6 | 1.56 | 0.70 |
| 25:BA:1678:G:N2 | 25:BA:1989:G:H22 | 1.88 | 0.70 |
| 38:BQ:110:LEU:HA | 38:BQ:112:PHE:CE1 | 2.26 | 0.70 |
| 28:DE:44:TYR:N | 28:DE:44:TYR:HD1 | 1.84 | 0.70 |
| 44:BU:81:LYS:HZ3 | 44:BU:96:ILE:HD12 | 1.56 | 0.70 |
| 35:DO:15:ARG:NH1 | 35:DO:15:ARG:CG | 2.39 | 0.70 |
| 36:BP:88:GLY:C | 36:BP:90:VAL:N | 2.43 | 0.70 |
| 1:AA:1004:A:C4 | 1:AA:1025:U:C2 | 2.79 | 0.70 |
| 3:CF:131:ARG:NH1 | 5:CH:50:GLU:HG3 | 2.06 | 0.70 |
| 2:AE:111:ARG:HH11 | 2:AE:111:ARG:HG2 | 1.55 | 0.70 |
| 7:CJ:79:ARG:HG2 | 7:CJ:84:ASN:HD21 | 1.56 | 0.70 |
| 25:BA:2419:U:H4' | 52:B6:23:THR:HG21 | 1.73 | 0.70 |
| 25:BA:1047:G:H2' | 25:BA:1110:G:N1 | 2.07 | 0.70 |
| 29:BF:34:TRP:NE1 | 35:BO:8:PRO:HD3 | 2.06 | 0.70 |
| 35:BO:63:PRO:CB | 54:B8:12:LYS:O | 2.39 | 0.70 |
| 31:DH:148:ILE:O | 31:DH:151:ILE:HG12 | 1.91 | 0.70 |
| 1:AA:1306:A:H61 | 1:AA:1331:G:H1' | 1.53 | 0.70 |
| 5:AH:126:ARG:HG3 | 5:AH:126:ARG:NH1 | 1.96 | 0.70 |
| 25:DA:270(I):G:H1 | 25:DA:270(Q):C:H42 | 1.37 | 0.70 |
| 31:BH:159:GLU:CG | 31:BH:170:ARG:HH12 | 2.02 | 0.70 |
| 1:CA:1298:C:C5 | 7:CJ:114:ARG:HD2 | 2.25 | 0.70 |
| 4:AG:111:ALA:HB2 | 4:AG:120:LEU:HD12 | 1.73 | 0.70 |
| 29:DF:53:THR:HG23 | 29:DF:55:GLY:H | 1.55 | 0.70 |
| 41:B2:29:PRO:HA | 41:B2:61:VAL:CG2 | 2.22 | 0.70 |
| 32:BK:2:LYS:HB2 | 32:BK:39:ALA:HB2 | 1.72 | 0.70 |
| 13:CP:81:LEU:HD13 | 13:CP:88:ARG:HH11 | 1.56 | 0.70 |
| 23:AC:20:G:C2 | 23:AC:58:A:N3 | 2.60 | 0.70 |
| 1:AA:1053:G:O3' | 1:AA:1054:C:H4' | 1.91 | 0.70 |
| 1:AA:1004:A:C2 | 1:AA:1024:G:C8 | 2.79 | 0.70 |
| 2:CE:111:ARG:HG2 | 2:CE:111:ARG:NH1 | 2.00 | 0.70 |
| 25:DA:71:A:C2 | 43:DT:31:HIS:CE1 | 2.75 | 0.70 |
| 28:BE:120:TRP:CE3 | 28:BE:155:LYS:HD3 | 2.26 | 0.70 |
| 35:DO:111:ARG:HG3 | 35:DO:128:HIS:CG | 2.26 | 0.70 |
| 1:CA:1392:G:N2 | 1:CA:1502:A:H8 | 1.89 | 0.70 |
| 45:BV:150:LEU:HD23 | 45:BV:154:ASP:HB2 | 1.74 | 0.70 |
| 36:DP:68:ILE:HD13 | 36:DP:103:MET:HB3 | 1.72 | 0.70 |
| 39:BR:124:ASP:O | 39:BR:128:GLU:N | 2.25 | 0.70 |
| 13:CP:86:CYS:O | 13:CP:89:GLY:N | 2.22 | 0.70 |
| 38:BQ:28:VAL:HG11 | 38:BQ:98:VAL:HG13 | 1.74 | 0.70 |
| 18:AU:66:LEU:O | 18:AU:70:ILE:HG13 | 1.91 | 0.70 |
| 25:DA:1771:C:H1' | 25:DA:1786:A:C8 | 2.27 | 0.70 |
| 36:BP:63:LYS:HD3 | 36:BP:65:PHE:CZ | 2.27 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:1149:C:H2' | 1:CA:1150:U:C6 | 2.26 | 0.70 |
| 35:BO:112:LEU:H | 35:BO:128:HIS:HD2 | 1.37 | 0.70 |
| 26:BB:3:C:H2' | 26:BB:4:C:C6 | 2.26 | 0.70 |
| 3:AF:64:VAL:HG23 | 3:AF:99:VAL:HA | 1.72 | 0.70 |
| 35:BO:58:THR:HG22 | 35:BO:58:THR:O | 1.92 | 0.70 |
| 28:BE:23:VAL:HG11 | 28:BE:173:VAL:CG2 | 2.22 | 0.70 |
| 1:AA:1125:U:OP2 | 1:AA:1145:C:N4 | 2.25 | 0.70 |
| 31:DH:150:ALA:C | 31:DH:152:ARG:H | 1.95 | 0.70 |
| 25:DA:310:A:OP1 | 44:DU:18:GLY:HA2 | 1.91 | 0.70 |
| 25:BA:2164:C:H2' | 25:BA:2165:G:H8 | 1.57 | 0.70 |
| 25:BA:10:G:N2 | 25:BA:2802:G:OP1 | 2.25 | 0.70 |
| 25:BA:1771:C:H1' | 25:BA:1786:A:C8 | 2.26 | 0.70 |
| 1:CA:1502:A:H4' | 1:CA:1503:A:OP2 | 1.90 | 0.70 |
| 1:AA:1008:C:H42 | 1:AA:1021:G:H1 | 1.38 | 0.70 |
| 1:AA:105:G:H2' | 1:AA:106:C:C6 | 2.25 | 0.70 |
| 25:BA:1925:C:C2' | 25:BA:1926:U:H5' | 2.22 | 0.70 |
| 5:AH:148:VAL:HG21 | 8:AK:107:LEU:HD22 | 1.73 | 0.70 |
| 31:DH:81:GLU:HG2 | 31:DH:83:TYR:HB2 | 1.74 | 0.70 |
| 16:CS:1:MET:HE1 | 16:CS:65:GLN:HG2 | 1.74 | 0.70 |
| 39:DR:8:LYS:NZ | 39:DR:8:LYS:HB3 | 2.07 | 0.70 |
| 41:D2:81:TYR:O | 41:D2:82:ARG:CG | 2.30 | 0.70 |
| 25:DA:997:G:C2' | 25:DA:998:C:H5' | 2.22 | 0.70 |
| 25:BA:442:G:N3 | 29:BF:48:THR:CG2 | 2.54 | 0.70 |
| 25:DA:528:A:H2 | 25:DA:2043:C:C5' | 2.05 | 0.70 |
| 27:DD:164:GLN:HG2 | 27:DD:166:GLN:HE22 | 1.55 | 0.70 |
| 25:BA:524:U:H2' | 25:BA:525:U:C6 | 2.27 | 0.70 |
| 10:CM:27:ALA:HB2 | 10:CM:85:LEU:HD11 | 1.73 | 0.70 |
| 36:BP:78:PRO:O | 36:BP:79:LEU:HD12 | 1.90 | 0.70 |
| 37:B0:74:LYS:C | 37:B0:76:VAL:H | 1.95 | 0.70 |
| 54:D8:34:TRP:O | 54:D8:36:LYS:CG | 2.30 | 0.70 |
| 27:DD:35:LYS:HD3 | 27:DD:63:ARG:C | 2.13 | 0.70 |
| 25:DA:2378:A:H4' | 38:DQ:23:ARG:HH11 | 1.57 | 0.70 |
| 25:DA:2371:G:H4' | 52:D6:45:LYS:HE2 | 1.72 | 0.70 |
| 28:BE:51:PHE:HD1 | 28:BE:52:LEU:HD23 | 1.46 | 0.70 |
| 28:BE:52:LEU:O | 28:BE:75:VAL:HG22 | 1.92 | 0.70 |
| 25:BA:2415:G:C4' | 35:BO:67:MET:H | 2.01 | 0.70 |
| 25:BA:259:G:O2' | 25:BA:621:A:O2' | 2.06 | 0.70 |
| 25:DA:2849:U:O4 | 39:DR:23:ARG:NH2 | 2.25 | 0.70 |
| 44:DU:97:ARG:H | 44:DU:97:ARG:HD3 | 1.57 | 0.70 |
| 38:BQ:36:TYR:N | 38:BQ:36:TYR:CD1 | 2.57 | 0.70 |
| 1:CA:250:A:H1' | 1:CA:251:G:OP2 | 1.91 | 0.70 |
| 13:CP:54:VAL:O | 13:CP:58:GLU:HG2 | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 35:BO:17:LYS:HE2 | 35:BO:27:HIS:CE1 | 2.27 | 0.70 |
| 41:D2:83:ARG:O | 41:D2:84:LYS:HB2 | 1.92 | 0.69 |
| 41:D2:83:ARG:O | 41:D2:84:LYS:CB | 2.40 | 0.69 |
| 27:BD:35:LYS:HD3 | 27:BD:63:ARG:CA | 2.21 | 0.69 |
| 39:DR:74:ARG:HG2 | 39:DR:74:ARG:NH1 | 1.89 | 0.69 |
| 23:CC:17:C:C3' | 23:CC:18:C:H5'' | 2.18 | 0.69 |
| 25:BA:607:U:N3 | 25:BA:621:A:C2 | 2.59 | 0.69 |
| 1:AA:792:A:H1' | 1:AA:794:A:N7 | 2.07 | 0.69 |
| 9:CL:28:VAL:HG22 | 9:CL:63:ILE:HB | 1.73 | 0.69 |
| 25:BA:593:G:H1' | 54:B8:4:MET:HE1 | 1.74 | 0.69 |
| 35:BO:38:GLN:HG2 | 35:BO:45:LEU:HD13 | 1.74 | 0.69 |
| 26:BB:12:C:O2 | 46:B3:74:ARG:NH1 | 2.24 | 0.69 |
| 1:AA:933:G:OP2 | 7:AJ:3:ARG:HB2 | 1.92 | 0.69 |
| 36:DP:43:THR:OG1 | 36:DP:46:GLN:HG3 | 1.92 | 0.69 |
| 39:BR:105:LEU:O | 39:BR:107:ASP:OD1 | 2.10 | 0.69 |
| 25:BA:1113:U:OP1 | 31:BH:2:SER:N | 2.24 | 0.69 |
| 44:BU:42:VAL:O | 44:BU:42:VAL:HG12 | 1.92 | 0.69 |
| 27:DD:5:LYS:HB2 | 27:DD:5:LYS:NZ | 2.06 | 0.69 |
| 50:D4:18:CYS:SG | 50:D4:19:GLY:HA2 | 2.32 | 0.69 |
| 42:DS:75:TYR:CZ | 42:DS:104:THR:HG21 | 2.27 | 0.69 |
| 52:D6:27:LYS:HZ1 | 52:D6:28:ARG:HH12 | 1.40 | 0.69 |
| 27:DD:30:GLU:CD | 27:DD:63:ARG:HH21 | 1.95 | 0.69 |
| 36:DP:66:ILE:CD1 | 36:DP:67:ARG:N | 2.30 | 0.69 |
| 35:DO:64:LYS:HD3 | 54:D8:25:MET:SD | 2.32 | 0.69 |
| 52:B6:15:GLU:CG | 52:B6:16:CYS:H | 2.05 | 0.69 |
| 14:AQ:41:ARG:HG2 | 14:AQ:41:ARG:HH11 | 1.58 | 0.69 |
| 27:DD:166:GLN:HA | 27:DD:166:GLN:NE2 | 2.06 | 0.69 |
| 1:AA:39:G:N7 | 1:AA:547:A:H8 | 1.90 | 0.69 |
| 54:D8:40:GLU:H | 54:D8:43:GLN:HG3 | 1.56 | 0.69 |
| 50:B4:61:ARG:NE | 50:B4:61:ARG:HA | 2.07 | 0.69 |
| 25:DA:1964:G:H4' | 25:DA:1965:C:OP2 | 1.91 | 0.69 |
| 25:DA:171:G:H2' | 25:DA:172:C:C6 | 2.28 | 0.69 |
| 8:AK:64:LYS:HB3 | 8:AK:79:VAL:HG21 | 1.74 | 0.69 |
| 51:B5:42:PRO:HB2 | 51:B5:43:HIS:HD2 | 1.57 | 0.69 |
| 1:AA:625:G:C5' | 16:AS:16:HIS:CD2 | 2.75 | 0.69 |
| 51:D5:4:HIS:HB3 | 51:D5:5:PRO:HD2 | 1.65 | 0.69 |
| 28:BE:78:LEU:CD1 | 28:BE:79:ARG:N | 2.50 | 0.69 |
| 25:BA:1900:A:H5' | 25:BA:1900:A:H8 | 1.57 | 0.69 |
| 25:DA:674:G:O2' | 29:DF:74:ARG:HG3 | 1.93 | 0.69 |
| 4:AG:173:TRP:CD1 | 4:AG:174:LEU:HG | 2.27 | 0.69 |
| 4:CG:122:ARG:NH2 | 4:CG:134:ASP:HB3 | 2.06 | 0.69 |
| 25:BA:847:U:O4 | 25:BA:933:A:N1 | 2.24 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 54:D8:39:LYS:HG2 | 54:D8:40:GLU:H | 1.57 | 0.69 |
| 37:B0:103:ARG:HH11 | 42:BS:40:ASN:HD22 | 1.37 | 0.69 |
| 23:AC:20:G:HO2' | 23:AC:21:U:H5 | 1.41 | 0.69 |
| 39:DR:56:GLY:O | 39:DR:58:ASN:N | 2.25 | 0.69 |
| 47:DZ:87:PRO:O | 47:DZ:91:LYS:N | 2.21 | 0.69 |
| 25:DA:2849:U:O2' | 25:DA:2866:U:O2 | 2.09 | 0.69 |
| 25:DA:273(D):C:H42 | 25:DA:363(B):G:H1 | 1.40 | 0.69 |
| 44:DU:81:LYS:HD3 | 44:DU:97:ARG:CZ | 2.23 | 0.69 |
| 1:CA:1306:A:N6 | 1:CA:1331:G:H1' | 2.08 | 0.69 |
| 25:BA:1021:A:C3' | 25:BA:1022:G:H5'' | 2.23 | 0.69 |
| 38:BQ:11:LYS:HD2 | 38:BQ:15:ARG:HH21 | 1.56 | 0.69 |
| 4:AG:122:ARG:CG | 4:AG:122:ARG:HH11 | 2.03 | 0.69 |
| 40:B1:92:ARG:CZ | 41:B2:11:GLN:H | 2.05 | 0.69 |
| 9:CL:85:LEU:HD13 | 9:CL:92:TYR:HD2 | 1.57 | 0.69 |
| 1:CA:537:G:H5'' | 12:CO:113:ARG:HH12 | 1.55 | 0.69 |
| 27:BD:6:PHE:CE1 | 27:BD:18:VAL:HG23 | 2.24 | 0.69 |
| 31:BH:12:PRO:HD3 | 31:BH:48:GLY:O | 1.92 | 0.69 |
| 29:DF:82:ILE:O | 29:DF:82:ILE:CD1 | 2.41 | 0.69 |
| 25:BA:1240:U:O2' | 25:BA:1241:A:H5' | 1.92 | 0.69 |
| 1:AA:658:G:C5 | 1:AA:659:U:C5 | 2.79 | 0.69 |
| 26:BB:78:A:C2 | 26:BB:99:A:C4 | 2.80 | 0.69 |
| 1:CA:197:A:H3' | 1:CA:197:A:OP2 | 1.93 | 0.69 |
| 45:BV:111:VAL:HG11 | 45:BV:146:ILE:HB | 1.72 | 0.69 |
| 32:DK:78:THR:HB | 32:DK:104:GLN:HE22 | 1.58 | 0.69 |
| 47:BZ:23:LYS:HB3 | 47:BZ:29:GLY:HA3 | 1.74 | 0.69 |
| 27:DD:85:ASP:OD2 | 27:DD:88:ARG:HD2 | 1.91 | 0.69 |
| 10:CM:49:VAL:O | 10:CM:60:ARG:HB2 | 1.93 | 0.69 |
| 31:BH:159:GLU:CG | 31:BH:170:ARG:HH11 | 2.03 | 0.69 |
| 45:BV:62:PRO:O | 45:BV:63:ASP:HB3 | 1.90 | 0.69 |
| 31:BH:83:TYR:HB2 | 31:BH:134:SER:HA | 1.73 | 0.69 |
| 1:CA:1442:G:H2' | 1:CA:1443:G:O5' | 1.93 | 0.69 |
| 25:DA:885:C:N3 | 25:DA:890:A:C6 | 2.60 | 0.69 |
| 1:CA:1297:C:H1' | 1:CA:1298:C:OP2 | 1.92 | 0.69 |
| 29:DF:181:LEU:CD2 | 29:DF:186:ILE:HD11 | 2.22 | 0.69 |
| 25:DA:2211:G:H3' | 25:DA:2212:A:N3 | 2.07 | 0.69 |
| 25:DA:148:C:H6 | 25:DA:148:C:H5' | 1.57 | 0.69 |
| 31:DH:168:PRO:O | 31:DH:169:VAL:HG12 | 1.92 | 0.69 |
| 5:CH:51:VAL:HB | 5:CH:52:PRO:HD3 | 1.74 | 0.69 |
| 1:CA:994:A:C5 | 1:CA:1216:G:H4' | 2.27 | 0.69 |
| 25:BA:1014:U:H2' | 25:BA:1015:G:H5'' | 1.72 | 0.69 |
| 43:DT:12:VAL:HG13 | 43:DT:27:THR:O | 1.92 | 0.69 |
| 48:BW:46:GLN:OE1 | 48:BW:46:GLN:HA | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 4:AG:201:GLN:HE21 | 4:AG:201:GLN:HA | 1.57 | 0.69 |
| 1:AA:1254:C:H41 | 10:AM:43:ARG:HH12 | 1.41 | 0.69 |
| 1:AA:1193:G:C2' | 1:AA:1194:U:H5' | 2.23 | 0.69 |
| 25:BA:2310:A:H2 | 30:BG:77:ILE:HG13 | 1.54 | 0.69 |
| 28:BE:19:ARG:HH12 | 34:BN:72:PRO:CG | 2.06 | 0.69 |
| 1:AA:1004:A:H2 | 1:AA:1024:G:C8 | 2.11 | 0.69 |
| 25:BA:881:G:H3' | 25:BA:882:G:C4' | 2.22 | 0.69 |
| 25:DA:2872:G:C8 | 25:DA:2873:A:C2 | 2.80 | 0.69 |
| 33:BM:132:ALA:HB1 | 33:BM:133:GLN:NE2 | 2.06 | 0.69 |
| 25:BA:1178:C:H4' | 25:BA:1179:C:OP1 | 1.91 | 0.69 |
| 27:DD:70:TRP:O | 27:DD:73:VAL:HG23 | 1.92 | 0.69 |
| 5:CH:51:VAL:O | 5:CH:55:VAL:HG23 | 1.93 | 0.69 |
| 29:BF:176:LEU:HD21 | 29:BF:180:GLY:O | 1.93 | 0.69 |
| 1:AA:1106:G:C4 | 1:AA:1107:C:C5 | 2.81 | 0.69 |
| 25:BA:2263:C:H5'' | 25:BA:2264:C:OP2 | 1.92 | 0.69 |
| 42:BS:79:GLY:CA | 42:BS:100:THR:HG22 | 2.22 | 0.69 |
| 28:DE:82:ARG:HG3 | 28:DE:82:ARG:O | 1.90 | 0.69 |
| 33:BM:40:PRO:HB3 | 40:B1:68:ALA:HB2 | 1.74 | 0.69 |
| 28:DE:48:GLN:HG2 | 28:DE:78:LEU:HB3 | 1.74 | 0.69 |
| 22:CB:18:G:O6 | 22:CB:71:U:O2 | 2.11 | 0.69 |
| 25:BA:71:A:C2 | 43:BT:31:HIS:CE1 | 2.70 | 0.69 |
| 25:DA:1826:G:C4' | 27:DD:242:ARG:HH21 | 2.03 | 0.69 |
| 45:BV:61:LEU:O | 45:BV:64:GLY:HA2 | 1.92 | 0.69 |
| 25:DA:2872:G:C4 | 25:DA:2873:A:C2 | 2.80 | 0.69 |
| 35:DO:36:LYS:CB | 35:DO:36:LYS:HZ3 | 2.03 | 0.69 |
| 23:CC:28:U:O2 | 23:CC:45:A:C2 | 2.45 | 0.69 |
| 3:AF:95:THR:HG22 | 3:AF:97:LYS:H | 1.58 | 0.69 |
| 25:BA:1113:U:H5' | 31:BH:2:SER:HB2 | 1.75 | 0.69 |
| 3:AF:81:GLY:O | 3:AF:85:ARG:HB2 | 1.92 | 0.69 |
| 25:BA:270(F):U:H2' | 25:BA:270(G):C:C6 | 2.27 | 0.69 |
| 19:AV:36:ARG:NH1 | 19:AV:52:TYR:O | 2.25 | 0.69 |
| 25:BA:1084:A:N6 | 25:BA:1085:A:H62 | 1.90 | 0.69 |
| 25:DA:2378:A:O5' | 25:DA:2378:A:H8 | 1.75 | 0.69 |
| 40:D1:92:ARG:HG3 | 40:D1:94:ASN:H | 1.56 | 0.69 |
| 28:BE:53:PRO:HA | 28:BE:74:PRO:HA | 1.75 | 0.69 |
| 25:BA:1899:G:N2 | 25:BA:1902:C:H5 | 1.90 | 0.69 |
| 1:CA:976:G:OP1 | 14:CQ:32:SER:N | 2.24 | 0.69 |
| 28:DE:39:PRO:HD3 | 28:DE:45:THR:OG1 | 1.91 | 0.69 |
| 25:BA:2344:U:O2' | 52:B6:37:ARG:HG2 | 1.92 | 0.69 |
| 51:B5:3:LYS:HA | 51:B5:3:LYS:HE3 | 1.75 | 0.69 |
| 44:DU:13:VAL:CG2 | 44:DU:72:VAL:HB | 2.22 | 0.69 |
| 22:AB:37:G:N2 | 24:A1:19:U:O2 | 2.19 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 7:CJ:115:ARG:HB2 | 7:CJ:118:VAL:HG12 | 1.75 | 0.69 |
| 25:BA:2115:G:H2' | 25:BA:2116:G:H8 | 1.56 | 0.69 |
| 25:BA:2799:A:H5'' | 25:BA:2801:A:OP2 | 1.92 | 0.69 |
| 25:BA:2261:C:H2' | 25:BA:2262:U:H5' | 1.75 | 0.69 |
| 27:BD:166:GLN:CA | 27:BD:166:GLN:HE21 | 2.05 | 0.69 |
| 30:BG:135:LEU:HD23 | 30:BG:140:ILE:HD11 | 1.74 | 0.69 |
| 1:AA:1346:A:H5'' | 9:AL:120:ARG:HH12 | 1.58 | 0.69 |
| 3:CF:35:GLU:HA | 3:CF:38:ARG:HE | 1.57 | 0.69 |
| 25:BA:2688:U:H5 | 25:BA:2720:U:OP2 | 1.76 | 0.69 |
| 25:DA:2150:U:H2' | 25:DA:2151:G:H8 | 1.56 | 0.69 |
| 25:DA:125:G:H5'' | 53:D7:19:ARG:HD3 | 1.74 | 0.69 |
| 25:DA:753:C:H2' | 25:DA:754:C:H6 | 1.58 | 0.69 |
| 30:BG:107:LEU:HD21 | 30:BG:178:PHE:CD1 | 2.27 | 0.69 |
| 1:CA:554:C:H2' | 1:CA:555:C:H6 | 1.57 | 0.69 |
| 9:CL:24:GLY:HA2 | 9:CL:59:PHE:O | 1.93 | 0.69 |
| 1:AA:524:G:H2' | 1:AA:525:C:C6 | 2.27 | 0.69 |
| 25:BA:2233:U:H2' | 25:BA:2234:G:C8 | 2.27 | 0.69 |
| 36:DP:137:TYR:CE1 | 45:DV:83:PRO:HG3 | 2.27 | 0.69 |
| 40:B1:110:VAL:O | 40:B1:113:ALA:HB3 | 1.93 | 0.69 |
| 1:AA:1159:U:C2 | 1:AA:1182:G:C2 | 2.81 | 0.69 |
| 25:BA:2310:A:C2' | 25:BA:2311:A:C5' | 2.70 | 0.69 |
| 52:D6:15:GLU:HG3 | 52:D6:47:THR:HG21 | 1.75 | 0.69 |
| 28:BE:59:VAL:O | 28:BE:60:ASN:CG | 2.30 | 0.69 |
| 25:BA:1899:G:H22 | 25:BA:1902:C:H41 | 0.73 | 0.69 |
| 1:AA:1003:G:C2' | 1:AA:1004:A:H5' | 2.22 | 0.69 |
| 2:CE:12:GLU:HB2 | 2:CE:16:HIS:CE1 | 2.28 | 0.69 |
| 25:BA:747:U:O2 | 25:BA:2014:A:H1' | 1.92 | 0.69 |
| 25:BA:2162:G:H2' | 25:BA:2163:C:H6 | 1.57 | 0.69 |
| 19:CV:18:LYS:O | 19:CV:22:LEU:HB2 | 1.93 | 0.69 |
| 25:DA:943:U:OP2 | 35:DO:36:LYS:HG3 | 1.92 | 0.69 |
| 25:BA:1869:G:H5' | 25:BA:1869:G:H8 | 1.55 | 0.69 |
| 25:BA:1165:U:H2' | 25:BA:1166:C:C6 | 2.28 | 0.69 |
| 6:AI:44:GLY:HA2 | 6:AI:59:TYR:CZ | 2.28 | 0.69 |
| 34:DN:4:PRO:O | 34:DN:5:GLN:HB2 | 1.93 | 0.69 |
| 25:BA:2315:G:OP1 | 30:BG:36:LYS:NZ | 2.26 | 0.69 |
| 5:CH:57:LYS:HG2 | 5:CH:61:TYR:HE2 | 1.57 | 0.69 |
| 50:B4:10:VAL:HG22 | 50:B4:11:PRO:HD2 | 1.75 | 0.69 |
| 15:AR:17:ARG:HG3 | 15:AR:17:ARG:HH11 | 1.57 | 0.69 |
| 19:AV:10:PHE:N | 19:AV:10:PHE:CD1 | 2.60 | 0.69 |
| 26:DB:50:G:OP1 | 38:DQ:63:THR:HG23 | 1.93 | 0.69 |
| 1:AA:1170:A:H2' | 1:AA:1171:G:O4' | 1.93 | 0.69 |
| 27:DD:64:ILE:O | 27:DD:64:ILE:CG1 | 2.41 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:1226:C:C4 | 13:CP:104:ARG:HB2 | 2.28 | 0.69 |
| 25:BA:259:G:H21 | 25:BA:621:A:H8 | 1.37 | 0.69 |
| 25:BA:61:G:H5' | 48:BW:50:ILE:HG12 | 1.74 | 0.69 |
| 25:BA:2577:A:H5'' | 25:BA:2578:G:C5' | 2.22 | 0.69 |
| 4:CG:108:LEU:CD2 | 4:CG:183:GLY:HA3 | 2.21 | 0.69 |
| 10:AM:49:VAL:HG22 | 14:AQ:41:ARG:HB2 | 1.74 | 0.69 |
| 25:BA:479:A:C2 | 25:BA:481:G:H5' | 2.28 | 0.69 |
| 31:BH:4:ILE:HD11 | 31:BH:7:LEU:HD11 | 1.75 | 0.69 |
| 7:AJ:22:LEU:HD23 | 7:AJ:62:PHE:HE2 | 1.58 | 0.69 |
| 25:BA:2680:C:O2' | 25:BA:2681:C:H5' | 1.93 | 0.69 |
| 30:DG:15:VAL:HG13 | 30:DG:175:LEU:HB2 | 1.73 | 0.69 |
| 26:BB:13:A:N1 | 26:BB:69:G:O2' | 2.19 | 0.69 |
| 31:DH:20:ALA:HB3 | 31:DH:23:ARG:HB2 | 1.74 | 0.69 |
| 3:CF:18:TRP:CD1 | 14:CQ:54:PRO:HA | 2.28 | 0.69 |
| 1:CA:279:A:H4' | 1:CA:280:C:O5' | 1.92 | 0.69 |
| 1:CA:243:A:H4' | 1:CA:244:U:O5' | 1.93 | 0.69 |
| 1:AA:1211:U:H5' | 1:AA:1212:U:OP1 | 1.93 | 0.69 |
| 45:DV:93:ASP:HA | 45:DV:130:PRO:HG2 | 1.74 | 0.69 |
| 25:DA:1310:G:OP2 | 53:D7:9:ARG:NH1 | 2.26 | 0.69 |
| 1:AA:310:G:P | 16:AS:27:LYS:HZ1 | 2.16 | 0.69 |
| 39:DR:22:PHE:CE1 | 39:DR:52:ILE:HD11 | 2.29 | 0.68 |
| 1:CA:426:G:P | 4:CG:36:ARG:HH21 | 2.16 | 0.68 |
| 29:BF:28:ILE:HG22 | 29:BF:112:MET:HB3 | 1.74 | 0.68 |
| 13:CP:15:VAL:HG12 | 13:CP:45:VAL:HG22 | 1.75 | 0.68 |
| 25:BA:1796:U:H2' | 25:BA:1797:C:C6 | 2.28 | 0.68 |
| 50:D4:16:CYS:HA | 50:D4:33:VAL:HG23 | 1.75 | 0.68 |
| 27:DD:186:HIS:CD2 | 27:DD:188:GLU:H | 2.10 | 0.68 |
| 50:B4:42:PHE:CD1 | 50:B4:42:PHE:O | 2.46 | 0.68 |
| 1:CA:1286:A:H5' | 21:CX:25:LYS:HD2 | 1.75 | 0.68 |
| 5:AH:98:THR:HG22 | 5:AH:99:GLY:N | 2.06 | 0.68 |
| 25:DA:1606:G:H5'' | 25:DA:1607:C:OP1 | 1.93 | 0.68 |
| 6:AI:69:GLU:O | 6:AI:72:VAL:HG12 | 1.93 | 0.68 |
| 42:BS:70:TYR:H | 42:BS:70:TYR:HD2 | 1.40 | 0.68 |
| 32:BK:114:LEU:O | 32:BK:115:ALA:HB3 | 1.93 | 0.68 |
| 28:DE:11:MET:HA | 28:DE:24:THR:HA | 1.75 | 0.68 |
| 41:D2:2:PHE:H | 41:D2:42:GLY:HA3 | 1.58 | 0.68 |
| 25:DA:1187:G:H4' | 41:D2:76:LYS:HZ2 | 1.58 | 0.68 |
| 2:AE:29:ALA:O | 2:AE:32:ILE:HG22 | 1.93 | 0.68 |
| 34:BN:104:ARG:HH22 | 39:BR:43:GLN:HE22 | 1.40 | 0.68 |
| 25:DA:1332:G:H21 | 25:DA:1610:A:H8 | 1.41 | 0.68 |
| 26:DB:44:G:H1' | 26:DB:47:C:H42 | 1.57 | 0.68 |
| 50:D4:20:ASN:CG | 50:D4:21:VAL:N | 2.47 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 31:BH:153:LYS:HB3 | 31:BH:154:PRO:CD | 2.23 | 0.68 |
| 17:CT:59:ILE:HG22 | 17:CT:71:PHE:CD1 | 2.27 | 0.68 |
| 40:B1:108:GLU:OE1 | 40:B1:112:ARG:NH1 | 2.27 | 0.68 |
| 25:BA:2336:A:H61 | 46:B3:43:THR:HG22 | 1.58 | 0.68 |
| 25:DA:204:A:O2' | 25:DA:205:G:OP2 | 2.09 | 0.68 |
| 25:BA:588:U:H2' | 25:BA:589:C:C6 | 2.29 | 0.68 |
| 45:DV:118:GLN:HB2 | 45:DV:173:ALA:O | 1.93 | 0.68 |
| 20:CW:89:ARG:NH1 | 20:CW:105:SER:OG | 2.27 | 0.68 |
| 1:AA:883:C:C2' | 1:AA:884:U:H5' | 2.22 | 0.68 |
| 28:DE:151:TYR:HD2 | 28:DE:154:LYS:HZ2 | 1.40 | 0.68 |
| 25:BA:85:G:OP2 | 44:BU:9:LYS:HB2 | 1.93 | 0.68 |
| 25:BA:1077:A:H3' | 25:BA:1078:U:H5' | 1.76 | 0.68 |
| 41:D2:71:LEU:HA | 41:D2:86:GLY:HA2 | 1.74 | 0.68 |
| 28:BE:80:GLU:O | 28:BE:82:ARG:N | 2.26 | 0.68 |
| 28:BE:82:ARG:O | 28:BE:84:PHE:N | 2.26 | 0.68 |
| 25:BA:1729:A:H2' | 25:BA:1731:G:N7 | 2.09 | 0.68 |
| 25:BA:1053:C:N4 | 25:BA:1106:G:H1 | 1.90 | 0.68 |
| 44:DU:96:ILE:HD12 | 44:DU:98:VAL:HG12 | 1.75 | 0.68 |
| 25:DA:259:G:N2 | 25:DA:621:A:H8 | 1.90 | 0.68 |
| 45:BV:27:VAL:HG12 | 45:BV:87:ASP:HB3 | 1.73 | 0.68 |
| 1:CA:685:G:H5'' | 1:CA:686:U:OP2 | 1.92 | 0.68 |
| 1:CA:413:G:O2' | 1:CA:414:A:OP2 | 2.08 | 0.68 |
| 36:DP:98:LYS:HB3 | 36:DP:99:PRO:HD2 | 1.75 | 0.68 |
| 25:DA:2148:G:H2' | 25:DA:2149:G:H8 | 1.58 | 0.68 |
| 47:DZ:65:SER:OG | 47:DZ:66:HIS:HD2 | 1.77 | 0.68 |
| 45:DV:15:PRO:HB2 | 45:DV:19:ARG:NH2 | 2.08 | 0.68 |
| 1:AA:1336:C:H4' | 1:AA:1336:C:OP1 | 1.93 | 0.68 |
| 46:B3:70:GLN:OE1 | 46:B3:72:ARG:HD3 | 1.93 | 0.68 |
| 25:BA:1056:G:H21 | 25:BA:1103:A:N6 | 1.76 | 0.68 |
| 1:CA:1004:A:C1' | 1:CA:1036:G:N1 | 2.49 | 0.68 |
| 4:CG:8:VAL:HG12 | 4:CG:21:LEU:HD22 | 1.73 | 0.68 |
| 22:CB:41:G:H2' | 22:CB:42:U:C6 | 2.28 | 0.68 |
| 45:BV:7:ALA:HB3 | 45:BV:61:LEU:CB | 2.24 | 0.68 |
| 13:CP:57:ARG:NH2 | 50:D4:34:GLU:HB2 | 2.07 | 0.68 |
| 1:CA:1285:A:H1' | 1:CA:1286:A:OP2 | 1.93 | 0.68 |
| 22:AB:52:U:H2' | 22:AB:53:A:H5' | 1.74 | 0.68 |
| 4:AG:79:PHE:HE1 | 4:AG:204:ILE:HG12 | 1.58 | 0.68 |
| 1:AA:186(E):C:N4 | 1:AA:191(B):G:H1 | 1.92 | 0.68 |
| 25:BA:1130:U:O2 | 28:BE:149:ARG:NH2 | 2.26 | 0.68 |
| 4:CG:62:GLN:NE2 | 4:CG:65:ARG:HE | 1.91 | 0.68 |
| 1:CA:273:A:H2' | 1:CA:274:A:H5' | 1.76 | 0.68 |
| 5:CH:9:LYS:HB2 | 5:CH:112:LEU:HD11 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:CF:94:LEU:HD12 | 3:CF:95:THR:H | 1.56 | 0.68 |
| 25:BA:405:U:H2' | 25:BA:405:U:O2 | 1.92 | 0.68 |
| 7:CJ:76:ARG:HG2 | 7:CJ:76:ARG:HH11 | 1.57 | 0.68 |
| 43:BT:15:GLU:CD | 43:BT:15:GLU:H | 1.96 | 0.68 |
| 25:BA:1085:A:C2 | 25:BA:1086:A:N7 | 2.61 | 0.68 |
| 38:BQ:106:ARG:CA | 38:BQ:110:LEU:HD21 | 2.24 | 0.68 |
| 54:D8:52:LYS:CB | 54:D8:53:PRO:HD3 | 2.23 | 0.68 |
| 25:DA:776:G:H4' | 25:DA:777:A:O5' | 1.92 | 0.68 |
| 40:D1:59:ARG:O | 40:D1:63:VAL:HG23 | 1.93 | 0.68 |
| 28:BE:35:GLN:CB | 28:BE:48:GLN:CG | 2.61 | 0.68 |
| 44:BU:76:CYS:HB3 | 44:BU:96:ILE:HD13 | 1.75 | 0.68 |
| 25:DA:1728:G:N1 | 25:DA:1730:U:OP2 | 2.26 | 0.68 |
| 1:CA:1127:G:H2' | 1:CA:1128:C:C6 | 2.29 | 0.68 |
| 36:DP:79:LEU:HD13 | 36:DP:80:GLU:HB2 | 1.75 | 0.68 |
| 25:BA:1533:C:H2' | 25:BA:1534:G:H8 | 1.55 | 0.68 |
| 2:CE:95:GLN:HB3 | 2:CE:148:TYR:HD1 | 1.59 | 0.68 |
| 25:DA:1651:G:OP1 | 37:D0:37:THR:HG21 | 1.94 | 0.68 |
| 3:CF:63:ASN:O | 3:CF:64:VAL:HB | 1.94 | 0.68 |
| 25:BA:2563:U:H1' | 25:BA:2566:A:N6 | 2.09 | 0.68 |
| 1:AA:498:A:H4' | 1:AA:500:G:OP1 | 1.93 | 0.68 |
| 25:BA:2864:G:O2' | 25:BA:2865:U:H5' | 1.94 | 0.68 |
| 39:DR:64:ARG:HB2 | 39:DR:73:GLU:HG3 | 1.76 | 0.68 |
| 1:AA:412:A:H1' | 1:AA:413:G:OP2 | 1.93 | 0.68 |
| 1:CA:942:G:H21 | 9:CL:124:GLN:NE2 | 1.91 | 0.68 |
| 41:D2:99:ILE:O | 41:D2:99:ILE:HG22 | 1.93 | 0.68 |
| 38:DQ:15:ARG:HD2 | 38:DQ:88:ASP:OD1 | 1.93 | 0.68 |
| 52:B6:28:ARG:HB3 | 52:B6:28:ARG:HH11 | 1.58 | 0.68 |
| 1:AA:872:A:C4 | 1:AA:874:G:N7 | 2.61 | 0.68 |
| 25:DA:2162:G:H2' | 25:DA:2163:C:H6 | 1.57 | 0.68 |
| 25:BA:1519:G:C2' | 25:BA:1520:U:H5' | 2.23 | 0.68 |
| 2:AE:187:LEU:HD23 | 2:AE:201:ILE:O | 1.94 | 0.68 |
| 2:AE:22:LYS:HZ3 | 2:AE:22:LYS:HA | 1.58 | 0.68 |
| 13:AP:3:ARG:HD3 | 13:AP:7:VAL:HG13 | 1.73 | 0.68 |
| 22:AB:52:U:C5 | 22:AB:53:A:C8 | 2.82 | 0.68 |
| 10:CM:33:GLN:HB2 | 10:CM:75:ILE:HG12 | 1.74 | 0.68 |
| 5:AH:76:ILE:HB | 5:AH:77:PRO:HD2 | 1.76 | 0.68 |
| 14:CQ:26:ARG:NH1 | 14:CQ:47:LEU:HD21 | 2.09 | 0.68 |
| 28:DE:64:LYS:HB3 | 28:DE:66:HIS:CD2 | 2.28 | 0.68 |
| 28:DE:82:ARG:O | 28:DE:83:ASP:CB | 2.42 | 0.68 |
| 38:BQ:83:LYS:O | 38:BQ:109:GLY:HA3 | 1.91 | 0.68 |
| 27:DD:35:LYS:HE3 | 27:DD:65:ILE:CA | 2.23 | 0.68 |
| 36:DP:134:ARG:HH22 | 45:DV:122:ARG:HD2 | 1.58 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 28:BE:41:LYS:NZ | 28:BE:41:LYS:HB3 | 2.04 | 0.68 |
| 28:BE:81:ILE:CG2 | 28:BE:84:PHE:CD1 | 2.70 | 0.68 |
| 1:AA:1124:G:H3' | 1:AA:1145:C:N4 | 2.05 | 0.68 |
| 1:AA:1025:U:O2' | 1:AA:1026:G:C5' | 2.42 | 0.68 |
| 29:DF:24:LEU:CD1 | 29:DF:25:PRO:HD3 | 2.20 | 0.68 |
| 45:BV:7:ALA:HB3 | 45:BV:61:LEU:HB3 | 1.75 | 0.68 |
| 22:CB:87:A:C8 | 25:DA:2583:G:N2 | 2.52 | 0.68 |
| 25:DA:1678:G:H22 | 25:DA:1989:G:N2 | 1.92 | 0.68 |
| 25:DA:607:U:H3 | 25:DA:621:A:H2 | 1.41 | 0.68 |
| 1:AA:1399:C:C2 | 1:AA:1502:A:N6 | 2.61 | 0.68 |
| 1:CA:164:U:H2' | 1:CA:165:C:C6 | 2.27 | 0.68 |
| 12:CO:32:PHE:HB3 | 12:CO:84:LEU:HD21 | 1.76 | 0.68 |
| 39:DR:8:LYS:NZ | 39:DR:8:LYS:CB | 2.57 | 0.68 |
| 25:DA:1011:G:H2' | 25:DA:1013:C:O4' | 1.92 | 0.68 |
| 5:AH:82:VAL:HB | 5:AH:138:ALA:HB2 | 1.76 | 0.68 |
| 25:DA:2500:U:H5'' | 25:DA:2501:C:OP2 | 1.94 | 0.68 |
| 4:CG:149:ALA:O | 4:CG:153:ARG:HG2 | 1.93 | 0.68 |
| 28:DE:46:ALA:HB2 | 28:DE:82:ARG:HB2 | 1.75 | 0.68 |
| 28:BE:79:ARG:HH22 | 28:BE:164:ARG:NH1 | 1.91 | 0.68 |
| 27:DD:35:LYS:HD3 | 27:DD:64:ILE:N | 2.08 | 0.68 |
| 23:AC:18:C:O2' | 23:AC:18:C:O2 | 2.09 | 0.68 |
| 23:AC:18:C:O2' | 23:AC:19:G:OP1 | 2.11 | 0.68 |
| 28:BE:21:VAL:HG23 | 28:BE:21:VAL:O | 1.93 | 0.68 |
| 25:DA:1022:G:H22 | 25:DA:1142(A):A:H2 | 1.40 | 0.68 |
| 48:BW:47:ASN:O | 48:BW:50:ILE:HG13 | 1.94 | 0.68 |
| 39:DR:91:ARG:HD2 | 39:DR:124:ASP:OD1 | 1.93 | 0.68 |
| 1:CA:1162:C:H42 | 1:CA:1174:G:H1 | 1.42 | 0.68 |
| 44:DU:17:SER:HB2 | 44:DU:71:LYS:CD | 2.23 | 0.68 |
| 45:BV:29:TYR:CE2 | 45:BV:87:ASP:HB2 | 2.26 | 0.68 |
| 45:BV:164:ALA:O | 45:BV:165:VAL:HG13 | 1.94 | 0.68 |
| 2:AE:97:TRP:HH2 | 2:AE:176:GLU:HG3 | 1.58 | 0.68 |
| 29:DF:110:LEU:HD22 | 29:DF:202:PHE:HE1 | 1.58 | 0.68 |
| 1:AA:129(A):G:C2 | 1:AA:188:U:O2' | 2.47 | 0.68 |
| 1:AA:464:G:O6 | 1:AA:466:C:H5' | 1.94 | 0.68 |
| 1:CA:1255:G:OP1 | 10:CM:45:ARG:NH1 | 2.20 | 0.68 |
| 1:CA:266:G:H5'' | 1:CA:268:C:H41 | 1.59 | 0.68 |
| 11:AN:66:LEU:HD21 | 11:AN:97:ALA:HB1 | 1.75 | 0.68 |
| 1:CA:534:U:H5' | 1:CA:535:A:OP2 | 1.94 | 0.68 |
| 38:DQ:86:ALA:O | 38:DQ:87:PHE:HB3 | 1.94 | 0.68 |
| 1:CA:1004:A:C1' | 1:CA:1036:G:H1 | 2.05 | 0.68 |
| 28:DE:80:GLU:O | 28:DE:81:ILE:HB | 1.94 | 0.68 |
| 4:CG:30:LYS:O | 4:CG:30:LYS:HG2 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1367:C:O2' | 10:AM:48:THR:HG21 | 1.94 | 0.68 |
| 1:CA:991:U:O2 | 1:CA:993:G:H8 | 1.77 | 0.68 |
| 1:CA:179:A:H2' | 1:CA:180:U:C6 | 2.29 | 0.68 |
| 50:D4:1:MET:C | 50:D4:2:LYS:HD3 | 2.14 | 0.68 |
| 38:BQ:35:ILE:C | 38:BQ:36:TYR:HD1 | 1.97 | 0.68 |
| 33:BM:13:TRP:O | 33:BM:135:PRO:HD2 | 1.93 | 0.68 |
| 25:BA:297:C:H5'' | 44:BU:85:VAL:CG2 | 2.24 | 0.68 |
| 25:BA:2470:G:O6 | 25:BA:2476:A:H1' | 1.93 | 0.68 |
| 26:BB:50:G:OP1 | 38:BQ:63:THR:HG23 | 1.92 | 0.68 |
| 35:DO:58:THR:O | 35:DO:58:THR:HG22 | 1.92 | 0.68 |
| 27:BD:235:GLY:O | 27:BD:237:GLU:OE1 | 2.12 | 0.68 |
| 7:AJ:74:GLU:HG2 | 7:AJ:91:VAL:HG22 | 1.75 | 0.68 |
| 10:AM:40:LEU:HB2 | 10:AM:69:ASN:CB | 2.24 | 0.68 |
| 31:BH:20:ALA:HB1 | 31:BH:21:PRO:HD2 | 1.74 | 0.68 |
| 16:AS:14:ASN:O | 16:AS:14:ASN:CG | 2.32 | 0.68 |
| 28:BE:79:ARG:HH22 | 28:BE:164:ARG:HH11 | 1.42 | 0.68 |
| 52:D6:44:ARG:HG3 | 52:D6:44:ARG:NH1 | 1.99 | 0.68 |
| 25:BA:2785:C:H2' | 25:BA:2786:U:O4' | 1.94 | 0.68 |
| 1:AA:1004:A:C5' | 1:AA:1025:U:H3 | 2.07 | 0.68 |
| 25:DA:1060:U:H5'' | 25:DA:1061:U:C5 | 2.29 | 0.68 |
| 25:BA:1379:A:C1' | 25:BA:1380:G:OP1 | 2.39 | 0.68 |
| 1:CA:1298:C:H4' | 1:CA:1299:A:C8 | 2.28 | 0.68 |
| 25:BA:2443:C:O2' | 25:BA:2444:G:H5' | 1.94 | 0.68 |
| 3:CF:84:ILE:HD11 | 3:CF:88:ARG:NH2 | 2.08 | 0.68 |
| 1:AA:1374:A:H2' | 1:AA:1375:A:H5' | 1.74 | 0.68 |
| 1:CA:1072:G:C5 | 1:CA:1073:U:C4 | 2.82 | 0.68 |
| 6:AI:78:GLU:O | 6:AI:81:ILE:HG13 | 1.93 | 0.68 |
| 25:DA:602:G:HO2' | 25:DA:604:G:HO2' | 1.40 | 0.68 |
| 25:BA:2376:A:N1 | 38:BQ:87:PHE:CD2 | 2.61 | 0.67 |
| 54:D8:49:VAL:CA | 54:D8:50:LEU:HD12 | 2.23 | 0.67 |
| 51:D5:40:LYS:HE3 | 51:D5:46:CYS:HB2 | 1.75 | 0.67 |
| 1:CA:182:U:H5 | 1:CA:183:G:C4 | 2.11 | 0.67 |
| 20:AW:71:THR:HG22 | 20:AW:72:LEU:N | 2.07 | 0.67 |
| 35:DO:11:GLY:C | 35:DO:13:ASN:H | 1.97 | 0.67 |
| 45:DV:128:VAL:HG23 | 45:DV:160:GLY:HA3 | 1.76 | 0.67 |
| 30:DG:111:LEU:HB3 | 30:DG:117:PHE:CE2 | 2.29 | 0.67 |
| 50:D4:61:ARG:HG3 | 50:D4:62:ARG:HH21 | 1.60 | 0.67 |
| 15:CR:21:ASP:OD1 | 15:CR:24:SER:HB2 | 1.93 | 0.67 |
| 32:DK:4:ILE:HG12 | 32:DK:18:VAL:HG22 | 1.76 | 0.67 |
| 2:AE:185:ILE:HB | 2:AE:199:TYR:HB2 | 1.76 | 0.67 |
| 26:DB:55:U:O2' | 26:DB:56:G:H5' | 1.94 | 0.67 |
| 25:BA:1983:C:C2' | 25:BA:1984:G:H5' | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 49:BX:19:GLN:HE22 | 49:BX:52:HIS:HE1 | 1.42 | 0.67 |
| 38:BQ:85:VAL:CG2 | 38:BQ:112:PHE:CE1 | 2.77 | 0.67 |
| 54:D8:50:LEU:N | 54:D8:50:LEU:HD12 | 2.08 | 0.67 |
| 1:CA:1023:G:H3' | 1:CA:1024:G:H5'' | 1.76 | 0.67 |
| 32:DK:82:ARG:HH11 | 32:DK:146:ALA:HA | 1.59 | 0.67 |
| 39:DR:88:ILE:HG13 | 39:DR:88:ILE:O | 1.94 | 0.67 |
| 25:DA:2776:A:H3' | 25:DA:2776:A:OP1 | 1.94 | 0.67 |
| 40:B1:92:ARG:HD2 | 40:B1:95:LEU:HD12 | 1.77 | 0.67 |
| 2:AE:7:VAL:HB | 2:AE:217:ARG:NH2 | 2.10 | 0.67 |
| 27:BD:270:ILE:HG22 | 27:BD:271:ILE:N | 2.09 | 0.67 |
| 2:CE:84:GLU:O | 2:CE:219:VAL:HG21 | 1.94 | 0.67 |
| 7:AJ:62:PHE:CD1 | 7:AJ:124:LEU:HD21 | 2.26 | 0.67 |
| 3:CF:58:GLU:O | 3:CF:59:ARG:HG3 | 1.95 | 0.67 |
| 2:CE:77:ALA:HB2 | 2:CE:211:ILE:HD13 | 1.75 | 0.67 |
| 25:BA:1827:C:C2' | 25:BA:1828:G:H5' | 2.25 | 0.67 |
| 1:CA:8:A:N6 | 4:CG:209:ARG:HB2 | 2.09 | 0.67 |
| 25:BA:1294:U:O2' | 37:B0:23:ASN:ND2 | 2.27 | 0.67 |
| 25:DA:1266:G:O5' | 42:DS:15:ARG:NH2 | 2.27 | 0.67 |
| 25:DA:1287:A:N7 | 37:D0:107:ASP:HB3 | 2.10 | 0.67 |
| 27:BD:35:LYS:CG | 27:BD:64:ILE:N | 2.53 | 0.67 |
| 39:DR:22:PHE:CE2 | 39:DR:86:ILE:HD11 | 2.29 | 0.67 |
| 25:DA:1056:G:H5'' | 25:DA:1057:A:H5' | 1.76 | 0.67 |
| 1:CA:1443:G:O2' | 39:DR:122:ASP:OD2 | 2.12 | 0.67 |
| 25:BA:1266:G:O4' | 42:BS:15:ARG:NH2 | 2.28 | 0.67 |
| 4:AG:119:GLN:HE21 | 4:AG:123:HIS:CD2 | 2.11 | 0.67 |
| 43:DT:53:LYS:HB3 | 43:DT:82:GLN:HB3 | 1.74 | 0.67 |
| 31:BH:131:VAL:HG12 | 31:BH:132:ARG:N | 2.10 | 0.67 |
| 22:AB:56:G:H2' | 22:AB:57:C:C6 | 2.28 | 0.67 |
| 25:BA:2035:G:H4' | 25:BA:2036:C:OP2 | 1.94 | 0.67 |
| 25:BA:1056:G:O6 | 25:BA:1104:C:N4 | 2.28 | 0.67 |
| 25:DA:2286:A:H4' | 25:DA:2287:A:O4' | 1.95 | 0.67 |
| 40:D1:91:ASP:C | 40:D1:93:LYS:H | 1.98 | 0.67 |
| 28:DE:37:ARG:HA | 28:DE:42:ASP:OD2 | 1.94 | 0.67 |
| 1:AA:1004:A:C1' | 1:AA:1036:G:O6 | 2.43 | 0.67 |
| 25:DA:1332:G:N2 | 25:DA:1609:A:HO2' | 1.91 | 0.67 |
| 45:DV:69:THR:HG22 | 45:DV:90:VAL:HA | 1.76 | 0.67 |
| 25:DA:1204:A:O2' | 25:DA:1205:U:OP2 | 2.10 | 0.67 |
| 30:BG:40:ASN:HD22 | 30:BG:91:ARG:HB2 | 1.59 | 0.67 |
| 35:DO:57:THR:C | 35:DO:59:LEU:H | 1.97 | 0.67 |
| 25:DA:1991:U:H2' | 25:DA:1992:G:H5'' | 1.75 | 0.67 |
| 1:AA:1221:G:O3' | 19:AV:77:THR:HG21 | 1.94 | 0.67 |
| 12:AO:24:VAL:HG13 | 12:AO:98:TYR:CE2 | 2.30 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 20:AW:75:ASN:N | 20:AW:75:ASN:OD1 | 2.27 | 0.67 |
| 10:CM:48:THR:HA | 10:CM:62:HIS:HB3 | 1.77 | 0.67 |
| 1:AA:618:C:H5'' | 1:AA:619:U:H5'' | 1.77 | 0.67 |
| 47:BZ:85:LEU:O | 47:BZ:87:PRO:HD2 | 1.92 | 0.67 |
| 36:DP:34:LEU:HB2 | 36:DP:118:LEU:HD22 | 1.77 | 0.67 |
| 38:DQ:24:LEU:CD2 | 38:DQ:24:LEU:H | 2.07 | 0.67 |
| 25:BA:860:U:H5 | 25:BA:917:A:N1 | 1.91 | 0.67 |
| 11:AN:79:SER:HB2 | 11:AN:106:LYS:HD2 | 1.75 | 0.67 |
| 23:CD:59:A:O2' | 23:CD:60:A:C8 | 2.47 | 0.67 |
| 46:B3:27:GLU:HG3 | 46:B3:68:GLU:HA | 1.75 | 0.67 |
| 13:CP:3:ARG:HG3 | 13:CP:9:ILE:CG1 | 2.24 | 0.67 |
| 32:BK:8:PRO:O | 32:BK:9:LEU:HD13 | 1.95 | 0.67 |
| 25:BA:1178:C:H2' | 25:BA:1179:C:C6 | 2.30 | 0.67 |
| 40:B1:69:CYS:SG | 40:B1:79:PHE:HD1 | 2.17 | 0.67 |
| 37:D0:38:VAL:HB | 37:D0:39:PRO:HD3 | 1.74 | 0.67 |
| 2:CE:132:LYS:HA | 2:CE:135:GLN:HE21 | 1.59 | 0.67 |
| 1:CA:1378:C:H5 | 1:CA:1379:G:N9 | 1.92 | 0.67 |
| 1:AA:1277:C:HO2' | 1:AA:1279:A:H8 | 1.40 | 0.67 |
| 20:AW:73:HIS:HB3 | 20:AW:74:LYS:HG2 | 1.77 | 0.67 |
| 1:CA:1004:A:H5'' | 1:CA:1025:U:C4 | 2.29 | 0.67 |
| 29:BF:46:ARG:HH11 | 29:BF:46:ARG:CG | 2.03 | 0.67 |
| 12:AO:18:VAL:HG23 | 12:AO:19:ARG:N | 2.07 | 0.67 |
| 1:CA:1129:C:N4 | 1:CA:1141:C:H41 | 1.93 | 0.67 |
| 36:DP:78:PRO:O | 36:DP:79:LEU:CD1 | 2.43 | 0.67 |
| 25:DA:1298:C:H5'' | 25:DA:1299:G:OP2 | 1.95 | 0.67 |
| 44:BU:47:LYS:HG3 | 44:BU:60:PHE:CE1 | 2.29 | 0.67 |
| 53:B7:8:ASN:O | 53:B7:8:ASN:ND2 | 2.22 | 0.67 |
| 25:DA:974:G:O2' | 25:DA:975:G:N7 | 2.27 | 0.67 |
| 1:CA:1014:A:H2' | 1:CA:1015:A:C8 | 2.29 | 0.67 |
| 25:BA:1568:G:H5' | 27:BD:60:ARG:HA | 1.75 | 0.67 |
| 1:CA:1321:C:H41 | 1:CA:1322:C:N4 | 1.90 | 0.67 |
| 15:CR:17:ARG:NH1 | 15:CR:17:ARG:HG3 | 1.97 | 0.67 |
| 25:DA:2748:A:N6 | 25:DA:2754:U:H3 | 1.92 | 0.67 |
| 35:BO:11:GLY:C | 35:BO:13:ASN:H | 1.94 | 0.67 |
| 25:BA:1019:U:O2' | 25:BA:1021:A:H2 | 1.78 | 0.67 |
| 9:CL:95:LYS:HD3 | 9:CL:96:LEU:H | 1.58 | 0.67 |
| 15:CR:87:ILE:HG22 | 15:CR:88:ARG:H | 1.60 | 0.67 |
| 25:DA:2531:A:C5' | 31:DH:157:TYR:HE2 | 2.08 | 0.67 |
| 1:AA:1266:G:N2 | 1:AA:1270:C:C2 | 2.63 | 0.67 |
| 8:AK:39:LEU:HB3 | 8:AK:45:ILE:HG12 | 1.75 | 0.67 |
| 31:DH:10:PRO:O | 31:DH:49:VAL:HG12 | 1.95 | 0.67 |
| 4:AG:29:PRO:C | 4:AG:30:LYS:HD3 | 2.14 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|---------------------|-------------|----------|
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.30 | 0.67 |
| 6:AI:24:GLU:HG2 | 6:AI:28:ARG:NH2 | 2.09 | 0.67 |
| 54:D8:34:TRP:O | 54:D8:35:GLN:C | 2.33 | 0.67 |
| 27:BD:181:GLU:HA | 27:BD:272:ALA:HB2 | 1.70 | 0.67 |
| 16:AS:22:THR:CG2 | 16:AS:23:ASP:N | 2.57 | 0.67 |
| 23:AC:21:U:O2' | 23:AC:22:A:H5' | 1.95 | 0.67 |
| 28:BE:14:ILE:CG2 | 28:BE:15:PHE:N | 2.30 | 0.67 |
| 1:CA:254:G:OP1 | 17:CT:67:LYS:O | 2.11 | 0.67 |
| 33:BM:21:LYS:HE2 | 33:BM:138:LEU:HD12 | 1.76 | 0.67 |
| 39:DR:3:ARG:HG2 | 39:DR:6:LEU:H | 1.60 | 0.67 |
| 41:B2:44:LYS:C | 41:B2:46:VAL:H | 1.98 | 0.67 |
| 32:BK:29:TYR:O | 32:BK:32:PRO:HD2 | 1.94 | 0.67 |
| 45:DV:164:ALA:O | 45:DV:165:VAL:HG13 | 1.95 | 0.67 |
| 31:DH:118:PRO:HD2 | 31:DH:121:ILE:HG13 | 1.75 | 0.67 |
| 35:BO:57:THR:C | 35:BO:59:LEU:H | 1.97 | 0.67 |
| 25:BA:2466:C:O2' | 25:BA:2467:C:H5' | 1.95 | 0.67 |
| 52:D6:26:ASN:O | 52:D6:28:ARG:HG2 | 1.95 | 0.67 |
| 25:BA:2308:G:H4' | 25:BA:2309:A:OP2 | 1.94 | 0.67 |
| 41:D2:71:LEU:H | 41:D2:86:GLY:CA | 2.08 | 0.67 |
| 25:BA:1899:G:H21 | 25:BA:1902:C:H5 | 1.43 | 0.67 |
| 1:CA:1126:U:O4 | 1:CA:1281:U:C6 | 2.47 | 0.67 |
| 1:CA:345:C:HO2' | 1:CA:346:G:P | 2.17 | 0.67 |
| 30:BG:166:ASP:HA | 30:BG:169:ALA:HB3 | 1.76 | 0.67 |
| 2:CE:185:ILE:CG2 | 2:CE:199:TYR:HB2 | 2.24 | 0.67 |
| 25:DA:2854:G:C2 | 25:DA:2864:G:C2 | 2.83 | 0.67 |
| 1:AA:250:A:H4' | 1:AA:251:G:H5'' | 1.77 | 0.67 |
| 25:DA:195:A:OP1 | 35:DO:46:LYS:HE2 | 1.95 | 0.67 |
| 25:BA:1932:A:H2' | 25:BA:1933:G:O4' | 1.95 | 0.67 |
| 41:D2:49:THR:O | 41:D2:51:VAL:N | 2.28 | 0.67 |
| 2:AE:233:SER:HB2 | 2:AE:234:PRO:HD2 | 1.76 | 0.67 |
| 28:BE:78:LEU:HD12 | 28:BE:79:ARG:HG2 | 1.75 | 0.67 |
| 36:DP:29:PHE:CB | 36:DP:65:PHE:CE1 | 2.78 | 0.67 |
| 28:BE:48:GLN:HE22 | 28:BE:77:ILE:HD12 | 1.60 | 0.67 |
| 2:AE:32:ILE:HD11 | 2:AE:40:HIS:CB | 2.21 | 0.67 |
| 25:DA:1021:A:H61 | 25:DA:1142(A):A:H61 | 1.41 | 0.67 |
| 26:DB:42:C:H4' | 30:DG:67:LYS:HD3 | 1.76 | 0.67 |
| 25:BA:792:G:H5'' | 25:BA:793:A:H5' | 1.76 | 0.67 |
| 25:BA:2125:G:N1 | 25:BA:2172:U:OP1 | 2.28 | 0.67 |
| 35:DO:128:HIS:HA | 35:DO:147:LEU:HA | 1.76 | 0.67 |
| 25:BA:242:G:H5' | 54:B8:62:LEU:HD22 | 1.77 | 0.67 |
| 1:AA:502:G:OP1 | 12:AO:118:SER:HB3 | 1.95 | 0.67 |
| 25:BA:2335:A:N7 | 25:BA:2337:G:C5 | 2.63 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:CF:14:ILE:HG12 | 3:CF:15:THR:N | 2.10 | 0.67 |
| 25:DA:796:C:H2' | 25:DA:797:C:C6 | 2.30 | 0.67 |
| 35:BO:126:VAL:HG12 | 35:BO:147:LEU:HD22 | 1.76 | 0.67 |
| 12:CO:82:VAL:HG23 | 12:CO:106:ASP:OD1 | 1.95 | 0.67 |
| 25:DA:1283:G:H22 | 25:DA:1286:A:H5' | 1.60 | 0.67 |
| 1:CA:946:A:H2' | 1:CA:947:G:C8 | 2.30 | 0.67 |
| 25:BA:234:C:H2' | 25:BA:235:U:H6 | 1.60 | 0.67 |
| 25:BA:1348:G:H2' | 25:BA:1349:A:H5'' | 1.77 | 0.67 |
| 25:DA:2393:A:OP1 | 54:D8:30:ARG:HB2 | 1.95 | 0.66 |
| 48:DW:70:GLN:HG2 | 48:DW:71:ASN:N | 2.10 | 0.66 |
| 25:DA:2275:C:H5' | 25:DA:2275:C:H6 | 1.59 | 0.66 |
| 31:DH:102:ALA:O | 31:DH:103:LEU:HB3 | 1.94 | 0.66 |
| 25:BA:2154:G:H2' | 25:BA:2155:G:H8 | 1.60 | 0.66 |
| 25:BA:1537:C:H2' | 25:BA:1538:G:C8 | 2.30 | 0.66 |
| 22:CB:55:G:H2' | 22:CB:56:G:C8 | 2.29 | 0.66 |
| 45:BV:76:LEU:CD2 | 45:BV:76:LEU:H | 2.08 | 0.66 |
| 28:BE:13:ARG:HG3 | 39:BR:58:ASN:OD1 | 1.95 | 0.66 |
| 25:BA:32:C:O2' | 25:BA:33:U:H5' | 1.95 | 0.66 |
| 43:DT:11:PRO:HD3 | 48:DW:37:PHE:CD2 | 2.30 | 0.66 |
| 1:AA:1194:U:H2' | 1:AA:1195:C:C6 | 2.30 | 0.66 |
| 1:AA:112:G:OP1 | 16:AS:27:LYS:HD2 | 1.94 | 0.66 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:C8 | 2.47 | 0.66 |
| 41:D2:49:THR:O | 41:D2:50:PRO:C | 2.34 | 0.66 |
| 24:A1:14:U:OP1 | 24:A1:14:U:H4' | 1.93 | 0.66 |
| 31:DH:68:THR:O | 31:DH:72:ILE:HG13 | 1.96 | 0.66 |
| 23:CD:18:C:O2 | 23:CD:18:C:H2' | 1.93 | 0.66 |
| 52:D6:27:LYS:HB3 | 52:D6:27:LYS:HZ3 | 1.60 | 0.66 |
| 25:BA:631:A:P | 54:B8:46:ARG:NH2 | 2.68 | 0.66 |
| 1:AA:1181:G:C2 | 1:AA:1182:G:N2 | 2.63 | 0.66 |
| 25:BA:1568:G:H5'' | 27:BD:61:LEU:HD22 | 1.76 | 0.66 |
| 23:CC:59:A:H4' | 23:CC:60:A:OP1 | 1.93 | 0.66 |
| 4:CG:13:ARG:HD3 | 4:CG:13:ARG:H | 1.60 | 0.66 |
| 47:DZ:92:LYS:HE3 | 47:DZ:97:LEU:HG | 1.77 | 0.66 |
| 25:BA:885:C:H2' | 25:BA:890:A:H61 | 1.59 | 0.66 |
| 25:BA:1689:A:N6 | 25:BA:1698:A:C2 | 2.51 | 0.66 |
| 7:CJ:16:LEU:CD1 | 9:CL:42:ARG:HA | 2.24 | 0.66 |
| 23:AD:19:G:H2' | 23:AD:58:A:N6 | 2.10 | 0.66 |
| 39:BR:50:ILE:HD11 | 39:BR:102:ILE:HD11 | 1.75 | 0.66 |
| 25:DA:2523:G:H8 | 25:DA:2523:G:H5' | 1.60 | 0.66 |
| 45:BV:51:ALA:HB1 | 45:BV:57:ILE:HD11 | 1.77 | 0.66 |
| 28:DE:119:ARG:HG2 | 28:DE:160:TYR:HB2 | 1.77 | 0.66 |
| 6:AI:86:ARG:O | 6:AI:87:ARG:HG2 | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:1819:A:H4' | 25:DA:1820:U:O5' | 1.95 | 0.66 |
| 11:AN:48:ILE:HG13 | 11:AN:63:LEU:HB3 | 1.75 | 0.66 |
| 40:B1:8:VAL:HG23 | 40:B1:11:ARG:HH21 | 1.60 | 0.66 |
| 25:DA:2473:U:O2 | 25:DA:2473:U:H2' | 1.95 | 0.66 |
| 10:AM:30:SER:OG | 10:AM:84:GLN:NE2 | 2.25 | 0.66 |
| 1:CA:581:G:OP1 | 15:CR:61:GLY:HA3 | 1.95 | 0.66 |
| 1:AA:890:G:O2' | 1:AA:906:G:O6 | 2.11 | 0.66 |
| 27:BD:65:ILE:HD11 | 27:BD:67:PHE:CE2 | 2.30 | 0.66 |
| 54:D8:47:LYS:O | 54:D8:48:PHE:HB3 | 1.96 | 0.66 |
| 19:AV:9:VAL:O | 19:AV:9:VAL:HG12 | 1.95 | 0.66 |
| 11:AN:40:ILE:CG2 | 11:AN:75:TYR:HD2 | 2.06 | 0.66 |
| 23:CD:14:A:OP1 | 23:CD:14:A:C8 | 2.49 | 0.66 |
| 23:CD:8:U:H1' | 23:CD:49:C:O4' | 1.94 | 0.66 |
| 25:DA:242:G:H5'' | 54:D8:62:LEU:HD13 | 1.76 | 0.66 |
| 1:CA:1202:G:N2 | 14:CQ:43:CYS:SG | 2.68 | 0.66 |
| 6:AI:3:ARG:O | 6:AI:93:SER:HB2 | 1.95 | 0.66 |
| 37:B0:117:VAL:HG22 | 37:B0:118:GLU:H | 1.60 | 0.66 |
| 48:BW:65:ASN:HD22 | 48:BW:69:ARG:HE | 1.40 | 0.66 |
| 25:BA:1464:C:HO2' | 25:BA:1528:A:H8 | 1.43 | 0.66 |
| 25:BA:1065:U:C5 | 25:BA:1066:U:H6 | 2.12 | 0.66 |
| 40:D1:90:VAL:HG22 | 41:D2:39:LEU:CB | 2.26 | 0.66 |
| 44:DU:97:ARG:NH2 | 44:DU:98:VAL:HB | 2.08 | 0.66 |
| 44:DU:98:VAL:HG13 | 44:DU:99:CYS:H | 1.59 | 0.66 |
| 40:B1:92:ARG:NH1 | 40:B1:94:ASN:HD22 | 1.94 | 0.66 |
| 31:BH:4:ILE:HB | 31:BH:6:ARG:HG3 | 1.78 | 0.66 |
| 25:BA:1359:A:H2' | 25:BA:1360:A:H5' | 1.77 | 0.66 |
| 45:BV:19:ARG:NH1 | 45:BV:84:GLU:HB2 | 2.10 | 0.66 |
| 2:AE:76:GLN:HB3 | 2:AE:211:ILE:CD1 | 2.25 | 0.66 |
| 25:BA:34:C:O2' | 25:BA:35:G:P | 2.53 | 0.66 |
| 14:AQ:46:GLU:O | 14:AQ:50:LYS:HG3 | 1.96 | 0.66 |
| 52:B6:25:LYS:NZ | 52:B6:27:LYS:HD3 | 2.11 | 0.66 |
| 23:CC:1:C:H2' | 23:CC:2:G:OP2 | 1.95 | 0.66 |
| 45:DV:148:ASP:CG | 45:DV:149:SER:N | 2.48 | 0.66 |
| 39:BR:112:ARG:HA | 39:BR:115:ARG:HD2 | 1.77 | 0.66 |
| 8:CK:82:HIS:CD2 | 8:CK:82:HIS:C | 2.68 | 0.66 |
| 46:B3:42:GLY:O | 46:B3:57:PHE:HD1 | 1.79 | 0.66 |
| 27:DD:43:ARG:HB3 | 27:DD:54:ARG:HB2 | 1.78 | 0.66 |
| 3:AF:40:ARG:HG3 | 3:AF:40:ARG:HH11 | 1.59 | 0.66 |
| 25:BA:2439:A:C5' | 25:BA:2439:A:H8 | 2.09 | 0.66 |
| 25:BA:784:A:H5' | 25:BA:785:G:OP1 | 1.95 | 0.66 |
| 29:DF:124:LEU:O | 29:DF:126:VAL:HG13 | 1.94 | 0.66 |
| 29:DF:82:ILE:HD12 | 29:DF:82:ILE:O | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 4:AG:138:TYR:CD2 | 4:AG:139:ARG:N | 2.64 | 0.66 |
| 25:DA:1430:C:H2' | 25:DA:1431:U:C6 | 2.30 | 0.66 |
| 27:DD:218:ARG:HB3 | 27:DD:219:PRO:HD2 | 1.78 | 0.66 |
| 25:BA:1652:A:OP1 | 37:B0:8:ARG:NH1 | 2.28 | 0.66 |
| 1:AA:1027:C:C4' | 1:AA:1028:C:OP1 | 2.43 | 0.66 |
| 17:AT:88:TYR:HD2 | 17:AT:89:LEU:HD23 | 1.61 | 0.66 |
| 28:DE:112:GLY:O | 28:DE:159:HIS:HA | 1.95 | 0.66 |
| 13:AP:107:ALA:HB3 | 13:AP:111:LYS:HD2 | 1.77 | 0.66 |
| 52:D6:45:LYS:HE3 | 52:D6:45:LYS:CA | 2.23 | 0.66 |
| 1:CA:973:G:N3 | 10:CM:55:LYS:NZ | 2.44 | 0.66 |
| 31:BH:159:GLU:HG3 | 31:BH:170:ARG:HH11 | 1.58 | 0.66 |
| 50:B4:15:ILE:HD12 | 50:B4:32:TYR:HD1 | 1.60 | 0.66 |
| 28:DE:11:MET:SD | 28:DE:24:THR:HG22 | 2.34 | 0.66 |
| 7:CJ:22:LEU:HD23 | 7:CJ:62:PHE:CE2 | 2.30 | 0.66 |
| 42:DS:12:ILE:HD13 | 42:DS:17:VAL:HG13 | 1.78 | 0.66 |
| 45:BV:11:GLU:O | 45:BV:36:LYS:NZ | 2.22 | 0.66 |
| 25:DA:2:G:H1 | 25:DA:2901:C:H42 | 1.41 | 0.66 |
| 25:BA:602:G:HO2' | 25:BA:604:G:HO2' | 1.42 | 0.66 |
| 13:AP:49:THR:HG22 | 13:AP:51:ALA:H | 1.61 | 0.66 |
| 54:B8:8:LYS:O | 54:B8:12:LYS:HG3 | 1.96 | 0.66 |
| 38:BQ:26:LEU:HD12 | 38:BQ:39:ILE:HD11 | 1.76 | 0.66 |
| 28:BE:53:PRO:HA | 28:BE:74:PRO:HB3 | 1.77 | 0.66 |
| 1:CA:976:G:H5' | 1:CA:1358:U:O2' | 1.95 | 0.66 |
| 36:BP:68:ILE:CD1 | 36:BP:103:MET:HG2 | 2.22 | 0.66 |
| 10:AM:57:LYS:HE3 | 10:AM:60:ARG:NH2 | 2.10 | 0.66 |
| 32:BK:106:GLY:C | 32:BK:107:VAL:CG2 | 2.63 | 0.66 |
| 2:CE:42:ILE:HD11 | 2:CE:202:PRO:CB | 2.26 | 0.66 |
| 25:BA:2061:G:OP1 | 29:BF:68:LYS:NZ | 2.29 | 0.66 |
| 6:AI:4:TYR:CD1 | 6:AI:92:LYS:HA | 2.28 | 0.66 |
| 5:CH:70:PRO:HB3 | 5:CH:144:THR:HG22 | 1.77 | 0.66 |
| 25:BA:309:G:N3 | 25:BA:329:G:O2' | 2.28 | 0.66 |
| 36:DP:7:MET:HB3 | 36:DP:10:ARG:HH22 | 1.60 | 0.66 |
| 25:DA:2531:A:H5' | 31:DH:157:TYR:CE2 | 2.31 | 0.66 |
| 22:CB:47:C:N3 | 22:CB:56:G:N2 | 2.40 | 0.66 |
| 43:BT:60:ARG:HH22 | 53:B7:47:ARG:HH12 | 1.43 | 0.66 |
| 25:BA:1388:G:O2' | 25:BA:1389:G:H5' | 1.96 | 0.66 |
| 25:BA:1297:C:OP1 | 25:BA:2710:C:H4' | 1.94 | 0.66 |
| 46:B3:60:PHE:N | 46:B3:60:PHE:CD2 | 2.64 | 0.66 |
| 37:D0:100:LEU:HD21 | 37:D0:113:LEU:HD13 | 1.77 | 0.66 |
| 36:DP:66:ILE:O | 36:DP:67:ARG:HB2 | 1.95 | 0.66 |
| 1:CA:1226:C:N4 | 13:CP:104:ARG:HB2 | 2.11 | 0.66 |
| 1:AA:1003:G:H2' | 1:AA:1004:A:H5' | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:1058:U:H3 | 25:DA:1080:A:H61 | 1.43 | 0.66 |
| 25:DA:528:A:C8 | 25:DA:528:A:H3' | 2.31 | 0.66 |
| 25:BA:1786:A:H2 | 25:BA:2606:C:H1' | 1.60 | 0.66 |
| 1:AA:1171:G:O2' | 1:AA:1172:C:H5' | 1.95 | 0.66 |
| 25:BA:654(V):A:H2 | 25:BA:655:A:C2 | 2.14 | 0.66 |
| 14:CQ:22:THR:OG1 | 14:CQ:33:VAL:HG11 | 1.95 | 0.66 |
| 12:AO:91:LYS:HG3 | 12:AO:91:LYS:O | 1.96 | 0.66 |
| 29:DF:101:LEU:O | 29:DF:106:ARG:NH1 | 2.29 | 0.66 |
| 47:BZ:49:VAL:HG11 | 47:BZ:70:VAL:HG11 | 1.75 | 0.66 |
| 2:CE:158:LEU:HD23 | 2:CE:182:ILE:HD11 | 1.78 | 0.66 |
| 25:DA:1671:U:HO2' | 25:DA:1673:U:H5 | 1.41 | 0.66 |
| 1:CA:973:G:N2 | 10:CM:55:LYS:HZ1 | 1.94 | 0.66 |
| 29:BF:177:ALA:HB1 | 29:BF:178:PRO:HD2 | 1.78 | 0.66 |
| 39:DR:92:GLY:HA2 | 39:DR:116:ALA:HA | 1.78 | 0.66 |
| 50:D4:11:PRO:HA | 50:D4:25:TYR:H | 1.58 | 0.66 |
| 26:DB:39:A:H61 | 50:D4:1:MET:HB3 | 1.58 | 0.66 |
| 25:BA:1478:G:H2' | 25:BA:1479:G:H8 | 1.60 | 0.66 |
| 27:BD:270:ILE:C | 27:BD:271:ILE:CG1 | 2.64 | 0.66 |
| 1:AA:192:U:H4' | 20:AW:102:GLY:O | 1.96 | 0.66 |
| 28:BE:111:ARG:HG2 | 37:B0:1:MET:HE1 | 1.77 | 0.66 |
| 25:DA:289:A:H5' | 25:DA:290:G:OP2 | 1.96 | 0.66 |
| 23:AD:45:A:H5'' | 23:AD:46:G:OP2 | 1.96 | 0.66 |
| 50:B4:12:ALA:CB | 50:B4:29:PRO:HA | 2.26 | 0.66 |
| 25:BA:1929:G:H4' | 25:BA:1930:G:OP1 | 1.95 | 0.66 |
| 25:BA:414:C:H2' | 25:BA:415:A:C8 | 2.31 | 0.66 |
| 17:AT:86:GLU:O | 17:AT:90:ILE:HG13 | 1.96 | 0.66 |
| 9:AL:8:GLY:HA3 | 9:AL:79:LEU:HB3 | 1.76 | 0.66 |
| 19:CV:42:PRO:HA | 19:CV:45:VAL:HG13 | 1.77 | 0.66 |
| 34:DN:35:VAL:HG21 | 34:DN:69:ILE:HD13 | 1.78 | 0.66 |
| 1:AA:814:A:N7 | 1:AA:816:A:C4 | 2.64 | 0.66 |
| 41:D2:85:LYS:CG | 41:D2:86:GLY:N | 2.54 | 0.66 |
| 30:BG:67:LYS:CE | 50:B4:6:HIS:CE1 | 2.74 | 0.66 |
| 29:BF:197:ASP:O | 29:BF:198:ALA:HB3 | 1.96 | 0.66 |
| 1:AA:843:U:H5' | 1:AA:848:C:C5 | 2.31 | 0.66 |
| 25:BA:67:U:N3 | 25:BA:74:A:C2 | 2.54 | 0.66 |
| 9:CL:28:VAL:CG2 | 9:CL:63:ILE:HB | 2.25 | 0.66 |
| 38:BQ:11:LYS:HD3 | 38:BQ:91:PRO:HD3 | 1.78 | 0.66 |
| 25:DA:1024:G:C3' | 25:DA:1025:G:H5'' | 2.25 | 0.66 |
| 33:BM:96:GLU:O | 33:BM:96:GLU:HG2 | 1.93 | 0.66 |
| 53:B7:8:ASN:HD21 | 53:B7:11:LYS:N | 1.81 | 0.66 |
| 35:DO:9:ASN:HB3 | 35:DO:10:PRO:CD | 2.26 | 0.66 |
| 2:CE:96:ARG:O | 2:CE:98:LEU:HD23 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 13:AP:17:VAL:O | 13:AP:20:THR:OG1 | 2.08 | 0.66 |
| 25:DA:287:C:H2' | 25:DA:288:C:C6 | 2.31 | 0.66 |
| 23:AD:20:G:C5' | 23:AD:60:A:H61 | 2.09 | 0.66 |
| 25:DA:147:U:H2' | 25:DA:148:C:H5'' | 1.77 | 0.66 |
| 1:CA:1378:C:H5 | 1:CA:1379:G:C4 | 2.14 | 0.66 |
| 25:DA:959:A:N6 | 25:DA:960:A:N1 | 2.44 | 0.66 |
| 25:BA:2756:U:H4' | 25:BA:2757:A:OP1 | 1.96 | 0.66 |
| 25:DA:1599:C:H5'' | 43:DT:35:THR:HG22 | 1.78 | 0.66 |
| 5:AH:84:PHE:HB3 | 5:AH:134:ALA:HB2 | 1.78 | 0.66 |
| 31:BH:94:TYR:CE1 | 31:BH:107:VAL:O | 2.48 | 0.66 |
| 30:BG:130:ASN:HB3 | 30:BG:160:VAL:HA | 1.76 | 0.66 |
| 25:BA:1931:U:H5 | 25:BA:1969:A:N7 | 1.94 | 0.66 |
| 40:D1:91:ASP:O | 40:D1:93:LYS:N | 2.28 | 0.65 |
| 27:BD:35:LYS:NZ | 27:BD:65:ILE:HA | 2.11 | 0.65 |
| 28:DE:42:ASP:HB3 | 28:DE:44:TYR:CE1 | 2.31 | 0.65 |
| 29:DF:25:PRO:CB | 29:DF:28:ILE:HG13 | 2.26 | 0.65 |
| 25:DA:2357:U:OP1 | 46:D3:20:ARG:NH1 | 2.28 | 0.65 |
| 25:BA:654(M):C:C2' | 25:BA:654(N):G:C8 | 2.79 | 0.65 |
| 23:CD:13:C:O2' | 23:CD:14:A:P | 2.53 | 0.65 |
| 4:AG:19:LEU:H | 4:AG:19:LEU:CD2 | 2.08 | 0.65 |
| 25:DA:2129:C:H2' | 25:DA:2130:U:H5' | 1.78 | 0.65 |
| 25:BA:443:A:H1' | 25:BA:1201:C:O4' | 1.96 | 0.65 |
| 45:DV:108:PRO:CB | 45:DV:143:GLY:CA | 2.74 | 0.65 |
| 35:DO:47:ASP:OD1 | 35:DO:50:ARG:NH1 | 2.29 | 0.65 |
| 15:CR:87:ILE:CG2 | 15:CR:88:ARG:N | 2.57 | 0.65 |
| 1:AA:188:U:H2' | 1:AA:189:U:H5'' | 1.77 | 0.65 |
| 33:BM:58:ASP:H | 33:BM:60:ILE:CD1 | 2.09 | 0.65 |
| 1:CA:1347:G:O2' | 1:CA:1373:G:O6 | 2.12 | 0.65 |
| 19:AV:32:LYS:HD2 | 19:AV:57:HIS:CD2 | 2.31 | 0.65 |
| 36:DP:135:ASP:OD1 | 36:DP:137:TYR:HD2 | 1.80 | 0.65 |
| 1:CA:1352:C:OP1 | 21:CX:3:LYS:NZ | 2.27 | 0.65 |
| 44:DU:20:TYR:CD1 | 44:DU:20:TYR:N | 2.63 | 0.65 |
| 32:BK:130:TYR:C | 32:BK:131:LYS:HD2 | 2.16 | 0.65 |
| 1:CA:1206:G:O2' | 3:CF:193:TYR:HA | 1.96 | 0.65 |
| 25:BA:2467:C:O2' | 25:BA:2468:G:C5' | 2.44 | 0.65 |
| 27:BD:272:ALA:CB | 27:BD:273:ARG:CA | 2.37 | 0.65 |
| 36:DP:29:PHE:HD2 | 36:DP:65:PHE:CZ | 2.12 | 0.65 |
| 31:DH:57:ASP:O | 31:DH:62:LYS:HE2 | 1.97 | 0.65 |
| 48:DW:15:LYS:HE2 | 48:DW:67:LYS:HE2 | 1.79 | 0.65 |
| 25:DA:2470:G:P | 36:DP:56:ARG:CZ | 2.84 | 0.65 |
| 1:CA:1305:G:H22 | 1:CA:1331:G:H2' | 1.60 | 0.65 |
| 42:BS:94:ASP:C | 42:BS:95:ILE:CG2 | 2.64 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 30:BG:120:LEU:HD22 | 30:BG:133:LEU:HD12 | 1.78 | 0.65 |
| 49:DX:59:VAL:HG12 | 49:DX:60:GLU:N | 2.10 | 0.65 |
| 7:CJ:20:ASP:HB3 | 7:CJ:23:VAL:CG2 | 2.26 | 0.65 |
| 36:BP:14:ARG:HG2 | 36:BP:41:TRP:CH2 | 2.31 | 0.65 |
| 25:BA:1264:G:H5' | 51:B5:11:THR:HG21 | 1.77 | 0.65 |
| 3:CF:58:GLU:HB2 | 3:CF:65:ALA:HB3 | 1.78 | 0.65 |
| 6:AI:44:GLY:HA2 | 6:AI:59:TYR:CE1 | 2.32 | 0.65 |
| 1:AA:652:U:O4 | 1:AA:752:G:O2' | 2.10 | 0.65 |
| 11:AN:22:HIS:HB3 | 11:AN:29:ILE:HG23 | 1.77 | 0.65 |
| 1:CA:736:C:H2' | 1:CA:737:A:C8 | 2.31 | 0.65 |
| 25:DA:2012:G:OP1 | 42:DS:11:ARG:NH2 | 2.29 | 0.65 |
| 43:DT:57:LEU:N | 43:DT:57:LEU:HD23 | 2.11 | 0.65 |
| 1:AA:160:A:H2' | 1:AA:161:A:O4' | 1.95 | 0.65 |
| 23:CC:30:G:O2' | 23:CC:31:G:H5' | 1.96 | 0.65 |
| 1:AA:1132:C:H2' | 1:AA:1133:G:H8 | 1.59 | 0.65 |
| 1:CA:1226:C:C5 | 13:CP:104:ARG:HB2 | 2.31 | 0.65 |
| 1:CA:1226:C:H4' | 19:CV:80:TYR:OH | 1.96 | 0.65 |
| 25:DA:2311:A:H5'' | 25:DA:2312:U:OP2 | 1.96 | 0.65 |
| 32:BK:104:GLN:O | 32:BK:105:HIS:CB | 2.45 | 0.65 |
| 25:BA:811:U:O5' | 35:BO:21:ARG:O | 2.14 | 0.65 |
| 16:AS:21:VAL:HG22 | 16:AS:34:GLU:O | 1.95 | 0.65 |
| 25:DA:142:G:H2' | 25:DA:143:C:H6 | 1.61 | 0.65 |
| 2:CE:132:LYS:O | 2:CE:136:VAL:HG23 | 1.95 | 0.65 |
| 50:B4:14:ILE:HA | 50:B4:31:ILE:O | 1.97 | 0.65 |
| 25:DA:2633:G:H1' | 28:DE:62:PRO:HG2 | 1.78 | 0.65 |
| 13:AP:115:LYS:O | 13:AP:117:VAL:HG13 | 1.95 | 0.65 |
| 16:AS:54:GLU:O | 16:AS:57:ARG:HB2 | 1.96 | 0.65 |
| 1:CA:652:U:O2' | 1:CA:653:A:N3 | 2.29 | 0.65 |
| 28:BE:183:LEU:HD12 | 28:BE:183:LEU:N | 2.11 | 0.65 |
| 25:DA:228:A:H3' | 25:DA:228:A:C8 | 2.32 | 0.65 |
| 25:BA:2467:C:H4' | 36:BP:123:HIS:CE1 | 2.31 | 0.65 |
| 25:BA:2394:C:OP1 | 35:BO:62:LEU:CB | 2.43 | 0.65 |
| 13:CP:102:ARG:HD3 | 13:CP:105:THR:HG23 | 1.79 | 0.65 |
| 25:DA:2402:C:N4 | 25:DA:2416:C:H1' | 2.12 | 0.65 |
| 19:AV:41:VAL:HB | 19:AV:42:PRO:CA | 2.25 | 0.65 |
| 3:CF:119:ARG:HH22 | 3:CF:140:ARG:CG | 2.07 | 0.65 |
| 25:BA:1557:C:OP2 | 25:BA:1558:A:O2' | 2.13 | 0.65 |
| 9:CL:26:VAL:HG22 | 9:CL:61:ALA:HB3 | 1.77 | 0.65 |
| 31:DH:102:ALA:CB | 31:DH:117:PRO:HD3 | 2.27 | 0.65 |
| 25:DA:2331:G:H4' | 46:D3:43:THR:H | 1.60 | 0.65 |
| 5:AH:11:ILE:HD11 | 5:AH:31:LEU:HB3 | 1.78 | 0.65 |
| 45:DV:158:PRO:HB2 | 45:DV:159:PRO:HD2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 10:AM:37:PRO:HA | 10:AM:72:VAL:HG22 | 1.79 | 0.65 |
| 25:BA:1799:G:O2' | 25:BA:1800:C:OP2 | 2.09 | 0.65 |
| 32:DK:125:GLU:HB2 | 32:DK:141:LYS:HD3 | 1.78 | 0.65 |
| 25:BA:1080:A:H2' | 25:BA:1081:U:C6 | 2.31 | 0.65 |
| 25:DA:2292:C:OP1 | 38:DQ:17:ARG:NH2 | 2.30 | 0.65 |
| 1:CA:922:G:H4' | 5:CH:20:GLN:HA | 1.78 | 0.65 |
| 26:BB:48:A:H4' | 38:BQ:95:HIS:HD2 | 1.61 | 0.65 |
| 25:BA:953:A:OP2 | 36:BP:16:ARG:HD3 | 1.95 | 0.65 |
| 32:DK:114:LEU:HD23 | 32:DK:114:LEU:O | 1.96 | 0.65 |
| 25:BA:2310:A:N3 | 30:BG:77:ILE:HG12 | 2.10 | 0.65 |
| 29:BF:29:ASN:HB3 | 29:BF:112:MET:HE1 | 1.79 | 0.65 |
| 50:D4:1:MET:O | 50:D4:2:LYS:HD3 | 1.97 | 0.65 |
| 4:AG:8:VAL:HG13 | 4:AG:21:LEU:HD13 | 1.79 | 0.65 |
| 25:DA:2128:C:H4' | 25:DA:2173:A:C6 | 2.31 | 0.65 |
| 35:DO:11:GLY:O | 35:DO:13:ASN:N | 2.30 | 0.65 |
| 25:DA:1862:G:C2' | 25:DA:1863:G:H5' | 2.26 | 0.65 |
| 29:DF:36:VAL:HG11 | 29:DF:183:VAL:HG11 | 1.79 | 0.65 |
| 25:BA:1734:C:H2' | 25:BA:1735:C:H5'' | 1.77 | 0.65 |
| 1:CA:728:A:H2' | 1:CA:729:A:C8 | 2.31 | 0.65 |
| 9:CL:32:ASP:HB3 | 9:CL:35:GLU:HB2 | 1.78 | 0.65 |
| 39:DR:51:ARG:HG3 | 39:DR:98:LYS:HG3 | 1.79 | 0.65 |
| 26:BB:73:A:H2' | 26:BB:74:U:H5' | 1.78 | 0.65 |
| 3:AF:78:GLY:HA3 | 3:AF:83:ARG:HB3 | 1.78 | 0.65 |
| 23:AC:56:U:O2 | 23:AC:58:A:C8 | 2.49 | 0.65 |
| 29:DF:68:LYS:NZ | 29:DF:68:LYS:HA | 2.11 | 0.65 |
| 30:BG:64:THR:HG23 | 30:BG:66:GLN:H | 1.61 | 0.65 |
| 25:BA:2371:G:H1' | 52:B6:45:LYS:HD2 | 1.79 | 0.65 |
| 1:AA:789:U:H5 | 1:AA:792:A:OP2 | 1.79 | 0.65 |
| 25:BA:654(N):G:H2' | 25:BA:654(O):G:C8 | 2.32 | 0.65 |
| 1:CA:1128:C:N4 | 1:CA:1139:G:C2 | 2.64 | 0.65 |
| 30:DG:102:PHE:HE2 | 30:DG:141:PHE:CE1 | 2.15 | 0.65 |
| 10:CM:78:ASN:HB2 | 10:CM:81:THR:H | 1.60 | 0.65 |
| 4:AG:110:PHE:HD1 | 4:AG:110:PHE:N | 1.94 | 0.65 |
| 25:DA:2572:A:C8 | 28:DE:144:ARG:HD2 | 2.31 | 0.65 |
| 25:BA:1025:G:C4 | 25:BA:1135:C:H1' | 2.32 | 0.65 |
| 2:CE:144:ARG:HD2 | 2:CE:148:TYR:HE2 | 1.61 | 0.65 |
| 25:DA:6:A:H4' | 33:DM:129:PRO:HB2 | 1.78 | 0.65 |
| 25:BA:1177:A:H4' | 25:BA:1178:C:H5'' | 1.78 | 0.65 |
| 4:CG:24:GLU:O | 4:CG:27:TYR:HB2 | 1.97 | 0.65 |
| 1:AA:737:A:H2' | 1:AA:738:C:C6 | 2.31 | 0.65 |
| 31:DH:26:VAL:HG21 | 31:DH:75:ALA:O | 1.97 | 0.65 |
| 25:DA:1262:A:N3 | 51:D5:10:LYS:HE3 | 2.12 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 4:AG:13:ARG:O | 4:AG:15:GLU:N | 2.30 | 0.65 |
| 28:DE:36:ARG:HG2 | 28:DE:36:ARG:HH11 | 1.60 | 0.65 |
| 28:DE:53:PRO:O | 28:DE:54:GLN:C | 2.35 | 0.65 |
| 1:AA:1004:A:H8 | 1:AA:1036:G:H22 | 1.43 | 0.65 |
| 9:CL:18:PHE:HD1 | 9:CL:62:TYR:HD2 | 1.45 | 0.65 |
| 42:BS:88:ARG:HB3 | 42:BS:92:ARG:HB3 | 1.79 | 0.65 |
| 25:DA:90:U:H2' | 25:DA:91:A:H5'' | 1.77 | 0.65 |
| 44:DU:17:SER:OG | 44:DU:18:GLY:O | 2.13 | 0.65 |
| 19:CV:31:ILE:HG22 | 19:CV:50:ALA:H | 1.61 | 0.65 |
| 40:B1:69:CYS:HG | 40:B1:79:PHE:HD1 | 1.40 | 0.65 |
| 45:BV:105:VAL:HG22 | 45:BV:106:GLY:H | 1.60 | 0.65 |
| 1:CA:422:C:O2' | 1:CA:423:G:C2 | 2.50 | 0.65 |
| 31:DH:48:GLY:O | 31:DH:49:VAL:HG13 | 1.97 | 0.65 |
| 4:CG:43:HIS:HA | 4:CG:46:LYS:HG3 | 1.79 | 0.65 |
| 25:DA:2364:C:C2' | 25:DA:2365:G:H5' | 2.27 | 0.65 |
| 25:DA:617:G:OP1 | 29:DF:40:GLN:HG2 | 1.95 | 0.65 |
| 37:B0:44:LEU:HD22 | 37:B0:48:VAL:CG2 | 2.26 | 0.65 |
| 50:B4:9:LEU:H | 50:B4:27:THR:HG23 | 1.61 | 0.65 |
| 36:DP:54:MET:CE | 36:DP:118:LEU:HD23 | 2.26 | 0.65 |
| 1:CA:1320:C:H2' | 1:CA:1321:C:H6 | 1.59 | 0.65 |
| 45:DV:115:GLY:HA3 | 45:DV:174:VAL:CG1 | 2.27 | 0.65 |
| 1:AA:1305:G:H22 | 1:AA:1331:G:C2' | 2.01 | 0.65 |
| 36:DP:88:GLY:O | 36:DP:89:ASN:HB2 | 1.95 | 0.65 |
| 30:BG:133:LEU:CD2 | 30:BG:157:ILE:HB | 2.27 | 0.65 |
| 25:DA:2137:C:N4 | 25:DA:2154:G:H1 | 1.94 | 0.65 |
| 38:BQ:9:ARG:O | 38:BQ:12:PHE:N | 2.30 | 0.65 |
| 42:BS:79:GLY:HA3 | 42:BS:100:THR:HG22 | 1.77 | 0.65 |
| 3:CF:29:TYR:OH | 14:CQ:54:PRO:HD2 | 1.96 | 0.65 |
| 4:CG:178:VAL:HG12 | 4:CG:179:GLU:H | 1.62 | 0.65 |
| 44:DU:87:LYS:HB3 | 44:DU:92:ASN:HB3 | 1.79 | 0.65 |
| 12:CO:110:VAL:CG2 | 12:CO:120:TYR:HB3 | 2.26 | 0.65 |
| 25:DA:627:A:N7 | 35:DO:84:ASN:ND2 | 2.45 | 0.65 |
| 25:DA:443:A:H1' | 25:DA:1201:C:O4' | 1.96 | 0.65 |
| 25:BA:581:C:H2' | 25:BA:582:G:H8 | 1.62 | 0.65 |
| 25:BA:2150:U:H2' | 25:BA:2151:G:C8 | 2.31 | 0.65 |
| 1:CA:660:G:H2' | 1:CA:661:G:O4' | 1.95 | 0.65 |
| 3:CF:138:VAL:HG23 | 3:CF:151:VAL:HG23 | 1.79 | 0.65 |
| 36:BP:39:PRO:HA | 36:BP:97:VAL:O | 1.97 | 0.65 |
| 27:DD:35:LYS:HG2 | 27:DD:64:ILE:H | 1.59 | 0.65 |
| 48:BW:50:ILE:O | 48:BW:54:LYS:HB2 | 1.96 | 0.65 |
| 25:DA:1332:G:N2 | 25:DA:1610:A:H8 | 1.95 | 0.65 |
| 38:BQ:88:ASP:OD1 | 38:BQ:90:GLY:N | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:827:U:C5 | 1:AA:872:A:N1 | 2.64 | 0.65 |
| 35:BO:47:ASP:OD1 | 35:BO:50:ARG:NH2 | 2.29 | 0.65 |
| 39:BR:60:THR:HG22 | 39:BR:77:PRO:HA | 1.77 | 0.65 |
| 19:CV:39:THR:HG22 | 19:CV:40:ILE:H | 1.61 | 0.65 |
| 13:CP:3:ARG:HH11 | 30:DG:113:ARG:HH21 | 1.45 | 0.65 |
| 25:DA:38:A:H2' | 25:DA:39:C:C6 | 2.32 | 0.65 |
| 41:B2:38:LEU:O | 41:B2:51:VAL:HG13 | 1.97 | 0.65 |
| 40:B1:79:PHE:HE1 | 40:B1:106:PHE:CZ | 2.15 | 0.65 |
| 25:BA:1188:U:C4' | 41:B2:79:VAL:HG22 | 2.27 | 0.65 |
| 44:DU:87:LYS:O | 44:DU:88:LYS:HD3 | 1.97 | 0.65 |
| 3:AF:123:GLN:O | 3:AF:128:PHE:HB2 | 1.97 | 0.65 |
| 25:DA:2820:A:O2' | 25:DA:2821:A:OP1 | 2.14 | 0.65 |
| 37:B0:9:LYS:HA | 37:B0:17:ARG:NE | 2.12 | 0.65 |
| 1:CA:920:U:H2' | 1:CA:921:U:C6 | 2.31 | 0.65 |
| 1:CA:719:C:C5 | 1:CA:720:C:C4 | 2.85 | 0.65 |
| 12:AO:40:VAL:HG21 | 12:AO:78:GLN:O | 1.96 | 0.65 |
| 39:DR:65:LYS:HE2 | 39:DR:67:SER:HB2 | 1.79 | 0.65 |
| 36:DP:26:TYR:HE1 | 36:DP:139:GLU:CB | 1.93 | 0.65 |
| 25:DA:932:G:H4' | 25:DA:933:A:O5' | 1.96 | 0.65 |
| 33:DM:42:TRP:O | 40:D1:64:ARG:NH2 | 2.30 | 0.65 |
| 26:BB:42:C:O2' | 30:BG:67:LYS:HE3 | 1.96 | 0.65 |
| 44:BU:81:LYS:HG2 | 44:BU:96:ILE:HB | 1.79 | 0.65 |
| 13:CP:40:ASN:HB3 | 13:CP:43:THR:HG23 | 1.77 | 0.65 |
| 25:BA:1021:A:H61 | 25:BA:1142(A):A:N6 | 1.94 | 0.65 |
| 36:DP:79:LEU:CD1 | 36:DP:80:GLU:HB2 | 2.26 | 0.65 |
| 25:DA:1678:G:N2 | 25:DA:1989:G:N2 | 2.44 | 0.65 |
| 38:BQ:35:ILE:HD11 | 38:BQ:101:LEU:HD23 | 1.79 | 0.65 |
| 2:AE:215:LEU:O | 2:AE:219:VAL:HG23 | 1.97 | 0.65 |
| 25:BA:594:U:H5' | 54:B8:61:LEU:CD1 | 2.27 | 0.65 |
| 25:DA:2854:G:N2 | 25:DA:2864:G:N3 | 2.45 | 0.65 |
| 25:DA:1485:G:C2' | 25:DA:1486:A:H5' | 2.27 | 0.65 |
| 36:BP:19:GLY:O | 36:BP:21:THR:OG1 | 2.10 | 0.65 |
| 25:DA:195:A:OP1 | 35:DO:46:LYS:HE3 | 1.96 | 0.65 |
| 47:DZ:4:VAL:HG11 | 47:DZ:11:ARG:NH1 | 2.12 | 0.65 |
| 1:AA:1432:G:OP1 | 39:BR:107:ASP:HB2 | 1.96 | 0.65 |
| 25:DA:797:C:OP2 | 29:DF:62:ARG:HG3 | 1.98 | 0.65 |
| 27:BD:130:ALA:C | 27:BD:131:LEU:HD12 | 2.17 | 0.65 |
| 28:DE:103:ASP:OD1 | 28:DE:201:THR:HG23 | 1.97 | 0.65 |
| 16:CS:48:TRP:HH2 | 16:CS:76:GLN:HE22 | 1.43 | 0.65 |
| 25:BA:323:G:H5' | 29:BF:169:ASN:HD21 | 1.62 | 0.65 |
| 25:DA:986:C:C2' | 25:DA:987:G:H5' | 2.27 | 0.65 |
| 51:B5:20:ARG:HG3 | 51:B5:23:HIS:CD2 | 2.32 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 31:BH:9:ILE:H | 31:BH:9:ILE:HD12 | 1.62 | 0.65 |
| 1:AA:723:U:H2' | 1:AA:723:U:O2 | 1.97 | 0.65 |
| 45:DV:76:LEU:HD23 | 45:DV:76:LEU:N | 2.11 | 0.64 |
| 28:BE:35:GLN:HG3 | 28:BE:36:ARG:N | 2.09 | 0.64 |
| 26:BB:15:A:O2' | 26:BB:109:G:C8 | 2.48 | 0.64 |
| 27:DD:28:GLU:HB3 | 27:DD:29:PRO:HD2 | 1.77 | 0.64 |
| 54:B8:26:LYS:HB3 | 54:B8:44:LYS:HG3 | 1.79 | 0.64 |
| 31:DH:4:ILE:HG13 | 31:DH:6:ARG:HG2 | 1.79 | 0.64 |
| 1:CA:1119:C:OP2 | 9:CL:9:ARG:NH2 | 2.30 | 0.64 |
| 23:AD:57:C:H42 | 25:BA:2112:G:H1 | 1.43 | 0.64 |
| 45:DV:108:PRO:HA | 45:DV:143:GLY:H | 1.62 | 0.64 |
| 30:DG:109:VAL:HG11 | 30:DG:142:PRO:HD3 | 1.79 | 0.64 |
| 1:CA:1190:G:H3' | 3:CF:3:ASN:ND2 | 2.12 | 0.64 |
| 2:CE:231:GLU:HB3 | 2:CE:232:PRO:HD2 | 1.77 | 0.64 |
| 2:CE:92:TYR:CD2 | 2:CE:151:GLY:HA3 | 2.31 | 0.64 |
| 29:DF:123:LEU:O | 29:DF:123:LEU:HD12 | 1.96 | 0.64 |
| 29:DF:34:TRP:CE3 | 35:DO:8:PRO:HB3 | 2.32 | 0.64 |
| 32:DK:25:TYR:CE2 | 32:DK:29:TYR:CD2 | 2.85 | 0.64 |
| 28:DE:128:SER:O | 28:DE:129:HIS:HB2 | 1.96 | 0.64 |
| 4:AG:107:ARG:HH22 | 4:AG:194:LEU:HD11 | 1.60 | 0.64 |
| 20:AW:9:ASN:ND2 | 20:AW:9:ASN:O | 2.30 | 0.64 |
| 20:CW:26:ASN:HB2 | 20:CW:71:THR:HG23 | 1.78 | 0.64 |
| 30:BG:83:ARG:CG | 30:BG:86:MET:HE1 | 2.20 | 0.64 |
| 31:DH:150:ALA:O | 31:DH:152:ARG:N | 2.30 | 0.64 |
| 19:AV:40:ILE:HD11 | 19:AV:62:ILE:CG2 | 2.26 | 0.64 |
| 32:BK:106:GLY:C | 32:BK:107:VAL:HG22 | 2.17 | 0.64 |
| 33:BM:96:GLU:O | 33:BM:96:GLU:CG | 2.45 | 0.64 |
| 25:DA:780:G:N2 | 25:DA:783:A:H62 | 1.91 | 0.64 |
| 25:DA:2689:U:C4' | 25:DA:2690:C:H5' | 2.28 | 0.64 |
| 7:AJ:22:LEU:HD23 | 7:AJ:62:PHE:CE2 | 2.32 | 0.64 |
| 1:CA:1090:U:H2' | 1:CA:1091:U:C6 | 2.32 | 0.64 |
| 40:B1:79:PHE:C | 40:B1:79:PHE:HD2 | 2.00 | 0.64 |
| 3:AF:152:ILE:HG13 | 3:AF:167:TRP:HB2 | 1.79 | 0.64 |
| 25:DA:1204:A:C2 | 25:DA:1241:A:N1 | 2.66 | 0.64 |
| 31:DH:169:VAL:HG13 | 31:DH:170:ARG:H | 1.62 | 0.64 |
| 25:BA:2312:U:O2 | 30:BG:42:GLY:HA3 | 1.97 | 0.64 |
| 25:BA:2590:A:OP2 | 27:BD:237:GLU:HB3 | 1.97 | 0.64 |
| 9:AL:83:ARG:HA | 9:AL:86:VAL:HG12 | 1.79 | 0.64 |
| 36:BP:17:LEU:HD13 | 36:BP:39:PRO:HB2 | 1.79 | 0.64 |
| 29:DF:153:SER:OG | 29:DF:190:GLU:HG3 | 1.97 | 0.64 |
| 25:BA:370:G:H4' | 25:BA:371:A:OP2 | 1.96 | 0.64 |
| 25:BA:598:G:H1' | 35:BO:12:ALA:HB2 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 39:BR:93:ARG:HG3 | 39:BR:93:ARG:HH11 | 1.63 | 0.64 |
| 16:AS:17:TYR:CE1 | 16:AS:41:PRO:HG3 | 2.33 | 0.64 |
| 27:DD:35:LYS:HD3 | 27:DD:63:ARG:HB3 | 1.79 | 0.64 |
| 38:DQ:85:VAL:HG12 | 38:DQ:86:ALA:H | 1.61 | 0.64 |
| 41:D2:75:PHE:CD2 | 41:D2:81:TYR:CD1 | 2.85 | 0.64 |
| 13:CP:91:ARG:NH2 | 13:CP:96:LEU:HD13 | 2.12 | 0.64 |
| 44:DU:81:LYS:HB3 | 44:DU:82:PRO:HD2 | 1.80 | 0.64 |
| 54:B8:36:LYS:CD | 54:B8:40:GLU:HG2 | 2.27 | 0.64 |
| 25:BA:1019:U:O2' | 25:BA:1021:A:C2 | 2.49 | 0.64 |
| 25:DA:2314:C:O2' | 25:DA:2315:G:H5' | 1.97 | 0.64 |
| 40:B1:90:VAL:HG12 | 40:B1:91:ASP:HA | 1.78 | 0.64 |
| 25:DA:2689:U:C5' | 25:DA:2690:C:H5' | 2.28 | 0.64 |
| 12:CO:26:ALA:HA | 12:CO:98:TYR:HE2 | 1.61 | 0.64 |
| 1:AA:1226:C:OP2 | 13:AP:103:THR:OG1 | 2.13 | 0.64 |
| 23:AD:15:G:H2' | 23:AD:60:A:H2 | 1.61 | 0.64 |
| 1:AA:195:A:C5 | 1:AA:196:A:N1 | 2.65 | 0.64 |
| 1:CA:77:C:H42 | 1:CA:92:G:H1 | 1.42 | 0.64 |
| 2:CE:121:LEU:HD23 | 2:CE:127:ILE:HG12 | 1.80 | 0.64 |
| 28:BE:81:ILE:HG21 | 28:BE:84:PHE:HD1 | 1.55 | 0.64 |
| 1:CA:973:G:N3 | 10:CM:55:LYS:CE | 2.60 | 0.64 |
| 1:CA:1160:G:O6 | 1:CA:1181:G:C6 | 2.51 | 0.64 |
| 41:B2:47:VAL:HG23 | 41:B2:48:GLY:N | 2.10 | 0.64 |
| 9:CL:16:ARG:O | 9:CL:63:ILE:HG23 | 1.98 | 0.64 |
| 25:BA:34:C:O4' | 25:BA:34:C:OP2 | 2.15 | 0.64 |
| 1:AA:105:G:H2' | 1:AA:106:C:H6 | 1.63 | 0.64 |
| 28:DE:62:PRO:C | 28:DE:64:LYS:H | 2.00 | 0.64 |
| 31:DH:9:ILE:HD12 | 31:DH:49:VAL:HG21 | 1.79 | 0.64 |
| 32:BK:131:LYS:HB3 | 32:BK:132:PRO:HA | 1.79 | 0.64 |
| 1:AA:724:G:O2' | 1:AA:725:G:H5' | 1.97 | 0.64 |
| 3:AF:7:PRO:O | 3:AF:11:ARG:HG2 | 1.97 | 0.64 |
| 1:AA:114:U:O2' | 1:AA:115:G:H5' | 1.97 | 0.64 |
| 25:BA:550:G:O2' | 25:BA:1220:A:N3 | 2.25 | 0.64 |
| 5:CH:73:ASN:OD1 | 5:CH:73:ASN:N | 2.31 | 0.64 |
| 1:AA:1263:C:H2' | 1:AA:1264:C:H6 | 1.62 | 0.64 |
| 1:AA:452:A:OP2 | 16:AS:43:LYS:NZ | 2.30 | 0.64 |
| 25:BA:1062:G:N3 | 25:BA:1077:A:N6 | 2.46 | 0.64 |
| 36:DP:65:PHE:O | 36:DP:66:ILE:C | 2.35 | 0.64 |
| 30:BG:78:SER:O | 30:BG:79:ASN:C | 2.36 | 0.64 |
| 28:BE:35:GLN:NE2 | 28:BE:37:ARG:HH12 | 1.95 | 0.64 |
| 1:CA:963:G:N2 | 10:CM:55:LYS:HD3 | 1.99 | 0.64 |
| 1:AA:1032(B):G:H2' | 1:AA:1033:G:C8 | 2.32 | 0.64 |
| 25:BA:592:G:H21 | 54:B8:4:MET:HE1 | 1.60 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 6:AI:89:MET:HE1 | 18:AU:76:LEU:HD23 | 1.78 | 0.64 |
| 25:DA:2125:G:N2 | 25:DA:2172:U:O5' | 2.28 | 0.64 |
| 45:BV:151:HIS:HD2 | 45:BV:168:GLU:HG3 | 1.62 | 0.64 |
| 25:DA:2772:C:H5' | 28:DE:168:MET:HE3 | 1.78 | 0.64 |
| 1:AA:719:C:O2' | 18:AU:49:LYS:HB3 | 1.96 | 0.64 |
| 36:DP:35:VAL:HG22 | 36:DP:130:LYS:HB3 | 1.79 | 0.64 |
| 38:DQ:88:ASP:OD2 | 38:DQ:89:ARG:N | 2.30 | 0.64 |
| 41:D2:72:VAL:O | 41:D2:84:LYS:HB3 | 1.96 | 0.64 |
| 39:DR:56:GLY:O | 39:DR:59:THR:HG23 | 1.97 | 0.64 |
| 45:DV:144:LEU:C | 45:DV:146:ILE:H | 1.99 | 0.64 |
| 25:DA:1012:U:C4 | 33:DM:25:ARG:HD3 | 2.32 | 0.64 |
| 29:DF:28:ILE:HA | 29:DF:112:MET:HE3 | 1.79 | 0.64 |
| 46:B3:23:VAL:HA | 46:B3:38:VAL:HG22 | 1.79 | 0.64 |
| 54:B8:36:LYS:HB2 | 54:B8:40:GLU:CG | 2.23 | 0.64 |
| 37:D0:87:TYR:CE1 | 37:D0:117:VAL:HG12 | 2.26 | 0.64 |
| 50:B4:16:CYS:SG | 50:B4:17:GLY:N | 2.71 | 0.64 |
| 39:DR:50:ILE:HD11 | 39:DR:102:ILE:CD1 | 2.25 | 0.64 |
| 25:DA:2191:G:HO2' | 25:DA:2192:G:P | 2.19 | 0.64 |
| 28:BE:26:ILE:CD1 | 28:BE:198:VAL:CG2 | 2.74 | 0.64 |
| 52:B6:24:GLU:HG3 | 52:B6:25:LYS:H | 1.63 | 0.64 |
| 1:AA:474:G:H2' | 1:AA:475:G:C8 | 2.33 | 0.64 |
| 28:BE:92:THR:O | 28:BE:95:ILE:HG12 | 1.97 | 0.64 |
| 32:BK:46:ALA:O | 32:BK:50:ARG:HD3 | 1.97 | 0.64 |
| 20:CW:49:ALA:HA | 20:CW:52:ALA:HB3 | 1.80 | 0.64 |
| 33:DM:62:VAL:HG22 | 33:DM:66:LYS:HD2 | 1.80 | 0.64 |
| 25:BA:2580:U:H4' | 28:BE:130:GLY:HA3 | 1.79 | 0.64 |
| 45:DV:116:VAL:HG12 | 45:DV:117:LEU:H | 1.61 | 0.64 |
| 25:DA:988:A:H3' | 49:DX:11:SER:OG | 1.98 | 0.64 |
| 16:AS:49:LEU:HD12 | 16:AS:50:LYS:N | 2.13 | 0.64 |
| 10:CM:4:ILE:HD13 | 10:CM:100:THR:CG2 | 2.27 | 0.64 |
| 3:CF:70:VAL:HG11 | 3:CF:76:VAL:HG11 | 1.79 | 0.64 |
| 3:CF:73:PRO:O | 3:CF:76:VAL:HG22 | 1.98 | 0.64 |
| 1:CA:1374:A:H2' | 1:CA:1375:A:H5' | 1.80 | 0.64 |
| 25:BA:1486:A:H2' | 25:BA:1487:G:H8 | 1.61 | 0.64 |
| 25:DA:2765:A:H2 | 25:DA:2766:G:O4' | 1.80 | 0.64 |
| 18:AU:36:ASN:H | 18:AU:36:ASN:HD22 | 1.44 | 0.64 |
| 38:BQ:111:GLU:HA | 38:BQ:111:GLU:OE1 | 1.97 | 0.64 |
| 25:BA:1061:U:H1' | 25:BA:1070:A:C2 | 2.33 | 0.64 |
| 28:BE:57:LYS:O | 28:BE:59:VAL:N | 2.30 | 0.64 |
| 28:DE:79:ARG:O | 28:DE:80:GLU:HG3 | 1.98 | 0.64 |
| 29:DF:25:PRO:HB3 | 29:DF:28:ILE:CG1 | 2.28 | 0.64 |
| 1:AA:976:G:OP1 | 14:AQ:32:SER:N | 2.29 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 23:CD:15:G:N2 | 23:CD:49:C:C2 | 2.64 | 0.64 |
| 1:CA:1142:G:H2' | 1:CA:1143:G:O4' | 1.98 | 0.64 |
| 1:CA:560:U:H5' | 1:CA:566:G:N2 | 2.12 | 0.64 |
| 25:DA:70:G:H21 | 25:DA:71:A:H62 | 1.46 | 0.64 |
| 25:DA:857:C:H4' | 46:D3:23:VAL:HG21 | 1.79 | 0.64 |
| 25:BA:2444:G:OP2 | 29:BF:68:LYS:CE | 2.46 | 0.64 |
| 2:AE:88:ALA:HB2 | 2:AE:219:VAL:HG13 | 1.80 | 0.64 |
| 30:DG:109:VAL:HG13 | 50:D4:33:VAL:CG1 | 2.27 | 0.64 |
| 31:BH:153:LYS:HD2 | 31:BH:153:LYS:N | 2.11 | 0.64 |
| 25:BA:140:A:H8 | 25:BA:1408:C:O2' | 1.81 | 0.64 |
| 22:CB:44:G:H2' | 22:CB:45:U:O4' | 1.97 | 0.64 |
| 1:AA:659:U:C2 | 1:AA:660:G:C8 | 2.86 | 0.64 |
| 1:CA:1216:G:H2' | 1:CA:1217:C:C6 | 2.32 | 0.64 |
| 28:DE:151:TYR:HD2 | 28:DE:154:LYS:NZ | 1.96 | 0.64 |
| 1:CA:273:A:C2' | 1:CA:274:A:H5' | 2.27 | 0.64 |
| 1:AA:411:A:N7 | 1:AA:413:G:N3 | 2.45 | 0.64 |
| 1:AA:1027:C:H4' | 1:AA:1028:C:OP1 | 1.97 | 0.64 |
| 26:BB:73:A:C2' | 26:BB:74:U:H5' | 2.28 | 0.64 |
| 25:DA:872:A:C5 | 25:DA:906:G:C2 | 2.86 | 0.64 |
| 27:DD:72:LYS:HE2 | 27:DD:101:GLU:OE2 | 1.98 | 0.64 |
| 25:DA:105:C:O2' | 44:DU:2:ARG:HD2 | 1.98 | 0.64 |
| 6:AI:62:TRP:CH2 | 6:AI:64:GLN:HG3 | 2.33 | 0.64 |
| 46:D3:72:ARG:HB2 | 46:D3:75:LEU:HB2 | 1.80 | 0.64 |
| 25:BA:1118:C:H2' | 25:BA:1119:C:C6 | 2.33 | 0.64 |
| 25:BA:1416:G:O2' | 25:BA:1417:C:O5' | 2.12 | 0.64 |
| 39:BR:31:SER:OG | 39:BR:85:LYS:HE2 | 1.98 | 0.64 |
| 8:AK:88:LYS:HB3 | 8:AK:89:PRO:HD2 | 1.77 | 0.64 |
| 22:CB:3:C:H6 | 22:CB:3:C:O5' | 1.80 | 0.64 |
| 3:CF:27:LYS:HB3 | 3:CF:27:LYS:NZ | 2.13 | 0.64 |
| 38:BQ:83:LYS:C | 38:BQ:109:GLY:HA2 | 2.12 | 0.64 |
| 25:BA:70:G:H21 | 25:BA:71:A:H62 | 1.43 | 0.64 |
| 22:CB:85:C:C6 | 25:DA:2555:U:O2 | 2.50 | 0.64 |
| 14:AQ:21:TYR:HE2 | 14:AQ:23:ARG:NE | 1.96 | 0.64 |
| 25:BA:1021:A:H8 | 25:BA:1022:G:H5'' | 1.62 | 0.64 |
| 1:CA:1128:C:C4 | 1:CA:1139:G:C2 | 2.85 | 0.64 |
| 9:CL:53:VAL:HG13 | 9:CL:95:LYS:HE3 | 1.78 | 0.64 |
| 1:AA:438:G:O2' | 1:AA:439:A:H5'' | 1.98 | 0.64 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:N2 | 1.95 | 0.64 |
| 22:CB:27:G:H5' | 22:CB:28:C:OP2 | 1.97 | 0.64 |
| 32:DK:77:LEU:HD12 | 32:DK:78:THR:H | 1.62 | 0.64 |
| 25:DA:2147:G:H2' | 25:DA:2148:G:O4' | 1.96 | 0.64 |
| 25:BA:2849:U:H4' | 25:BA:2868:A:C2 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:2199:A:H3' | 25:BA:2205:C:H6 | 1.63 | 0.64 |
| 1:AA:695:A:OP1 | 11:AN:52:GLY:HA3 | 1.97 | 0.64 |
| 16:AS:15:PRO:O | 16:AS:16:HIS:ND1 | 2.30 | 0.64 |
| 36:DP:33:GLY:HA2 | 36:DP:105:GLU:CB | 2.27 | 0.64 |
| 38:DQ:110:LEU:HD23 | 38:DQ:112:PHE:CE2 | 2.33 | 0.64 |
| 28:BE:51:PHE:O | 28:BE:52:LEU:C | 2.34 | 0.64 |
| 28:BE:59:VAL:C | 28:BE:60:ASN:ND2 | 2.51 | 0.64 |
| 44:BU:96:ILE:HG12 | 44:BU:99:CYS:O | 1.98 | 0.64 |
| 23:CD:55:U:N3 | 23:CD:56:U:C5 | 2.66 | 0.64 |
| 25:BA:2171:A:H2' | 25:BA:2172:U:H6 | 1.62 | 0.64 |
| 35:DO:85:LEU:HA | 35:DO:88:LEU:CB | 2.28 | 0.64 |
| 25:DA:140:A:H8 | 25:DA:1408:C:O2' | 1.81 | 0.64 |
| 35:DO:39:LYS:HD2 | 35:DO:45:LEU:CD2 | 2.28 | 0.64 |
| 40:B1:112:ARG:HG3 | 40:B1:112:ARG:HH11 | 1.61 | 0.64 |
| 37:B0:104:ARG:HH11 | 37:B0:104:ARG:CG | 2.11 | 0.64 |
| 51:B5:40:LYS:CD | 51:B5:46:CYS:HB3 | 2.27 | 0.64 |
| 1:CA:421:U:O2 | 1:CA:421:U:H2' | 1.98 | 0.64 |
| 1:CA:652:U:H1' | 1:CA:653:A:H2 | 1.62 | 0.64 |
| 32:DK:25:TYR:HE2 | 32:DK:29:TYR:CD2 | 2.16 | 0.64 |
| 33:DM:19:GLU:HG3 | 33:DM:59:LYS:HB3 | 1.80 | 0.64 |
| 10:CM:17:ASP:HB2 | 10:CM:70:ARG:NH2 | 2.12 | 0.64 |
| 25:BA:1216:G:P | 40:B1:12:ARG:HH21 | 2.20 | 0.64 |
| 1:CA:1121:U:C2' | 1:CA:1122:U:H5' | 2.28 | 0.64 |
| 20:AW:10:LEU:HD23 | 20:AW:12:ALA:HB3 | 1.75 | 0.64 |
| 54:D8:49:VAL:HG23 | 54:D8:50:LEU:N | 2.13 | 0.64 |
| 28:BE:23:VAL:CB | 28:BE:185:LYS:HA | 2.26 | 0.64 |
| 35:BO:11:GLY:O | 35:BO:13:ASN:N | 2.30 | 0.64 |
| 28:DE:199:ARG:HG2 | 28:DE:200:GLU:H | 1.61 | 0.64 |
| 16:CS:8:ARG:HD2 | 16:CS:17:TYR:CE2 | 2.33 | 0.64 |
| 25:BA:2562:U:H1' | 34:BN:23:ARG:NH1 | 2.13 | 0.64 |
| 25:DA:2446:G:C2' | 25:DA:2447:G:H5'' | 2.28 | 0.64 |
| 19:CV:41:VAL:HG22 | 50:D4:63:TYR:OH | 1.98 | 0.64 |
| 25:BA:1171:G:C5 | 25:BA:1174:A:N6 | 2.66 | 0.64 |
| 25:BA:1192:G:C2' | 25:BA:1193:G:H5' | 2.28 | 0.64 |
| 1:AA:667:G:H4' | 15:AR:51:HIS:CE1 | 2.33 | 0.64 |
| 45:BV:157:LEU:HD11 | 45:BV:163:LEU:HD21 | 1.79 | 0.64 |
| 29:BF:134:GLY:HA2 | 29:BF:166:ALA:HB2 | 1.79 | 0.64 |
| 19:AV:63:THR:O | 19:AV:66:MET:HG3 | 1.98 | 0.64 |
| 47:BZ:83:GLU:HG2 | 47:BZ:84:GLY:N | 2.13 | 0.63 |
| 23:CC:32:G:C4 | 23:CC:33:C:C5 | 2.86 | 0.63 |
| 43:DT:50:LYS:N | 43:DT:87:GLN:HE22 | 1.95 | 0.63 |
| 1:CA:1178:G:H5' | 9:CL:93:ARG:HH21 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:1332:G:N2 | 25:DA:1610:A:C8 | 2.66 | 0.63 |
| 25:BA:2137:C:N4 | 25:BA:2154:G:H1 | 1.95 | 0.63 |
| 52:B6:12:GLU:HB3 | 52:B6:23:THR:HG22 | 1.81 | 0.63 |
| 3:CF:18:TRP:HE1 | 14:CQ:55:GLY:H | 1.45 | 0.63 |
| 25:DA:1310:G:OP2 | 53:D7:9:ARG:HD2 | 1.97 | 0.63 |
| 3:AF:78:GLY:O | 3:AF:79:ARG:HG2 | 1.98 | 0.63 |
| 1:AA:51:A:OP2 | 1:AA:52:G:H8 | 1.80 | 0.63 |
| 25:DA:2187:G:H2' | 25:DA:2188:C:O4' | 1.98 | 0.63 |
| 1:AA:8:A:N6 | 4:AG:205:GLU:O | 2.31 | 0.63 |
| 23:AC:48:U:H4' | 23:AC:49:C:H5' | 1.80 | 0.63 |
| 31:DH:86:GLU:HA | 31:DH:132:ARG:HB2 | 1.78 | 0.63 |
| 21:AX:5:ASP:O | 21:AX:11:GLY:HA3 | 1.97 | 0.63 |
| 1:CA:689:C:C2' | 1:CA:690:G:H5' | 2.28 | 0.63 |
| 23:CC:7:G:H1 | 23:CC:67:C:H42 | 1.46 | 0.63 |
| 1:AA:173:U:H5'' | 1:AA:197:A:O4' | 1.98 | 0.63 |
| 27:BD:35:LYS:HZ3 | 27:BD:104:TYR:HB2 | 1.63 | 0.63 |
| 28:BE:35:GLN:HB3 | 28:BE:48:GLN:CB | 2.28 | 0.63 |
| 28:DE:48:GLN:HE22 | 28:DE:78:LEU:HD13 | 1.60 | 0.63 |
| 28:DE:12:THR:HG22 | 39:DR:58:ASN:HD21 | 1.63 | 0.63 |
| 25:DA:2401:U:H2' | 25:DA:2402:C:H5'' | 1.81 | 0.63 |
| 52:B6:15:GLU:CG | 52:B6:16:CYS:N | 2.61 | 0.63 |
| 25:DA:1342:A:C6 | 25:DA:1397:U:C5 | 2.86 | 0.63 |
| 25:DA:1065:U:H3 | 25:DA:1073:A:H61 | 1.45 | 0.63 |
| 23:CD:7:G:H3' | 23:CD:8:U:C5' | 2.27 | 0.63 |
| 9:CL:77:ILE:O | 9:CL:81:ILE:HG12 | 1.97 | 0.63 |
| 39:BR:16:ARG:HE | 39:BR:19:LEU:HD21 | 1.62 | 0.63 |
| 25:BA:1188:U:C2' | 25:BA:1189:A:H5' | 2.28 | 0.63 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:H8 | 1.63 | 0.63 |
| 10:AM:96:ILE:H | 10:AM:96:ILE:HD13 | 1.62 | 0.63 |
| 4:CG:178:VAL:HG12 | 4:CG:179:GLU:N | 2.13 | 0.63 |
| 12:AO:126:LYS:HG3 | 12:AO:128:ALA:H | 1.63 | 0.63 |
| 1:AA:1065:U:H1' | 1:AA:1066:C:OP2 | 1.98 | 0.63 |
| 1:AA:7:G:H5' | 1:AA:298:A:O4' | 1.97 | 0.63 |
| 8:AK:41:ARG:HG3 | 8:AK:41:ARG:HH11 | 1.63 | 0.63 |
| 19:AV:24:ALA:O | 19:AV:25:LYS:HB3 | 1.97 | 0.63 |
| 25:DA:907:U:O2' | 36:DP:101:ARG:NH2 | 2.30 | 0.63 |
| 7:AJ:16:LEU:HD12 | 9:AL:42:ARG:HA | 1.80 | 0.63 |
| 13:AP:60:VAL:HG12 | 13:AP:66:LEU:HD11 | 1.80 | 0.63 |
| 27:DD:49:ILE:CD1 | 27:DD:52:ARG:HA | 2.25 | 0.63 |
| 25:DA:1225:C:O3' | 41:D2:85:LYS:HA | 1.97 | 0.63 |
| 25:DA:673:C:H5' | 25:DA:673:C:H6 | 1.63 | 0.63 |
| 1:AA:1004:A:H5'' | 1:AA:1025:U:O4 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:1062:G:O6 | 25:DA:1075:C:N4 | 2.31 | 0.63 |
| 23:CD:15:G:N7 | 23:CD:16:C:H5 | 1.96 | 0.63 |
| 2:CE:237:ALA:O | 2:CE:238:LEU:HB3 | 1.98 | 0.63 |
| 1:CA:1252:A:H61 | 1:CA:1285:A:H61 | 1.45 | 0.63 |
| 2:AE:111:ARG:NH1 | 2:AE:111:ARG:HG2 | 2.12 | 0.63 |
| 1:AA:310:G:P | 16:AS:27:LYS:NZ | 2.71 | 0.63 |
| 34:DN:68:GLU:HB3 | 34:DN:78:ARG:HH11 | 1.62 | 0.63 |
| 27:DD:137:PRO:O | 27:DD:140:THR:HG23 | 1.98 | 0.63 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.47 | 0.63 |
| 4:AG:153:ARG:NH1 | 4:AG:181:MET:HG3 | 2.13 | 0.63 |
| 25:DA:1856:G:C2' | 25:DA:1857:G:H5' | 2.27 | 0.63 |
| 25:BA:957:A:N1 | 25:BA:2458:G:H4' | 2.13 | 0.63 |
| 30:BG:83:ARG:HG3 | 30:BG:86:MET:HE1 | 1.67 | 0.63 |
| 38:DQ:87:PHE:CZ | 38:DQ:102:ALA:HB2 | 2.32 | 0.63 |
| 38:DQ:26:LEU:HB3 | 38:DQ:87:PHE:HA | 1.81 | 0.63 |
| 28:BE:59:VAL:HG13 | 28:BE:63:LEU:HB3 | 1.81 | 0.63 |
| 26:BB:108:C:H5' | 26:BB:109:G:O5' | 1.98 | 0.63 |
| 25:DA:67:U:N3 | 25:DA:74:A:H2 | 1.94 | 0.63 |
| 28:DE:137:HIS:HB3 | 28:DE:138:PRO:HD2 | 1.80 | 0.63 |
| 9:CL:88:TYR:HB3 | 9:CL:89:ASN:ND2 | 2.13 | 0.63 |
| 25:DA:1025:G:C4 | 25:DA:1135:C:H1' | 2.34 | 0.63 |
| 41:D2:29:PRO:O | 41:D2:61:VAL:HG12 | 1.99 | 0.63 |
| 2:CE:185:ILE:HG22 | 2:CE:199:TYR:HB2 | 1.80 | 0.63 |
| 25:BA:2131:G:H1' | 25:BA:2158:A:H62 | 1.62 | 0.63 |
| 25:BA:1771:C:HO2' | 25:BA:1786:A:H8 | 1.44 | 0.63 |
| 12:AO:6:THR:H | 12:AO:9:GLN:NE2 | 1.97 | 0.63 |
| 25:BA:404:C:H1' | 25:BA:405:U:OP2 | 1.98 | 0.63 |
| 12:AO:126:LYS:HE3 | 12:AO:128:ALA:HB3 | 1.81 | 0.63 |
| 25:DA:1856:G:H2' | 25:DA:1857:G:H5' | 1.81 | 0.63 |
| 25:DA:2745:C:H4' | 31:DH:142:GLY:O | 1.98 | 0.63 |
| 25:BA:1761:C:H42 | 25:BA:1762:A:H62 | 1.47 | 0.63 |
| 25:DA:303:U:H2' | 25:DA:304:G:O4' | 1.98 | 0.63 |
| 16:AS:17:TYR:HE1 | 16:AS:41:PRO:HG3 | 1.64 | 0.63 |
| 54:D8:50:LEU:O | 54:D8:51:ALA:CB | 2.46 | 0.63 |
| 36:DP:34:LEU:HD11 | 36:DP:129:THR:HB | 1.81 | 0.63 |
| 28:BE:81:ILE:CG2 | 28:BE:84:PHE:HB3 | 2.26 | 0.63 |
| 28:DE:38:THR:CG2 | 28:DE:40:GLU:HB2 | 2.29 | 0.63 |
| 26:BB:66:A:H61 | 26:BB:107:U:H2' | 1.63 | 0.63 |
| 44:BU:97:ARG:NE | 44:BU:98:VAL:HG23 | 2.12 | 0.63 |
| 47:DZ:91:LYS:HG3 | 47:DZ:92:LYS:N | 2.13 | 0.63 |
| 1:AA:1004:A:C8 | 1:AA:1036:G:N1 | 2.59 | 0.63 |
| 25:DA:2470:G:OP2 | 36:DP:56:ARG:NH2 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:1306:A:N6 | 1:CA:1331:G:O2' | 2.32 | 0.63 |
| 25:BA:1021:A:H62 | 25:BA:1141:U:H3 | 1.47 | 0.63 |
| 25:BA:2552:U:H2' | 25:BA:2554:U:OP2 | 1.99 | 0.63 |
| 2:AE:61:LEU:HD23 | 2:AE:68:ILE:HD12 | 1.80 | 0.63 |
| 1:AA:428:G:C8 | 1:AA:430:A:C4 | 2.86 | 0.63 |
| 19:CV:45:VAL:HA | 19:CV:62:ILE:HG22 | 1.80 | 0.63 |
| 28:DE:202:LYS:N | 28:DE:202:LYS:HD2 | 2.14 | 0.63 |
| 31:BH:9:ILE:HD12 | 31:BH:9:ILE:N | 2.14 | 0.63 |
| 27:DD:267:SER:O | 27:DD:268:ARG:HB3 | 1.98 | 0.63 |
| 45:DV:53:ILE:HG22 | 45:DV:71:VAL:O | 1.99 | 0.63 |
| 10:AM:32:ALA:HB3 | 10:AM:76:ASN:HB2 | 1.79 | 0.63 |
| 1:AA:1490:C:O2' | 1:AA:1491:G:H5' | 1.98 | 0.63 |
| 15:CR:2:PRO:HB2 | 15:CR:3:ILE:HD13 | 1.81 | 0.63 |
| 1:CA:1386:G:C2 | 1:CA:1387:G:C8 | 2.85 | 0.63 |
| 1:AA:262:A:H2' | 1:AA:263:A:C8 | 2.32 | 0.63 |
| 14:CQ:27:CYS:SG | 14:CQ:27:CYS:O | 2.56 | 0.63 |
| 25:DA:671:C:OP1 | 35:DO:42:SER:O | 2.15 | 0.63 |
| 25:DA:846:C:C2 | 25:DA:847:U:C5 | 2.87 | 0.63 |
| 38:DQ:11:LYS:HD2 | 38:DQ:15:ARG:NH2 | 2.13 | 0.63 |
| 40:D1:98:LEU:O | 40:D1:99:ALA:HB3 | 1.98 | 0.63 |
| 41:D2:71:LEU:N | 41:D2:86:GLY:CA | 2.62 | 0.63 |
| 28:DE:51:PHE:O | 28:DE:74:PRO:CB | 2.46 | 0.63 |
| 26:DB:104:A:H2' | 26:DB:105:G:O4' | 1.99 | 0.63 |
| 35:DO:64:LYS:HD2 | 54:D8:25:MET:CE | 2.28 | 0.63 |
| 22:CB:21:A:H1' | 22:CB:22:G:C5' | 2.27 | 0.63 |
| 25:BA:889:C:H3' | 25:BA:890:A:C4' | 2.29 | 0.63 |
| 23:CD:15:G:H2' | 23:CD:15:G:N3 | 2.11 | 0.63 |
| 25:DA:486:C:H4' | 42:DS:60:ASN:ND2 | 2.14 | 0.63 |
| 25:BA:2789:C:H1' | 25:BA:2892:A:H2 | 1.63 | 0.63 |
| 35:DO:47:ASP:OD2 | 35:DO:49:ARG:NE | 2.32 | 0.63 |
| 2:AE:80:ILE:HD13 | 2:AE:212:GLN:HB2 | 1.81 | 0.63 |
| 31:BH:109:PHE:CE2 | 31:BH:152:ARG:NH1 | 2.67 | 0.63 |
| 25:BA:1777:U:O2' | 25:BA:1778:U:H5' | 1.98 | 0.63 |
| 25:BA:1049:C:H2' | 25:BA:1050:A:C5' | 2.28 | 0.63 |
| 26:DB:56:G:H4' | 26:DB:57:A:C8 | 2.33 | 0.63 |
| 41:D2:49:THR:HB | 41:D2:50:PRO:HD3 | 1.80 | 0.63 |
| 9:AL:45:ALA:O | 9:AL:78:LYS:NZ | 2.26 | 0.63 |
| 10:AM:35:SER:OG | 10:AM:73:ASP:HB2 | 1.99 | 0.63 |
| 1:CA:1084:G:H2' | 1:CA:1085:U:C6 | 2.33 | 0.63 |
| 2:AE:174:VAL:HG13 | 2:AE:184:VAL:HG11 | 1.81 | 0.63 |
| 25:BA:2065:C:H2' | 25:BA:2066:C:C6 | 2.34 | 0.63 |
| 25:BA:142:G:H1' | 43:BT:37:THR:CG2 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 36:DP:84:GLY:O | 36:DP:85:LYS:HB2 | 1.98 | 0.63 |
| 23:CD:6:G:H1 | 23:CD:68:C:H42 | 1.44 | 0.63 |
| 9:CL:18:PHE:HD1 | 9:CL:62:TYR:CD2 | 2.16 | 0.63 |
| 25:DA:2162:G:H2' | 25:DA:2163:C:C6 | 2.33 | 0.63 |
| 25:DA:2173:A:N3 | 25:DA:2173:A:H2' | 2.14 | 0.63 |
| 26:DB:89:G:OP2 | 26:DB:89:G:H8 | 1.81 | 0.63 |
| 35:DO:85:LEU:HB3 | 35:DO:114:ILE:CD1 | 2.28 | 0.63 |
| 3:AF:70:VAL:HG12 | 3:AF:72:LYS:N | 2.13 | 0.63 |
| 25:BA:142:G:H1' | 43:BT:37:THR:HG21 | 1.81 | 0.63 |
| 11:CN:99:GLN:HG2 | 11:CN:105:VAL:HG21 | 1.81 | 0.63 |
| 25:BA:1916:A:H5' | 25:BA:1917:U:OP2 | 1.99 | 0.63 |
| 1:AA:486:U:H2' | 1:AA:487:A:C8 | 2.34 | 0.63 |
| 25:DA:2724:C:OP1 | 28:DE:118:LYS:HE3 | 1.98 | 0.63 |
| 36:DP:57:HIS:O | 36:DP:57:HIS:ND1 | 2.32 | 0.63 |
| 23:AD:41:C:H2' | 23:AD:42:C:H6 | 1.63 | 0.63 |
| 25:DA:635:C:O2' | 25:DA:639:U:OP1 | 2.15 | 0.63 |
| 47:BZ:91:LYS:O | 47:BZ:93:GLU:N | 2.32 | 0.63 |
| 1:CA:1028(A):C:H42 | 1:CA:1032(B):G:H1 | 1.47 | 0.63 |
| 39:DR:53:ARG:HG3 | 39:DR:53:ARG:O | 1.97 | 0.63 |
| 3:AF:181:ASN:ND2 | 3:AF:204:LEU:HB2 | 2.12 | 0.63 |
| 36:DP:54:MET:HE1 | 36:DP:118:LEU:HD23 | 1.80 | 0.63 |
| 41:D2:37:VAL:HG21 | 41:D2:57:VAL:HG13 | 1.81 | 0.63 |
| 1:AA:229:U:O2' | 16:AS:23:ASP:OD2 | 2.17 | 0.63 |
| 25:DA:2371:G:C4' | 52:D6:45:LYS:CE | 2.71 | 0.63 |
| 45:DV:146:ILE:HD13 | 45:DV:175:VAL:HG23 | 1.79 | 0.63 |
| 25:DA:67:U:N3 | 25:DA:74:A:C2 | 2.57 | 0.63 |
| 25:DA:1328:G:H2' | 25:DA:1330:C:C5 | 2.34 | 0.63 |
| 26:BB:30:C:OP2 | 38:BQ:32:LEU:HD11 | 1.99 | 0.63 |
| 1:AA:397:A:N6 | 1:AA:548:G:C5 | 2.66 | 0.63 |
| 25:DA:138:G:H22 | 43:DT:44:GLU:CD | 2.02 | 0.63 |
| 35:DO:47:ASP:OD2 | 35:DO:49:ARG:CD | 2.45 | 0.63 |
| 25:BA:2473:U:C2' | 25:BA:2474:C:H5'' | 2.28 | 0.63 |
| 23:CD:22:A:H2' | 23:CD:47:G:O6 | 1.99 | 0.63 |
| 1:CA:994:A:N7 | 1:CA:1216:G:H4' | 2.13 | 0.63 |
| 3:CF:18:TRP:HE1 | 14:CQ:55:GLY:N | 1.96 | 0.63 |
| 3:CF:94:LEU:HD12 | 3:CF:95:THR:N | 2.14 | 0.63 |
| 25:DA:566:U:OP1 | 35:DO:29:LYS:HE3 | 1.98 | 0.63 |
| 2:AE:47:THR:O | 2:AE:51:LEU:HB2 | 1.97 | 0.63 |
| 25:DA:479:A:H4' | 25:DA:480:A:OP1 | 1.98 | 0.63 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:H8 | 1.64 | 0.63 |
| 25:BA:1056:G:O4' | 25:BA:1086:A:H8 | 1.81 | 0.63 |
| 28:BE:78:LEU:HD12 | 28:BE:79:ARG:CA | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 52:B6:15:GLU:HG2 | 52:B6:16:CYS:H | 1.62 | 0.63 |
| 36:DP:75:THR:CG2 | 36:DP:87:LYS:HE2 | 2.29 | 0.63 |
| 35:BO:64:LYS:HD3 | 54:B8:25:MET:SD | 2.38 | 0.63 |
| 1:CA:328:C:H4' | 1:CA:329:A:H5' | 1.80 | 0.63 |
| 44:DU:81:LYS:HB3 | 44:DU:82:PRO:CD | 2.29 | 0.63 |
| 13:CP:40:ASN:OD1 | 13:CP:41:PRO:HD2 | 1.99 | 0.63 |
| 1:AA:749:C:O2 | 1:AA:749:C:H2' | 1.98 | 0.63 |
| 25:BA:674:G:O2' | 29:BF:74:ARG:HD3 | 1.99 | 0.63 |
| 29:DF:132:VAL:O | 29:DF:133:ASN:HB2 | 1.99 | 0.63 |
| 45:DV:61:LEU:HD11 | 45:DV:67:LEU:HD12 | 1.79 | 0.63 |
| 25:BA:2734:A:H5' | 25:BA:2734:A:H8 | 1.63 | 0.63 |
| 48:DW:17:SER:OG | 48:DW:21:LEU:HD12 | 1.99 | 0.63 |
| 25:BA:587:C:N3 | 35:BO:33:ARG:NH1 | 2.46 | 0.63 |
| 25:DA:1600:C:O2' | 53:D7:49:ARG:HD3 | 1.99 | 0.63 |
| 3:CF:113:ALA:HB2 | 3:CF:202:ILE:HG13 | 1.80 | 0.63 |
| 1:CA:255:G:O6 | 1:CA:270:A:N6 | 2.32 | 0.63 |
| 1:AA:1112:C:C4 | 3:AF:178:LEU:HD23 | 2.33 | 0.63 |
| 25:BA:1870:C:O2 | 25:BA:1870:C:H2' | 1.98 | 0.63 |
| 31:DH:124:GLU:OE1 | 31:DH:124:GLU:N | 2.30 | 0.63 |
| 13:AP:58:GLU:O | 13:AP:62:ASN:HB2 | 1.98 | 0.63 |
| 8:CK:84:ARG:O | 8:CK:135:CYS:HB2 | 1.98 | 0.63 |
| 28:BE:53:PRO:HA | 28:BE:74:PRO:CA | 2.29 | 0.62 |
| 23:CC:24:C:C2 | 23:CC:25:U:C5 | 2.87 | 0.62 |
| 45:DV:175:VAL:HG13 | 45:DV:176:PRO:CD | 2.29 | 0.62 |
| 1:AA:1305:G:H5' | 21:AX:4:GLY:HA3 | 1.80 | 0.62 |
| 28:DE:130:GLY:O | 28:DE:131:ALA:C | 2.38 | 0.62 |
| 48:BW:50:ILE:CD1 | 48:BW:51:ARG:N | 2.61 | 0.62 |
| 1:AA:1367:C:H5' | 10:AM:60:ARG:NH1 | 2.14 | 0.62 |
| 3:CF:119:ARG:NH2 | 3:CF:140:ARG:HG2 | 2.09 | 0.62 |
| 25:DA:1047:G:H2' | 25:DA:1110:G:H1 | 1.64 | 0.62 |
| 25:BA:1138:G:N2 | 33:BM:106:MET:HE3 | 2.10 | 0.62 |
| 31:BH:4:ILE:C | 31:BH:6:ARG:H | 2.01 | 0.62 |
| 25:BA:443:A:C8 | 29:BF:45:ARG:HD2 | 2.33 | 0.62 |
| 29:DF:31:HIS:HB2 | 35:DO:9:ASN:OD1 | 1.98 | 0.62 |
| 30:DG:113:ARG:HD2 | 50:D4:33:VAL:HG12 | 1.80 | 0.62 |
| 4:AG:5:ILE:CG2 | 4:AG:6:GLY:H | 2.12 | 0.62 |
| 51:D5:6:VAL:HG13 | 51:D5:7:PRO:N | 2.13 | 0.62 |
| 45:DV:4:ARG:HD3 | 45:DV:58:VAL:HG11 | 1.81 | 0.62 |
| 1:AA:149:A:C2 | 1:AA:150:C:N3 | 2.67 | 0.62 |
| 1:CA:1028(A):C:N4 | 1:CA:1028(B):C:H41 | 1.97 | 0.62 |
| 43:DT:72:LYS:NZ | 43:DT:75:ASP:OD1 | 2.32 | 0.62 |
| 46:D3:42:GLY:H | 46:D3:57:PHE:HD2 | 1.47 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:1126:A:H4' | 25:BA:1127:A:O5' | 1.98 | 0.62 |
| 25:DA:900:A:H3' | 25:DA:901:A:H8 | 1.64 | 0.62 |
| 13:CP:7:VAL:HG22 | 30:DG:115:ARG:HB3 | 1.81 | 0.62 |
| 23:CD:20:G:H2' | 23:CD:20:G:N3 | 2.14 | 0.62 |
| 23:CC:41:C:H2' | 23:CC:42:C:H6 | 1.64 | 0.62 |
| 28:DE:179:GLU:O | 28:DE:180:ASN:HB2 | 1.97 | 0.62 |
| 35:BO:61:ARG:O | 35:BO:62:LEU:CD2 | 2.45 | 0.62 |
| 27:DD:35:LYS:CE | 27:DD:65:ILE:HA | 2.29 | 0.62 |
| 33:DM:45:ASN:ND2 | 33:DM:45:ASN:O | 2.32 | 0.62 |
| 25:DA:2747:G:O6 | 25:DA:2755:C:H5'' | 2.00 | 0.62 |
| 36:DP:87:LYS:O | 36:DP:88:GLY:C | 2.37 | 0.62 |
| 1:CA:1446:A:OP1 | 1:CA:1446:A:H4' | 1.97 | 0.62 |
| 25:DA:329:G:C6 | 44:DU:19:LYS:HG2 | 2.34 | 0.62 |
| 2:CE:137:ARG:NH1 | 2:CE:140:HIS:HB2 | 2.11 | 0.62 |
| 4:AG:110:PHE:N | 4:AG:110:PHE:CD1 | 2.66 | 0.62 |
| 1:AA:688:G:H2' | 1:AA:689:C:H6 | 1.64 | 0.62 |
| 40:B1:112:ARG:HG2 | 40:B1:112:ARG:HH11 | 1.64 | 0.62 |
| 25:BA:1469:A:H2' | 25:BA:1470:G:O5' | 1.99 | 0.62 |
| 25:BA:2335:A:C8 | 25:BA:2337:G:C5 | 2.86 | 0.62 |
| 26:BB:40:U:H1' | 26:BB:45:A:N6 | 2.14 | 0.62 |
| 25:DA:1203:G:H3' | 25:DA:1204:A:H5'' | 1.80 | 0.62 |
| 36:DP:102:VAL:HG12 | 36:DP:102:VAL:O | 1.98 | 0.62 |
| 32:DK:77:LEU:HB2 | 32:DK:141:LYS:HB3 | 1.81 | 0.62 |
| 31:DH:10:PRO:HG2 | 31:DH:50:VAL:HG13 | 1.81 | 0.62 |
| 45:DV:149:SER:HB3 | 45:DV:172:ALA:O | 1.99 | 0.62 |
| 5:CH:110:LEU:O | 5:CH:115:VAL:HG22 | 1.99 | 0.62 |
| 25:BA:1858:G:O2' | 25:BA:1883:G:N2 | 2.31 | 0.62 |
| 1:AA:960:U:O2 | 1:AA:960:U:H2' | 1.97 | 0.62 |
| 3:CF:23:TYR:CD2 | 3:CF:24:ALA:N | 2.67 | 0.62 |
| 1:AA:517:G:N1 | 1:AA:533:A:OP2 | 2.31 | 0.62 |
| 25:BA:2372:G:H1' | 52:B6:46:HIS:CE1 | 2.35 | 0.62 |
| 36:BP:86:GLY:C | 36:BP:88:GLY:N | 2.52 | 0.62 |
| 54:B8:44:LYS:N | 54:B8:44:LYS:HD2 | 2.14 | 0.62 |
| 25:DA:1899:G:H21 | 25:DA:1902:C:H5 | 1.45 | 0.62 |
| 44:DU:17:SER:HB2 | 44:DU:71:LYS:CE | 2.29 | 0.62 |
| 25:BA:2168:G:N3 | 25:BA:2168:G:H2' | 2.15 | 0.62 |
| 25:BA:2895:U:H2' | 25:BA:2896:C:O4' | 1.98 | 0.62 |
| 1:AA:606:G:H5'' | 1:AA:607:A:H5' | 1.81 | 0.62 |
| 1:AA:1316:G:N2 | 1:AA:1318:A:H3' | 2.14 | 0.62 |
| 39:BR:123:GLN:O | 39:BR:124:ASP:HB2 | 1.99 | 0.62 |
| 26:BB:71:C:C2 | 26:BB:72:G:C8 | 2.88 | 0.62 |
| 7:CJ:22:LEU:HD23 | 7:CJ:62:PHE:HE2 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 32:DK:128:LEU:O | 32:DK:138:ILE:HG22 | 1.99 | 0.62 |
| 47:BZ:51:VAL:HG21 | 47:BZ:74:VAL:HG21 | 1.81 | 0.62 |
| 1:AA:1455:G:H5' | 20:AW:32:ALA:HB2 | 1.81 | 0.62 |
| 27:DD:35:LYS:CG | 27:DD:64:ILE:N | 2.62 | 0.62 |
| 23:AC:20:G:C4 | 23:AC:58:A:H2 | 2.18 | 0.62 |
| 35:BO:65:ARG:NH1 | 35:BO:65:ARG:CG | 2.58 | 0.62 |
| 54:D8:25:MET:O | 54:D8:48:PHE:HE1 | 1.81 | 0.62 |
| 19:AV:40:ILE:HG12 | 19:AV:41:VAL:HG22 | 1.80 | 0.62 |
| 51:D5:3:LYS:HE3 | 51:D5:3:LYS:HA | 1.80 | 0.62 |
| 30:BG:7:LEU:HD23 | 30:BG:100:TRP:CZ3 | 2.34 | 0.62 |
| 25:DA:887:A:H3' | 25:DA:888:C:C5' | 2.30 | 0.62 |
| 25:DA:2127:G:N2 | 25:DA:2173:A:H8 | 1.95 | 0.62 |
| 13:AP:108:ARG:NH1 | 13:AP:113:PRO:O | 2.32 | 0.62 |
| 1:AA:1126:U:C5 | 1:AA:1127:G:C4 | 2.87 | 0.62 |
| 39:BR:128:GLU:O | 39:BR:128:GLU:HG2 | 1.99 | 0.62 |
| 35:BO:59:LEU:HD23 | 35:BO:59:LEU:O | 1.99 | 0.62 |
| 1:CA:689:C:H2' | 1:CA:690:G:H5' | 1.81 | 0.62 |
| 27:BD:121:PRO:HB3 | 27:BD:135:PHE:CE1 | 2.34 | 0.62 |
| 51:D5:20:ARG:HG2 | 51:D5:23:HIS:CD2 | 2.33 | 0.62 |
| 1:CA:612:C:O2 | 1:CA:629:G:N2 | 2.32 | 0.62 |
| 1:CA:1523:G:OP1 | 11:CN:123:LYS:HD2 | 1.99 | 0.62 |
| 4:CG:61:LYS:HA | 4:CG:203:VAL:HG22 | 1.80 | 0.62 |
| 20:CW:64:ASP:OD1 | 20:CW:81:LYS:HD2 | 1.99 | 0.62 |
| 1:AA:1410:G:H2' | 1:AA:1411:C:H6 | 1.63 | 0.62 |
| 52:D6:25:LYS:HE3 | 54:D8:34:TRP:HH2 | 1.64 | 0.62 |
| 28:BE:105:THR:OG1 | 28:BE:199:ARG:NH2 | 2.31 | 0.62 |
| 25:DA:7:G:H1 | 25:DA:2896:C:H42 | 1.47 | 0.62 |
| 40:D1:61:TRP:HB3 | 40:D1:93:LYS:HB3 | 1.82 | 0.62 |
| 40:B1:60:LEU:O | 40:B1:60:LEU:HD22 | 1.98 | 0.62 |
| 36:DP:30:GLY:HA3 | 36:DP:107:ALA:HB2 | 1.81 | 0.62 |
| 47:DZ:85:LEU:HB2 | 47:DZ:87:PRO:HD2 | 1.80 | 0.62 |
| 25:BA:259:G:N2 | 25:BA:621:A:H8 | 1.97 | 0.62 |
| 39:DR:93:ARG:HG2 | 39:DR:117:ASP:HB2 | 1.80 | 0.62 |
| 25:DA:1827:C:C2' | 25:DA:1828:G:H5' | 2.30 | 0.62 |
| 14:AQ:22:THR:O | 14:AQ:23:ARG:HD2 | 1.98 | 0.62 |
| 25:BA:2712:U:OP1 | 25:BA:2714:G:H4' | 2.00 | 0.62 |
| 1:AA:953:G:H2' | 1:AA:954:G:O4' | 1.99 | 0.62 |
| 29:DF:164:ARG:NH1 | 29:DF:177:ALA:HB2 | 2.14 | 0.62 |
| 15:CR:39:LEU:CD1 | 15:CR:56:LEU:HB2 | 2.29 | 0.62 |
| 42:BS:29:LEU:HD21 | 42:BS:33:ARG:NE | 2.15 | 0.62 |
| 23:AD:17:C:N4 | 23:AD:20:G:OP1 | 2.33 | 0.62 |
| 25:DA:1582:C:HO2' | 25:DA:1586:A:H8 | 1.45 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 48:DW:33:MET:O | 48:DW:37:PHE:HD1 | 1.83 | 0.62 |
| 25:DA:986:C:H2' | 25:DA:987:G:H5' | 1.81 | 0.62 |
| 19:AV:66:MET:HB3 | 19:AV:74:PHE:CZ | 2.34 | 0.62 |
| 25:DA:1784:A:H4' | 25:DA:1785:A:C5' | 2.30 | 0.62 |
| 25:DA:296:C:O2' | 25:DA:297:C:H5' | 1.98 | 0.62 |
| 25:BA:270(O):U:H5'' | 25:BA:270(P):C:OP2 | 1.99 | 0.62 |
| 25:BA:271(B):G:H4' | 25:BA:271(C):U:O5' | 1.98 | 0.62 |
| 25:BA:2303:G:C2' | 25:BA:2304:G:H5' | 2.30 | 0.62 |
| 36:BP:81:VAL:C | 36:BP:82:ARG:HG2 | 2.19 | 0.62 |
| 22:AB:68:A:H2' | 22:AB:69:A:H5' | 1.81 | 0.62 |
| 45:BV:81:ARG:HG3 | 45:BV:81:ARG:O | 1.99 | 0.62 |
| 25:DA:769:G:H5' | 25:DA:1379:A:N6 | 2.15 | 0.62 |
| 2:AE:124:SER:HB2 | 2:AE:125:PRO:HD2 | 1.81 | 0.62 |
| 1:AA:375:U:OP1 | 16:AS:69:THR:HG21 | 1.97 | 0.62 |
| 25:DA:2629:A:O2' | 25:DA:2630:G:H5' | 2.00 | 0.62 |
| 36:DP:104:PHE:O | 36:DP:105:GLU:HB3 | 1.99 | 0.62 |
| 27:BD:35:LYS:CE | 27:BD:104:TYR:HB2 | 2.28 | 0.62 |
| 28:BE:38:THR:HG22 | 28:BE:45:THR:CG2 | 2.28 | 0.62 |
| 1:CA:1028:C:N4 | 1:CA:1033:G:H1 | 1.98 | 0.62 |
| 25:BA:1899:G:N2 | 25:BA:1902:C:N4 | 2.27 | 0.62 |
| 35:BO:15:ARG:NH1 | 35:BO:15:ARG:CG | 2.39 | 0.62 |
| 35:DO:16:ARG:NH1 | 35:DO:16:ARG:HG3 | 2.15 | 0.62 |
| 25:DA:1140:C:C1' | 25:DA:1143:A:C8 | 2.82 | 0.62 |
| 1:AA:973:G:H3' | 1:AA:974:A:H5'' | 1.81 | 0.62 |
| 44:DU:96:ILE:HD12 | 44:DU:98:VAL:CG1 | 2.29 | 0.62 |
| 30:DG:67:LYS:HD2 | 50:D4:6:HIS:NE2 | 2.14 | 0.62 |
| 39:BR:53:ARG:CZ | 39:BR:53:ARG:HB3 | 2.28 | 0.62 |
| 1:CA:812:C:C1' | 1:CA:813:U:OP2 | 2.46 | 0.62 |
| 41:B2:39:LEU:CD1 | 41:B2:51:VAL:HG22 | 2.29 | 0.62 |
| 22:AB:50:A:C2 | 22:AB:52:U:H5'' | 2.34 | 0.62 |
| 25:BA:2470:G:O6 | 25:BA:2476:A:O2' | 2.08 | 0.62 |
| 3:AF:188:LEU:HD13 | 3:AF:195:VAL:HG13 | 1.82 | 0.62 |
| 25:BA:1067:A:N3 | 25:BA:1067:A:H2' | 2.14 | 0.62 |
| 26:DB:59:A:H2' | 26:DB:60:C:O4' | 1.98 | 0.62 |
| 19:AV:40:ILE:CG1 | 19:AV:41:VAL:HG13 | 2.29 | 0.62 |
| 19:AV:9:VAL:HG21 | 50:B4:66:SER:OG | 1.99 | 0.62 |
| 9:AL:114:TYR:HE1 | 10:AM:60:ARG:O | 1.82 | 0.62 |
| 25:DA:89:G:H3' | 25:DA:90:U:H5'' | 1.80 | 0.62 |
| 25:BA:2343:C:O2' | 25:BA:2373:G:O2' | 2.16 | 0.62 |
| 35:BO:46:LYS:O | 35:BO:47:ASP:HB3 | 2.00 | 0.62 |
| 25:BA:998:C:H2' | 25:BA:999:U:O5' | 2.00 | 0.62 |
| 45:DV:108:PRO:CA | 45:DV:143:GLY:CA | 2.78 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:1862:G:O2' | 25:DA:1863:G:H5' | 2.00 | 0.62 |
| 37:B0:104:ARG:HH11 | 37:B0:104:ARG:HG2 | 1.65 | 0.62 |
| 25:BA:592:G:H21 | 54:B8:4:MET:CE | 2.13 | 0.62 |
| 2:AE:166:ASP:HB3 | 2:AE:169:LYS:HB2 | 1.80 | 0.62 |
| 50:B4:37:SER:CB | 50:B4:42:PHE:HB3 | 2.29 | 0.62 |
| 1:AA:377:G:OP1 | 16:AS:3:LYS:HD2 | 1.98 | 0.62 |
| 1:CA:540:G:H2' | 1:CA:541:G:O4' | 2.00 | 0.62 |
| 23:AD:29:C:H2' | 23:AD:30:G:H8 | 1.64 | 0.62 |
| 8:CK:16:ALA:HB1 | 8:CK:21:LYS:HB3 | 1.81 | 0.62 |
| 52:B6:26:ASN:ND2 | 52:B6:35:GLU:OE1 | 2.32 | 0.62 |
| 1:CA:468:A:H2' | 1:CA:474:G:H5' | 1.82 | 0.62 |
| 45:DV:49:ARG:HB2 | 45:DV:50:GLN:HE21 | 1.64 | 0.62 |
| 27:BD:8:PRO:HB3 | 27:BD:14:ARG:HB2 | 1.81 | 0.62 |
| 25:BA:1061:U:H4' | 25:BA:1070:A:C1' | 2.30 | 0.62 |
| 30:BG:78:SER:O | 30:BG:81:LYS:N | 2.33 | 0.62 |
| 40:D1:40:PHE:CZ | 41:D2:81:TYR:CE2 | 2.88 | 0.62 |
| 23:CC:30:G:H2' | 23:CC:31:G:C5' | 2.19 | 0.62 |
| 10:AM:38:ILE:O | 10:AM:38:ILE:HG13 | 1.98 | 0.62 |
| 1:CA:1316:G:N2 | 1:CA:1319:A:OP2 | 2.32 | 0.62 |
| 22:CB:39:U:H2' | 22:CB:40:G:C8 | 2.29 | 0.62 |
| 36:BP:63:LYS:HD3 | 36:BP:65:PHE:CE2 | 2.35 | 0.62 |
| 25:DA:883:G:H2' | 25:DA:884:C:C6 | 2.35 | 0.62 |
| 29:BF:46:ARG:NH1 | 29:BF:46:ARG:HG2 | 2.06 | 0.62 |
| 29:DF:32:LEU:HD11 | 29:DF:105:VAL:HG13 | 1.80 | 0.62 |
| 1:AA:1236:A:O2' | 1:AA:1304:G:H4' | 1.99 | 0.62 |
| 50:D4:56:VAL:HG22 | 50:D4:57:GLU:H | 1.65 | 0.62 |
| 1:CA:1109:C:H2' | 1:CA:1110:A:O4' | 2.00 | 0.62 |
| 29:DF:164:ARG:HG2 | 29:DF:175:THR:OG1 | 2.00 | 0.62 |
| 28:BE:66:HIS:ND1 | 28:BE:66:HIS:C | 2.48 | 0.62 |
| 25:BA:2733:A:C2' | 25:BA:2734:A:H5'' | 2.29 | 0.62 |
| 1:CA:1217:C:H2' | 1:CA:1218:C:O4' | 1.99 | 0.62 |
| 45:DV:19:ARG:NH1 | 45:DV:84:GLU:HB2 | 2.15 | 0.62 |
| 1:AA:1228:C:OP1 | 13:AP:115:LYS:HE3 | 1.99 | 0.62 |
| 25:BA:1174:A:H3' | 25:BA:1175:U:H5'' | 1.80 | 0.62 |
| 25:BA:155:C:H42 | 25:BA:171:G:H1 | 1.46 | 0.62 |
| 25:BA:2349:G:OP2 | 54:B8:42:ARG:HD3 | 2.00 | 0.62 |
| 4:AG:95:GLY:O | 4:AG:99:SER:OG | 2.18 | 0.62 |
| 1:AA:942:G:H21 | 9:AL:124:GLN:NE2 | 1.97 | 0.62 |
| 37:B0:84:ALA:HB3 | 37:B0:85:PRO:HD3 | 1.82 | 0.62 |
| 15:CR:54:ARG:NH1 | 15:CR:58:MET:SD | 2.73 | 0.62 |
| 44:DU:63:LYS:HA | 44:DU:63:LYS:NZ | 2.14 | 0.62 |
| 1:AA:1240:U:O2' | 7:AJ:38:LEU:HG | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 5:CH:11:ILE:HG21 | 5:CH:105:VAL:HG22 | 1.81 | 0.62 |
| 30:DG:16:ARG:NH2 | 30:DG:28:VAL:O | 2.33 | 0.62 |
| 38:DQ:78:LEU:HD11 | 38:DQ:107:GLU:CB | 2.23 | 0.62 |
| 41:D2:35:LEU:C | 41:D2:37:VAL:HG13 | 2.21 | 0.62 |
| 28:BE:27:LEU:CD1 | 39:BR:1:MET:HE2 | 2.30 | 0.62 |
| 25:DA:1188:U:H2' | 25:DA:1189:A:H5' | 1.80 | 0.62 |
| 32:DK:82:ARG:HB3 | 32:DK:89:TYR:CD2 | 2.35 | 0.62 |
| 1:AA:255:G:H1' | 17:AT:16:GLN:NE2 | 2.14 | 0.62 |
| 42:BS:88:ARG:NH1 | 42:BS:94:ASP:OD1 | 2.30 | 0.62 |
| 25:BA:2154:G:H2' | 25:BA:2155:G:C8 | 2.35 | 0.62 |
| 25:BA:573:G:O2' | 25:BA:574:C:H3' | 2.00 | 0.62 |
| 30:DG:117:PHE:C | 30:DG:117:PHE:CD1 | 2.72 | 0.62 |
| 39:BR:136:GLN:HG3 | 39:BR:137:LYS:N | 2.14 | 0.62 |
| 25:BA:2335:A:C8 | 25:BA:2337:G:N7 | 2.68 | 0.62 |
| 45:DV:158:PRO:O | 45:DV:161:VAL:HG13 | 2.00 | 0.62 |
| 16:AS:4:ILE:HB | 16:AS:66:PRO:HB3 | 1.81 | 0.62 |
| 1:CA:32:A:C2 | 1:CA:33:A:C4 | 2.88 | 0.62 |
| 25:DA:911:A:C5 | 36:DP:9:TYR:CD2 | 2.88 | 0.62 |
| 1:CA:1032:A:H3' | 1:CA:1032(A):G:C5' | 2.30 | 0.62 |
| 2:AE:180:LEU:O | 2:AE:181:PHE:HB2 | 2.00 | 0.62 |
| 25:DA:813:U:OP2 | 35:DO:23:PRO:O | 2.18 | 0.62 |
| 4:CG:107:ARG:HH11 | 4:CG:107:ARG:HG2 | 1.65 | 0.62 |
| 4:CG:146:ILE:HD12 | 4:CG:146:ILE:N | 2.15 | 0.62 |
| 2:CE:28:PHE:CD1 | 2:CE:190:THR:HG22 | 2.34 | 0.62 |
| 2:CE:28:PHE:CE1 | 2:CE:31:TYR:HB2 | 2.35 | 0.62 |
| 25:BA:1056:G:N2 | 25:BA:1103:A:C6 | 2.68 | 0.62 |
| 25:BA:2376:A:N1 | 38:BQ:87:PHE:HD2 | 1.97 | 0.62 |
| 27:BD:35:LYS:HG2 | 27:BD:64:ILE:HG23 | 1.81 | 0.62 |
| 33:DM:45:ASN:O | 33:DM:45:ASN:CG | 2.38 | 0.62 |
| 1:AA:1139:G:C2 | 1:AA:1143:G:O6 | 2.53 | 0.62 |
| 1:AA:1004:A:C5' | 1:AA:1025:U:N3 | 2.63 | 0.62 |
| 41:B2:48:GLY:O | 41:B2:49:THR:O | 2.18 | 0.62 |
| 30:DG:47:LYS:HG2 | 30:DG:48:GLU:H | 1.63 | 0.62 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:C4 | 2.34 | 0.62 |
| 2:AE:16:HIS:HE2 | 2:AE:213:LEU:HD13 | 1.65 | 0.62 |
| 25:BA:2168:G:N2 | 25:BA:2170:A:OP2 | 2.32 | 0.62 |
| 26:DB:89:G:OP2 | 26:DB:89:G:C8 | 2.53 | 0.62 |
| 25:DA:1420:U:O2' | 25:DA:1421:G:P | 2.58 | 0.62 |
| 25:BA:572:A:H5'' | 25:BA:573:G:OP2 | 2.00 | 0.62 |
| 35:DO:37:GLY:O | 35:DO:38:GLN:C | 2.38 | 0.62 |
| 25:DA:654(D):G:N2 | 25:DA:654(R):C:N3 | 2.48 | 0.62 |
| 4:AG:114:ARG:HH11 | 4:AG:114:ARG:HG2 | 1.63 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:2439:A:O2' | 25:DA:2440:C:OP2 | 2.18 | 0.62 |
| 8:CK:20:TYR:HD1 | 8:CK:65:TYR:CD2 | 2.18 | 0.62 |
| 1:AA:353:A:H2' | 1:AA:354:G:OP2 | 2.00 | 0.62 |
| 1:AA:1410:G:H2' | 1:AA:1411:C:C6 | 2.35 | 0.62 |
| 12:CO:11:VAL:HG11 | 17:CT:36:ILE:HG21 | 1.80 | 0.62 |
| 14:AQ:29:ARG:HD3 | 14:AQ:40:CYS:HB2 | 1.82 | 0.62 |
| 31:DH:12:PRO:O | 31:DH:15:VAL:HG22 | 2.00 | 0.62 |
| 25:BA:2662:A:H2' | 25:BA:2663:G:O4' | 2.00 | 0.62 |
| 33:DM:67:LEU:HD23 | 33:DM:88:GLU:HG2 | 1.81 | 0.62 |
| 33:DM:95:PRO:O | 33:DM:98:VAL:HG22 | 1.99 | 0.62 |
| 25:BA:232:G:OP2 | 25:BA:232:G:H8 | 1.81 | 0.62 |
| 2:CE:17:PHE:CE2 | 2:CE:44:LEU:HA | 2.35 | 0.62 |
| 25:BA:1077:A:H2' | 25:BA:1077:A:N3 | 2.15 | 0.61 |
| 38:DQ:24:LEU:O | 38:DQ:85:VAL:HG12 | 2.00 | 0.61 |
| 40:D1:66:ASN:HB2 | 40:D1:76:TYR:HB2 | 1.81 | 0.61 |
| 23:CC:56:U:O2 | 23:CC:58:A:C8 | 2.53 | 0.61 |
| 25:DA:1005:C:N1 | 25:DA:1143:A:C2 | 2.68 | 0.61 |
| 29:BF:9:ILE:HD11 | 29:BF:125:LEU:CG | 2.28 | 0.61 |
| 25:DA:2128:C:O2' | 25:DA:2173:A:C2 | 2.51 | 0.61 |
| 1:CA:1368:G:H5' | 9:CL:112:LYS:HB3 | 1.81 | 0.61 |
| 25:DA:142:G:H2' | 25:DA:143:C:C6 | 2.35 | 0.61 |
| 36:DP:69:PHE:CD1 | 36:DP:70:PRO:HD2 | 2.35 | 0.61 |
| 1:AA:466:C:H5'' | 1:AA:467:G:OP2 | 2.00 | 0.61 |
| 42:BS:18:ARG:HG2 | 42:BS:76:VAL:HG13 | 1.83 | 0.61 |
| 4:AG:28:SER:HB3 | 4:AG:29:PRO:HD2 | 1.82 | 0.61 |
| 7:AJ:113:GLU:HB2 | 7:AJ:119:ARG:HG2 | 1.82 | 0.61 |
| 23:CC:9:G:O2' | 23:CC:10:G:N7 | 2.29 | 0.61 |
| 1:AA:69:G:N2 | 1:AA:73:G:C8 | 2.68 | 0.61 |
| 16:AS:72:ARG:HD3 | 16:AS:73:LEU:HD23 | 1.82 | 0.61 |
| 2:CE:180:LEU:O | 2:CE:181:PHE:HB2 | 2.00 | 0.61 |
| 25:BA:1063:G:H2' | 25:BA:1064:C:H6 | 1.65 | 0.61 |
| 52:D6:31:PRO:O | 52:D6:32:ASN:HB2 | 2.00 | 0.61 |
| 27:DD:65:ILE:HD11 | 27:DD:67:PHE:CZ | 2.35 | 0.61 |
| 25:BA:2415:G:H4' | 35:BO:66:GLY:HA3 | 1.81 | 0.61 |
| 39:DR:16:ARG:NH2 | 39:DR:19:LEU:HD21 | 2.15 | 0.61 |
| 13:CP:91:ARG:HH22 | 13:CP:96:LEU:HD13 | 1.65 | 0.61 |
| 43:DT:39:ILE:O | 43:DT:43:VAL:HG13 | 1.99 | 0.61 |
| 45:BV:60:GLU:O | 45:BV:61:LEU:HD23 | 2.00 | 0.61 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:H6 | 1.65 | 0.61 |
| 25:BA:252:G:OP2 | 35:BO:50:ARG:NH1 | 2.25 | 0.61 |
| 42:DS:59:VAL:HA | 42:DS:64:MET:H | 1.65 | 0.61 |
| 52:B6:10:LEU:HD23 | 54:B8:34:TRP:CD2 | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:1869:G:H5' | 25:DA:1869:G:H8 | 1.65 | 0.61 |
| 35:DO:146:VAL:HG13 | 35:DO:147:LEU:HD13 | 1.81 | 0.61 |
| 1:AA:438:G:OP1 | 4:AG:125:HIS:HE1 | 1.83 | 0.61 |
| 25:DA:774:A:C2 | 25:DA:787:U:O2' | 2.51 | 0.61 |
| 25:BA:2109:U:H1' | 25:BA:2181:G:N2 | 2.15 | 0.61 |
| 35:DO:59:LEU:HD23 | 35:DO:59:LEU:O | 1.99 | 0.61 |
| 50:B4:12:ALA:HB1 | 50:B4:29:PRO:HA | 1.82 | 0.61 |
| 21:CX:9:ARG:HG3 | 21:CX:10:ARG:H | 1.65 | 0.61 |
| 22:CB:3:C:H2' | 22:CB:4:G:H8 | 1.64 | 0.61 |
| 1:AA:49:U:O2' | 1:AA:50:A:H3' | 2.00 | 0.61 |
| 46:D3:24:LYS:O | 46:D3:25:ARG:HD3 | 1.98 | 0.61 |
| 25:DA:1165:U:H2' | 25:DA:1166:C:C6 | 2.35 | 0.61 |
| 25:DA:1169:G:H2' | 25:DA:1170:G:O4' | 2.01 | 0.61 |
| 1:CA:564:C:O2' | 8:CK:91:ARG:NH2 | 2.33 | 0.61 |
| 12:AO:37:CYS:O | 12:AO:79:GLU:O | 2.18 | 0.61 |
| 12:AO:11:VAL:HG13 | 17:AT:29:HIS:CD2 | 2.34 | 0.61 |
| 17:AT:29:HIS:CE1 | 17:AT:32:TYR:HD1 | 2.18 | 0.61 |
| 25:DA:1404:C:O2 | 25:DA:1404:C:H2' | 2.00 | 0.61 |
| 3:CF:164:ARG:HG2 | 3:CF:165:THR:H | 1.64 | 0.61 |
| 38:DQ:110:LEU:HD23 | 38:DQ:112:PHE:CZ | 2.36 | 0.61 |
| 25:DA:1225:C:H4' | 41:D2:85:LYS:HB2 | 1.83 | 0.61 |
| 28:BE:60:ASN:HB2 | 28:BE:62:PRO:HD2 | 1.81 | 0.61 |
| 23:AC:62:C:C5 | 23:AC:63:C:H5 | 2.18 | 0.61 |
| 14:AQ:23:ARG:CG | 14:AQ:23:ARG:HH11 | 2.12 | 0.61 |
| 1:CA:991:U:H6 | 1:CA:991:U:OP2 | 1.82 | 0.61 |
| 25:BA:1803:A:H4' | 27:BD:259:THR:HG23 | 1.82 | 0.61 |
| 1:CA:1278:U:H2' | 1:CA:1278:U:O2 | 2.00 | 0.61 |
| 1:CA:1148:U:OP1 | 9:CL:7:THR:HG21 | 2.01 | 0.61 |
| 1:CA:1442:G:C2' | 1:CA:1443:G:O5' | 2.47 | 0.61 |
| 26:DB:13:A:N1 | 26:DB:69:G:O2' | 2.28 | 0.61 |
| 25:BA:2157:G:HO2' | 25:BA:2158:A:P | 2.22 | 0.61 |
| 2:AE:80:ILE:HD11 | 2:AE:208:ILE:HG23 | 1.82 | 0.61 |
| 6:AI:101:ALA:HB2 | 18:AU:28:GLU:CG | 2.29 | 0.61 |
| 1:CA:1095:U:P | 1:CA:1108:G:H1 | 2.23 | 0.61 |
| 25:BA:1209:G:H21 | 25:BA:1210:A:H62 | 1.48 | 0.61 |
| 6:AI:89:MET:HE3 | 18:AU:76:LEU:HD23 | 1.82 | 0.61 |
| 27:DD:70:TRP:CZ3 | 27:DD:150:LYS:HA | 2.36 | 0.61 |
| 22:AB:50:A:H3' | 22:AB:51:A:C5' | 2.28 | 0.61 |
| 7:CJ:62:PHE:HD1 | 7:CJ:124:LEU:HD11 | 1.65 | 0.61 |
| 34:BN:60:ALA:HB1 | 34:BN:84:ALA:HB1 | 1.81 | 0.61 |
| 25:DA:2543:G:H5' | 25:DA:2543:G:H8 | 1.65 | 0.61 |
| 25:DA:243:U:OP1 | 54:D8:6:THR:OG1 | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:1665:A:H4' | 34:DN:67:LYS:HB2 | 1.81 | 0.61 |
| 25:DA:2845:G:O2' | 25:DA:2846:G:H5' | 2.00 | 0.61 |
| 1:CA:575:G:O2' | 1:CA:821:G:H5' | 2.00 | 0.61 |
| 32:BK:135:GLU:OE2 | 32:BK:135:GLU:N | 2.32 | 0.61 |
| 9:AL:127:LYS:HG2 | 9:AL:127:LYS:O | 1.99 | 0.61 |
| 4:CG:9:CYS:HA | 4:CG:12:CYS:HB2 | 1.83 | 0.61 |
| 25:DA:127:A:H5'' | 25:DA:128:C:C6 | 2.36 | 0.61 |
| 28:DE:46:ALA:HB1 | 28:DE:82:ARG:CA | 1.96 | 0.61 |
| 27:BD:273:ARG:HG3 | 27:BD:273:ARG:O | 2.00 | 0.61 |
| 27:DD:35:LYS:HZ1 | 27:DD:104:TYR:N | 1.95 | 0.61 |
| 23:CC:49:C:O2 | 23:CC:60:A:H1' | 2.00 | 0.61 |
| 31:DH:109:PHE:CZ | 31:DH:152:ARG:NE | 2.68 | 0.61 |
| 25:BA:2383:G:O2' | 25:BA:2384:G:H5' | 2.00 | 0.61 |
| 35:BO:9:ASN:CB | 35:BO:10:PRO:HD2 | 2.22 | 0.61 |
| 23:CD:13:C:HO2' | 23:CD:14:A:P | 2.23 | 0.61 |
| 26:DB:44:G:O2' | 26:DB:47:C:N4 | 2.33 | 0.61 |
| 43:BT:49:VAL:CG1 | 43:BT:50:LYS:N | 2.63 | 0.61 |
| 25:BA:2131:G:H5' | 25:BA:2132:U:OP1 | 2.00 | 0.61 |
| 23:CC:28:U:O2 | 23:CC:45:A:H2 | 1.79 | 0.61 |
| 25:BA:2312:U:O2 | 30:BG:42:GLY:CA | 2.48 | 0.61 |
| 1:CA:652:U:O4 | 1:CA:752:G:H1' | 2.00 | 0.61 |
| 39:DR:51:ARG:HG2 | 39:DR:98:LYS:HE3 | 1.80 | 0.61 |
| 1:AA:8:A:H5' | 5:AH:101:ILE:HG22 | 1.83 | 0.61 |
| 25:BA:2111:C:H41 | 25:BA:2147:G:N2 | 1.99 | 0.61 |
| 25:BA:1657:C:H2' | 25:BA:1658:C:C6 | 2.35 | 0.61 |
| 9:AL:43:ALA:HA | 9:AL:74:ILE:HD13 | 1.82 | 0.61 |
| 13:CP:76:ALA:HA | 13:CP:79:LYS:HB2 | 1.82 | 0.61 |
| 25:DA:483:A:C5' | 44:DU:49:VAL:HA | 2.30 | 0.61 |
| 38:DQ:62:LYS:HB3 | 38:DQ:97:ARG:HD3 | 1.82 | 0.61 |
| 26:DB:30:C:H2' | 26:DB:31:C:H5' | 1.81 | 0.61 |
| 4:CG:161:ASN:O | 4:CG:165:MET:HG2 | 2.00 | 0.61 |
| 1:CA:1226:C:H2' | 13:CP:103:THR:HB | 1.80 | 0.61 |
| 31:BH:169:VAL:C | 31:BH:170:ARG:HG3 | 2.19 | 0.61 |
| 1:AA:1004:A:C5' | 1:AA:1025:U:O4 | 2.48 | 0.61 |
| 29:DF:18:ARG:HG2 | 29:DF:19:GLU:N | 2.15 | 0.61 |
| 22:CB:85:C:C5 | 25:DA:2555:U:O2 | 2.54 | 0.61 |
| 1:CA:1127:G:H1' | 1:CA:1147:C:H42 | 1.66 | 0.61 |
| 1:CA:1127:G:H1' | 1:CA:1147:C:N4 | 2.15 | 0.61 |
| 25:DA:545:G:N2 | 25:DA:548:A:H62 | 1.93 | 0.61 |
| 3:AF:20:SER:HB2 | 3:AF:40:ARG:HH22 | 1.65 | 0.61 |
| 26:BB:30:C:C2' | 26:BB:31:C:O5' | 2.47 | 0.61 |
| 25:BA:330:A:H2 | 25:BA:1210:A:HO2' | 1.45 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:2786:U:H4' | 28:DE:64:LYS:C | 2.20 | 0.61 |
| 3:CF:73:PRO:HG3 | 3:CF:105:GLU:HB2 | 1.83 | 0.61 |
| 8:AK:41:ARG:NH2 | 8:AK:123:GLU:OE1 | 2.34 | 0.61 |
| 3:CF:40:ARG:HG2 | 3:CF:55:VAL:HG11 | 1.82 | 0.61 |
| 4:CG:191:ARG:NH1 | 4:CG:200:GLU:OE1 | 2.34 | 0.61 |
| 25:BA:1316:U:H2' | 25:BA:1317:A:H8 | 1.63 | 0.61 |
| 25:DA:581:C:H2' | 25:DA:582:G:H8 | 1.65 | 0.61 |
| 32:BK:98:ALA:HB2 | 32:BK:111:PRO:HB3 | 1.81 | 0.61 |
| 25:DA:77:C:OP1 | 48:DW:59:ARG:HD3 | 2.00 | 0.61 |
| 25:DA:2393:A:C5' | 35:DO:62:LEU:HB3 | 2.11 | 0.61 |
| 28:BE:47:VAL:HG22 | 28:BE:84:PHE:O | 2.00 | 0.61 |
| 23:AC:18:C:C2' | 23:AC:18:C:O2 | 2.48 | 0.61 |
| 1:CA:1026:G:O6 | 1:CA:1036:G:C2 | 2.53 | 0.61 |
| 31:DH:153:LYS:O | 31:DH:161:GLY:CA | 2.48 | 0.61 |
| 1:CA:1330:U:H4' | 13:CP:23:TYR:CD2 | 2.35 | 0.61 |
| 25:DA:1049:C:H42 | 31:DH:2:SER:HB3 | 1.66 | 0.61 |
| 25:DA:2168:G:H2' | 25:DA:2168:G:N3 | 2.16 | 0.61 |
| 1:AA:192:U:H4' | 20:AW:103:GLY:HA2 | 1.82 | 0.61 |
| 31:DH:116:GLU:HG2 | 31:DH:117:PRO:HD2 | 1.83 | 0.61 |
| 54:B8:34:TRP:O | 54:B8:35:GLN:CB | 2.48 | 0.61 |
| 25:DA:2262:U:OP2 | 46:D3:19:LYS:NZ | 2.34 | 0.61 |
| 52:B6:25:LYS:HZ3 | 52:B6:27:LYS:HE2 | 1.66 | 0.61 |
| 22:AB:49:C:N3 | 22:AB:54:G:N2 | 2.48 | 0.61 |
| 14:CQ:29:ARG:HD2 | 14:CQ:31:ARG:O | 1.99 | 0.61 |
| 19:CV:41:VAL:HG12 | 19:CV:42:PRO:HD2 | 1.83 | 0.61 |
| 1:CA:1123:A:H4' | 10:CM:36:GLY:HA3 | 1.83 | 0.61 |
| 23:AD:41:C:O2' | 23:AD:42:C:H5' | 2.00 | 0.61 |
| 50:B4:13:ARG:HB2 | 50:B4:30:GLU:HA | 1.81 | 0.61 |
| 1:CA:316:G:OP2 | 1:CA:351:G:O2' | 2.18 | 0.61 |
| 25:DA:1171:G:H1 | 25:DA:1178:C:H42 | 1.46 | 0.61 |
| 1:CA:1001:G:H1 | 1:CA:1039:C:H42 | 1.49 | 0.61 |
| 1:AA:136:C:H42 | 1:AA:227:G:H1 | 1.48 | 0.61 |
| 30:DG:96:ARG:HH11 | 30:DG:96:ARG:HG2 | 1.66 | 0.61 |
| 1:CA:1513:A:H2' | 1:CA:1514:C:C6 | 2.35 | 0.61 |
| 2:CE:197:VAL:HG12 | 2:CE:200:ILE:HG12 | 1.81 | 0.61 |
| 30:BG:73:ALA:HB1 | 30:BG:82:LEU:HD11 | 1.82 | 0.61 |
| 35:DO:61:ARG:O | 35:DO:62:LEU:CD2 | 2.45 | 0.61 |
| 27:DD:64:ILE:O | 27:DD:64:ILE:HG12 | 2.01 | 0.61 |
| 28:DE:4:ILE:HD12 | 28:DE:28:ALA:HB1 | 1.82 | 0.61 |
| 30:BG:67:LYS:HG3 | 50:B4:6:HIS:CE1 | 2.36 | 0.61 |
| 25:BA:1026:U:C4' | 25:BA:1027:A:OP1 | 2.48 | 0.61 |
| 22:CB:86:C:H2' | 22:CB:87:A:C4 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 48:DW:67:LYS:O | 48:DW:72:ALA:HB2 | 2.00 | 0.61 |
| 1:CA:1277:C:O2' | 1:CA:1279:A:H8 | 1.84 | 0.61 |
| 26:DB:40:U:H2' | 26:DB:45:A:H61 | 1.66 | 0.61 |
| 17:CT:44:ALA:HB1 | 17:CT:73:VAL:HG12 | 1.83 | 0.61 |
| 25:BA:594:U:OP1 | 54:B8:61:LEU:HD22 | 2.00 | 0.61 |
| 49:BX:8:LEU:HD13 | 49:BX:31:LEU:HD23 | 1.82 | 0.61 |
| 19:AV:10:PHE:H | 19:AV:10:PHE:HD1 | 1.43 | 0.61 |
| 14:CQ:37:PHE:HZ | 14:CQ:56:VAL:HG21 | 1.64 | 0.61 |
| 1:AA:186(E):C:H42 | 1:AA:191(B):G:H1 | 1.48 | 0.61 |
| 9:AL:79:LEU:O | 9:AL:83:ARG:HG3 | 2.01 | 0.61 |
| 1:AA:390:C:O3' | 16:AS:28:ARG:NH2 | 2.31 | 0.61 |
| 2:CE:28:PHE:HD1 | 2:CE:32:ILE:HG22 | 1.63 | 0.61 |
| 12:CO:58:VAL:O | 12:CO:65:GLU:HA | 2.00 | 0.61 |
| 25:BA:1099:G:H2' | 25:BA:1100:C:O4' | 2.01 | 0.61 |
| 6:CI:97:PHE:CD2 | 18:CU:65:ILE:HD11 | 2.36 | 0.61 |
| 25:BA:1060:U:H5' | 25:BA:1061:U:C5 | 2.36 | 0.61 |
| 25:BA:2377:A:H2' | 25:BA:2378:A:C8 | 2.36 | 0.61 |
| 23:AC:20:G:C5 | 23:AC:58:A:C2 | 2.89 | 0.61 |
| 28:DE:50:GLY:O | 28:DE:51:PHE:HB3 | 1.99 | 0.61 |
| 44:BU:81:LYS:HZ3 | 44:BU:96:ILE:CD1 | 2.14 | 0.61 |
| 36:BP:75:THR:HA | 36:BP:88:GLY:O | 2.01 | 0.61 |
| 25:BA:1728:G:N1 | 25:BA:1730:U:OP2 | 2.33 | 0.61 |
| 25:BA:479:A:N3 | 25:BA:481:G:H5' | 2.16 | 0.61 |
| 19:CV:27:GLU:HG2 | 19:CV:47:HIS:CD2 | 2.35 | 0.61 |
| 1:CA:619:U:O2 | 4:CG:135:LEU:HD22 | 2.01 | 0.61 |
| 25:DA:2522:U:C2' | 25:DA:2523:G:H5'' | 2.30 | 0.61 |
| 5:CH:144:THR:O | 5:CH:148:VAL:HG23 | 1.99 | 0.61 |
| 25:BA:1520:U:H2' | 25:BA:1521:G:O4' | 2.01 | 0.61 |
| 1:AA:606:G:H1 | 1:AA:631:G:H5'' | 1.65 | 0.61 |
| 45:DV:37:VAL:HG23 | 45:DV:38:TYR:N | 2.14 | 0.61 |
| 25:BA:2689:U:OP2 | 25:BA:2719:G:N2 | 2.32 | 0.61 |
| 23:AD:20:G:H5'' | 23:AD:60:A:H61 | 1.65 | 0.61 |
| 25:BA:518:G:H4' | 42:BS:18:ARG:NH1 | 2.15 | 0.61 |
| 31:DH:169:VAL:HG13 | 31:DH:170:ARG:N | 2.16 | 0.61 |
| 25:BA:613:U:O2 | 25:BA:613:U:O5' | 2.18 | 0.61 |
| 1:AA:411:A:C8 | 1:AA:413:G:H1' | 2.36 | 0.61 |
| 5:AH:102:ALA:HB1 | 5:AH:106:PRO:HG2 | 1.83 | 0.61 |
| 25:DA:1323:U:H2' | 25:DA:1324:G:H5' | 1.81 | 0.61 |
| 23:AD:25:U:H2' | 23:AD:26:C:C6 | 2.35 | 0.61 |
| 32:DK:95:LYS:NZ | 32:DK:99:GLU:OE2 | 2.33 | 0.61 |
| 41:B2:25:LEU:H | 41:B2:92:THR:CG2 | 2.13 | 0.61 |
| 25:BA:856:C:H2' | 25:BA:857:C:H6 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 48:DW:25:VAL:HG12 | 48:DW:60:LEU:HD23 | 1.80 | 0.61 |
| 4:CG:13:ARG:C | 4:CG:15:GLU:N | 2.51 | 0.61 |
| 1:AA:1004:A:C5' | 1:AA:1025:U:C4 | 2.84 | 0.61 |
| 25:DA:1062:G:OP1 | 25:DA:1062:G:H8 | 1.83 | 0.61 |
| 25:BA:882:G:C2' | 25:BA:883:G:C8 | 2.80 | 0.61 |
| 9:AL:118:LYS:O | 9:AL:119:ALA:HB3 | 2.00 | 0.61 |
| 25:DA:2310:A:C5' | 25:DA:2311:A:OP2 | 2.49 | 0.61 |
| 25:BA:2164:C:H2' | 25:BA:2165:G:C8 | 2.35 | 0.61 |
| 25:BA:2032:G:N2 | 28:BE:146:THR:HG23 | 2.12 | 0.61 |
| 8:AK:86:ILE:HG22 | 8:AK:87:SER:N | 2.14 | 0.61 |
| 25:DA:2261:C:O2' | 25:DA:2262:U:H5' | 2.01 | 0.61 |
| 25:BA:330:A:H2 | 25:BA:1210:A:H2' | 1.65 | 0.61 |
| 25:BA:2698:U:H2' | 25:BA:2699:C:C6 | 2.36 | 0.61 |
| 40:B1:79:PHE:HE2 | 40:B1:83:LEU:CD2 | 2.14 | 0.61 |
| 3:AF:166:GLU:HG3 | 3:AF:167:TRP:N | 2.15 | 0.61 |
| 25:DA:322:A:H5' | 25:DA:340:A:H1' | 1.82 | 0.61 |
| 1:AA:316:G:OP2 | 1:AA:351:G:O2' | 2.19 | 0.61 |
| 35:BO:57:THR:O | 35:BO:59:LEU:N | 2.34 | 0.61 |
| 1:AA:736:C:H2' | 1:AA:737:A:C8 | 2.35 | 0.61 |
| 25:BA:2389:G:H5'' | 25:BA:2390:U:H5' | 1.82 | 0.61 |
| 25:BA:1586:A:H3' | 25:BA:1587:A:H8 | 1.65 | 0.61 |
| 4:AG:196:LEU:HB3 | 4:AG:197:PRO:HD2 | 1.83 | 0.61 |
| 45:DV:11:GLU:HG2 | 45:DV:12:GLY:N | 2.14 | 0.61 |
| 17:CT:9:VAL:HG23 | 17:CT:56:VAL:HG22 | 1.83 | 0.61 |
| 48:DW:16:LEU:H | 48:DW:16:LEU:HD12 | 1.66 | 0.61 |
| 1:CA:84:U:O2 | 1:CA:84:U:H2' | 2.00 | 0.61 |
| 32:DK:117:GLU:CD | 32:DK:117:GLU:H | 2.04 | 0.61 |
| 44:DU:47:LYS:N | 44:DU:60:PHE:HB3 | 2.15 | 0.61 |
| 25:BA:1084:A:N6 | 25:BA:1085:A:N6 | 2.48 | 0.61 |
| 25:DA:9:U:C2 | 25:DA:2629:A:N6 | 2.52 | 0.61 |
| 16:AS:20:VAL:CG2 | 16:AS:32:TYR:CD2 | 2.84 | 0.61 |
| 28:BE:38:THR:C | 28:BE:40:GLU:H | 2.04 | 0.61 |
| 33:BM:42:TRP:CA | 33:BM:48:MET:HE1 | 2.12 | 0.61 |
| 4:AG:13:ARG:O | 4:AG:14:ARG:C | 2.38 | 0.61 |
| 1:CA:1322:C:H2' | 1:CA:1322:C:O2 | 2.00 | 0.61 |
| 31:BH:159:GLU:CD | 31:BH:170:ARG:HH12 | 2.04 | 0.61 |
| 36:BP:66:ILE:CG1 | 36:BP:67:ARG:H | 2.06 | 0.61 |
| 1:AA:1057:G:H2' | 1:AA:1058:G:O4' | 2.01 | 0.61 |
| 33:BM:59:LYS:HE3 | 33:BM:61:ARG:HH22 | 1.64 | 0.61 |
| 25:BA:1535:U:C2 | 25:BA:1536:A:H3' | 2.35 | 0.61 |
| 28:BE:119:ARG:CG | 28:BE:119:ARG:HH11 | 2.14 | 0.61 |
| 25:BA:774:A:H2 | 25:BA:787:U:O2' | 1.84 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 21:CX:25:LYS:HE2 | 21:CX:26:LYS:HE2 | 1.83 | 0.61 |
| 2:AE:60:ASP:O | 2:AE:64:ARG:HG2 | 2.01 | 0.61 |
| 15:AR:26:GLU:OE2 | 15:AR:77:ARG:NH1 | 2.33 | 0.61 |
| 25:BA:270(G):C:H2' | 25:BA:270(H):C:O4' | 2.00 | 0.61 |
| 12:AO:90:VAL:O | 12:AO:91:LYS:HB3 | 2.01 | 0.61 |
| 1:AA:941:G:C2 | 1:AA:942:G:H1' | 2.36 | 0.61 |
| 44:DU:53:PRO:HD2 | 44:DU:57:GLN:O | 2.01 | 0.61 |
| 44:DU:47:LYS:HG2 | 44:DU:60:PHE:CD1 | 2.36 | 0.61 |
| 2:CE:105:PHE:O | 2:CE:109:SER:N | 2.30 | 0.61 |
| 25:BA:2074:U:H2' | 25:BA:2075:U:C6 | 2.36 | 0.61 |
| 5:AH:9:LYS:O | 5:AH:33:VAL:HG23 | 2.01 | 0.61 |
| 39:BR:5:ALA:HA | 39:BR:8:LYS:HE2 | 1.83 | 0.61 |
| 31:BH:117:PRO:HB3 | 31:BH:123:PHE:CE1 | 2.36 | 0.61 |
| 25:BA:2127:G:H5' | 25:BA:2128:C:OP2 | 2.00 | 0.61 |
| 2:AE:63:MET:HB3 | 2:AE:225:ALA:HB1 | 1.82 | 0.61 |
| 1:AA:87:A:H2' | 1:AA:88:C:C6 | 2.36 | 0.61 |
| 3:CF:34:LEU:O | 3:CF:34:LEU:HD12 | 2.01 | 0.61 |
| 32:BK:73:GLU:HG3 | 32:BK:137:PRO:HG2 | 1.82 | 0.61 |
| 8:CK:64:LYS:HD2 | 8:CK:79:VAL:HG21 | 1.82 | 0.61 |
| 28:BE:41:LYS:C | 28:BE:42:ASP:OD2 | 2.39 | 0.60 |
| 19:CV:80:TYR:CZ | 19:CV:82:GLY:HA2 | 2.36 | 0.60 |
| 26:DB:75:G:C5' | 26:DB:75:G:H8 | 2.11 | 0.60 |
| 1:CA:973:G:C4 | 10:CM:55:LYS:HE2 | 2.36 | 0.60 |
| 39:DR:93:ARG:HG2 | 39:DR:117:ASP:HB3 | 1.82 | 0.60 |
| 10:AM:48:THR:CG2 | 10:AM:62:HIS:HB3 | 2.30 | 0.60 |
| 1:CA:1091:U:O2 | 1:CA:1093:A:H8 | 1.84 | 0.60 |
| 2:CE:82:ARG:HA | 2:CE:92:TYR:CE1 | 2.35 | 0.60 |
| 28:DE:182:LEU:HD12 | 28:DE:183:LEU:N | 2.15 | 0.60 |
| 1:CA:407:G:H2' | 1:CA:408:A:C8 | 2.36 | 0.60 |
| 25:BA:2733:A:C3' | 25:BA:2734:A:H5'' | 2.31 | 0.60 |
| 1:CA:1268:A:H2' | 1:CA:1269:A:C8 | 2.36 | 0.60 |
| 4:AG:79:PHE:CE1 | 4:AG:204:ILE:HG12 | 2.35 | 0.60 |
| 25:BA:1348:G:C2' | 25:BA:1349:A:H5'' | 2.31 | 0.60 |
| 1:AA:652:U:C4 | 1:AA:752:G:N3 | 2.69 | 0.60 |
| 8:AK:9:MET:SD | 8:AK:32:LYS:HG2 | 2.41 | 0.60 |
| 18:AU:26:LEU:HD22 | 18:AU:42:ARG:NH1 | 2.15 | 0.60 |
| 5:AH:91:LEU:HD12 | 5:AH:120:THR:HG22 | 1.81 | 0.60 |
| 25:DA:2052:G:O4' | 28:DE:142:GLY:HA3 | 2.01 | 0.60 |
| 43:BT:27:THR:HB | 43:BT:80:ILE:HG22 | 1.83 | 0.60 |
| 30:BG:15:VAL:HG22 | 30:BG:175:LEU:HB2 | 1.83 | 0.60 |
| 29:DF:10:PRO:HA | 29:DF:127:GLU:HB3 | 1.82 | 0.60 |
| 3:AF:119:ARG:HE | 3:AF:140:ARG:CZ | 2.14 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 22:AB:23:A:H3' | 22:AB:24:C:C5 | 2.36 | 0.60 |
| 28:BE:78:LEU:HD11 | 28:BE:79:ARG:HG2 | 1.82 | 0.60 |
| 25:DA:7:G:O2' | 25:DA:8:A:H5' | 2.02 | 0.60 |
| 27:DD:34:VAL:O | 27:DD:34:VAL:HG13 | 2.01 | 0.60 |
| 28:BE:14:ILE:HB | 28:BE:21:VAL:HG22 | 1.82 | 0.60 |
| 31:DH:152:ARG:C | 31:DH:154:PRO:CD | 2.69 | 0.60 |
| 1:CA:1227:A:O3' | 13:CP:115:LYS:HD2 | 2.01 | 0.60 |
| 25:BA:481:G:H1' | 25:BA:507:A:N1 | 2.15 | 0.60 |
| 40:B1:92:ARG:NH1 | 40:B1:94:ASN:ND2 | 2.49 | 0.60 |
| 1:CA:1239:A:O2' | 1:CA:1298:C:N4 | 2.34 | 0.60 |
| 25:BA:2169:A:C6 | 25:BA:2170:A:N1 | 2.69 | 0.60 |
| 45:DV:108:PRO:HB3 | 45:DV:141:VAL:O | 2.00 | 0.60 |
| 25:DA:857:C:H2' | 25:DA:858:U:C6 | 2.36 | 0.60 |
| 1:AA:1028(B):C:N3 | 1:AA:1032(A):G:N2 | 2.49 | 0.60 |
| 25:DA:1459:G:C2' | 25:DA:1460:A:H5' | 2.29 | 0.60 |
| 25:BA:2629:A:O2' | 25:BA:2630:G:H5'' | 2.01 | 0.60 |
| 25:BA:1332:G:H5' | 25:BA:1332:G:C8 | 2.36 | 0.60 |
| 25:BA:1786:A:C2 | 25:BA:2606:C:H1' | 2.35 | 0.60 |
| 1:CA:1184:G:H2' | 1:CA:1185:G:H5' | 1.83 | 0.60 |
| 1:AA:605:U:H2' | 1:AA:606:G:O4' | 2.00 | 0.60 |
| 25:DA:242:G:H5' | 54:D8:62:LEU:HB3 | 1.82 | 0.60 |
| 45:DV:139:VAL:HA | 45:DV:156:LYS:HE3 | 1.82 | 0.60 |
| 45:DV:126:VAL:HG12 | 45:DV:163:LEU:HA | 1.81 | 0.60 |
| 7:CJ:86:GLN:NE2 | 23:CD:32:G:H21 | 2.00 | 0.60 |
| 32:DK:75:LEU:HD23 | 32:DK:76:THR:H | 1.65 | 0.60 |
| 53:D7:19:ARG:HG2 | 53:D7:19:ARG:HH11 | 1.66 | 0.60 |
| 1:AA:1510:U:H2' | 1:AA:1511:G:C8 | 2.35 | 0.60 |
| 25:DA:873:G:C2 | 25:DA:905:U:O2 | 2.54 | 0.60 |
| 29:BF:123:LEU:HD12 | 29:BF:124:LEU:N | 2.17 | 0.60 |
| 49:DX:40:THR:HG23 | 49:DX:43:ILE:HG12 | 1.82 | 0.60 |
| 25:BA:755:C:O2' | 25:BA:756:C:H5' | 2.00 | 0.60 |
| 18:AU:58:LEU:HD22 | 18:AU:62:GLU:HB3 | 1.82 | 0.60 |
| 1:AA:177:C:OP2 | 20:AW:65:LYS:HD3 | 2.01 | 0.60 |
| 11:AN:78:GLN:O | 11:AN:103:LEU:HA | 2.00 | 0.60 |
| 25:BA:2820:A:C8 | 28:BE:109:LYS:HE2 | 2.36 | 0.60 |
| 35:DO:61:ARG:CZ | 35:DO:61:ARG:HB2 | 2.26 | 0.60 |
| 25:BA:2308:G:N3 | 25:BA:2308:G:H2' | 2.15 | 0.60 |
| 23:AC:59:A:H4' | 23:AC:60:A:OP1 | 2.02 | 0.60 |
| 23:CD:15:G:C2' | 23:CD:60:A:H2 | 2.11 | 0.60 |
| 26:DB:44:G:C2 | 26:DB:48:A:C2 | 2.89 | 0.60 |
| 27:BD:186:HIS:CD2 | 27:BD:188:GLU:H | 2.11 | 0.60 |
| 1:AA:38:G:C2 | 1:AA:397:A:C2 | 2.90 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:2467:C:H2' | 25:DA:2468:G:O4' | 2.02 | 0.60 |
| 31:DH:137:ASP:CB | 31:DH:140:LYS:HB2 | 2.31 | 0.60 |
| 14:CQ:45:ARG:O | 14:CQ:49:HIS:CD2 | 2.55 | 0.60 |
| 25:DA:2210:G:H4' | 25:DA:2211:G:OP2 | 2.01 | 0.60 |
| 25:DA:322:A:H3' | 29:DF:169:ASN:ND2 | 2.15 | 0.60 |
| 4:AG:30:LYS:N | 4:AG:30:LYS:HD3 | 2.16 | 0.60 |
| 20:AW:9:ASN:C | 20:AW:9:ASN:HD22 | 2.05 | 0.60 |
| 1:AA:667:G:H4' | 15:AR:51:HIS:ND1 | 2.17 | 0.60 |
| 1:AA:50:A:H4' | 1:AA:51:A:O5' | 2.01 | 0.60 |
| 1:AA:97:U:H2' | 1:AA:99:C:C6 | 2.36 | 0.60 |
| 22:AB:27:G:O6 | 22:AB:45:U:O2 | 2.19 | 0.60 |
| 3:CF:77:ILE:O | 3:CF:83:ARG:HB3 | 2.01 | 0.60 |
| 1:CA:928:G:O2' | 1:CA:1533:C:OP1 | 2.19 | 0.60 |
| 23:CD:37:U:O4 | 23:CD:38:A:N6 | 2.34 | 0.60 |
| 27:DD:48:ARG:NH1 | 27:DD:48:ARG:HG3 | 2.15 | 0.60 |
| 5:AH:12:LEU:O | 5:AH:30:ALA:HA | 2.01 | 0.60 |
| 30:BG:94:LEU:HD23 | 30:BG:94:LEU:H | 1.66 | 0.60 |
| 3:AF:53:ALA:HB2 | 3:AF:115:LEU:HD11 | 1.83 | 0.60 |
| 8:AK:101:PRO:HG2 | 8:AK:133:LEU:HD11 | 1.84 | 0.60 |
| 25:BA:2466:C:H2' | 25:BA:2467:C:H5' | 1.83 | 0.60 |
| 38:DQ:83:LYS:O | 38:DQ:109:GLY:HA3 | 2.01 | 0.60 |
| 41:D2:5:VAL:HA | 41:D2:37:VAL:HB | 1.83 | 0.60 |
| 45:DV:144:LEU:O | 45:DV:146:ILE:N | 2.35 | 0.60 |
| 25:DA:2415:G:H4' | 35:DO:66:GLY:HA3 | 1.83 | 0.60 |
| 43:BT:31:HIS:CD2 | 43:BT:33:LYS:H | 2.20 | 0.60 |
| 25:BA:2418:A:OP2 | 54:B8:29:LYS:HE2 | 2.02 | 0.60 |
| 1:CA:126:G:HO2' | 1:CA:634:C:HO2' | 1.49 | 0.60 |
| 25:BA:2212:A:H1' | 25:BA:2215:G:C5 | 2.37 | 0.60 |
| 1:AA:872:A:C4 | 1:AA:874:G:C8 | 2.89 | 0.60 |
| 16:CS:8:ARG:NH1 | 16:CS:8:ARG:HG2 | 2.16 | 0.60 |
| 12:CO:27:LEU:CD2 | 12:CO:33:ARG:HG2 | 2.31 | 0.60 |
| 2:CE:178:ARG:NH2 | 8:CK:74:PRO:HG3 | 2.17 | 0.60 |
| 5:AH:55:VAL:O | 5:AH:58:ALA:HB3 | 2.02 | 0.60 |
| 39:BR:121:ILE:O | 39:BR:123:GLN:O | 2.20 | 0.60 |
| 1:AA:73:G:H2' | 1:AA:74:C:C6 | 2.36 | 0.60 |
| 3:CF:37:GLN:O | 3:CF:41:GLY:N | 2.35 | 0.60 |
| 25:BA:1688:U:O2 | 25:BA:1700:A:H5'' | 2.01 | 0.60 |
| 1:CA:87:A:N3 | 1:CA:87:A:H2' | 2.16 | 0.60 |
| 5:CH:96:PRO:HA | 5:CH:117:ASP:OD2 | 2.01 | 0.60 |
| 25:DA:867:C:C5 | 25:DA:868:U:C5 | 2.90 | 0.60 |
| 28:BE:61:ARG:N | 28:BE:62:PRO:CD | 2.64 | 0.60 |
| 25:BA:2318:G:H22 | 38:BQ:2:ALA:HB2 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|---------------------|-------------|----------|
| 1:CA:1320:C:O2 | 19:CV:72:GLY:HA3 | 2.01 | 0.60 |
| 25:BA:2285:C:OP1 | 52:B6:28:ARG:HD3 | 2.01 | 0.60 |
| 52:B6:44:ARG:O | 52:B6:45:LYS:CB | 2.46 | 0.60 |
| 35:BO:9:ASN:O | 35:BO:10:PRO:C | 2.40 | 0.60 |
| 45:BV:6:LYS:HA | 45:BV:60:GLU:CB | 2.26 | 0.60 |
| 25:BA:1019:U:H3 | 25:BA:1142(A):A:H62 | 1.47 | 0.60 |
| 1:AA:1298:C:C6 | 7:AJ:114:ARG:NH1 | 2.69 | 0.60 |
| 25:BA:1469:A:C2' | 25:BA:1470:G:O5' | 2.49 | 0.60 |
| 1:AA:309:G:H1' | 1:AA:608:A:C2 | 2.35 | 0.60 |
| 33:BM:57:ALA:O | 33:BM:58:ASP:CG | 2.39 | 0.60 |
| 12:CO:32:PHE:HE1 | 12:CO:86:ARG:HG3 | 1.65 | 0.60 |
| 1:CA:828:A:H2' | 1:CA:829:G:O4' | 2.02 | 0.60 |
| 1:AA:1193:G:H2' | 1:AA:1194:U:H5' | 1.83 | 0.60 |
| 25:BA:612:G:H2' | 25:BA:613:U:O2 | 2.01 | 0.60 |
| 12:CO:110:VAL:HG23 | 12:CO:120:TYR:HB3 | 1.84 | 0.60 |
| 1:CA:342:C:C2' | 1:CA:343:U:H5' | 2.31 | 0.60 |
| 25:DA:155:C:H2' | 25:DA:155:C:O2 | 2.00 | 0.60 |
| 22:AB:42:U:H5' | 22:AB:43:A:OP2 | 2.01 | 0.60 |
| 11:CN:57:THR:HG22 | 11:CN:58:PRO:HD2 | 1.83 | 0.60 |
| 25:DA:524:U:H2' | 25:DA:525:U:C6 | 2.37 | 0.60 |
| 15:AR:82:ILE:HG22 | 15:AR:83:GLU:N | 2.16 | 0.60 |
| 25:DA:2251:G:OP1 | 36:DP:82:ARG:NH1 | 2.34 | 0.60 |
| 27:BD:146:GLU:HB2 | 27:BD:189:CYS:HB3 | 1.83 | 0.60 |
| 27:DD:35:LYS:HE3 | 27:DD:65:ILE:N | 2.17 | 0.60 |
| 28:BE:23:VAL:CA | 28:BE:185:LYS:HA | 2.31 | 0.60 |
| 41:D2:35:LEU:HG | 41:D2:37:VAL:CG1 | 2.27 | 0.60 |
| 52:D6:48:VAL:CG1 | 52:D6:49:HIS:N | 2.33 | 0.60 |
| 23:AC:20:G:C5 | 23:AC:58:A:H2 | 2.18 | 0.60 |
| 27:DD:25:THR:C | 27:DD:27:THR:H | 2.03 | 0.60 |
| 25:DA:2404:C:H1' | 35:DO:67:MET:HE1 | 1.81 | 0.60 |
| 1:AA:1004:A:C6 | 1:AA:1025:U:H1' | 2.37 | 0.60 |
| 28:DE:126:PRO:O | 28:DE:131:ALA:HB2 | 2.01 | 0.60 |
| 25:BA:442:G:C4' | 29:BF:46:ARG:HD3 | 2.32 | 0.60 |
| 42:BS:94:ASP:C | 42:BS:95:ILE:HG23 | 2.21 | 0.60 |
| 25:DA:2354:G:O2' | 46:D3:36:ILE:HD12 | 2.02 | 0.60 |
| 32:DK:101:LEU:H | 32:DK:101:LEU:CD2 | 2.14 | 0.60 |
| 44:DU:61:ILE:HG22 | 44:DU:62:GLU:N | 2.17 | 0.60 |
| 31:BH:115:VAL:HG11 | 31:BH:148:ILE:HG12 | 1.84 | 0.60 |
| 48:BW:58:ALA:O | 48:BW:62:THR:HG22 | 2.02 | 0.60 |
| 35:DO:57:THR:O | 35:DO:59:LEU:N | 2.34 | 0.60 |
| 25:DA:1820:U:O2' | 27:DD:159:ALA:O | 2.14 | 0.60 |
| 1:CA:652:U:O2' | 1:CA:653:A:H5'' | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:1778:U:H2' | 25:DA:1784:A:N6 | 2.15 | 0.60 |
| 25:DA:476:G:H4' | 25:DA:502:A:N1 | 2.16 | 0.60 |
| 25:DA:2632:A:O2' | 25:DA:2811:G:O2' | 1.98 | 0.60 |
| 11:AN:12:ARG:HG2 | 11:AN:13:GLN:N | 2.17 | 0.60 |
| 1:AA:880:C:OP1 | 12:AO:8:ASN:ND2 | 2.34 | 0.60 |
| 29:BF:20:LEU:HD12 | 29:BF:21:ALA:N | 2.17 | 0.60 |
| 22:CB:7:G:H3' | 22:CB:8:U:C5' | 2.31 | 0.60 |
| 28:BE:197:ILE:O | 28:BE:197:ILE:HG12 | 2.01 | 0.60 |
| 40:D1:98:LEU:C | 40:D1:100:VAL:H | 2.03 | 0.60 |
| 28:BE:34:VAL:HG13 | 28:BE:49:LEU:O | 2.00 | 0.60 |
| 28:BE:59:VAL:C | 28:BE:60:ASN:CG | 2.61 | 0.60 |
| 33:BM:38:HIS:CE1 | 33:BM:50:ASP:OD2 | 2.55 | 0.60 |
| 1:CA:972:C:OP2 | 10:CM:57:LYS:HD2 | 2.00 | 0.60 |
| 4:CG:31:CYS:C | 4:CG:33:MET:H | 2.04 | 0.60 |
| 1:AA:1022:G:H2' | 1:AA:1023:G:O4' | 2.02 | 0.60 |
| 1:CA:328:C:O2' | 1:CA:329:A:OP2 | 2.13 | 0.60 |
| 54:B8:32:LEU:O | 54:B8:36:LYS:NZ | 2.34 | 0.60 |
| 25:DA:1044:G:O3' | 25:DA:1045:A:H4' | 2.01 | 0.60 |
| 7:CJ:113:GLU:CB | 7:CJ:119:ARG:HG2 | 2.30 | 0.60 |
| 1:AA:1028(A):C:C2 | 1:AA:1028(B):C:C5 | 2.89 | 0.60 |
| 31:DH:137:ASP:HB3 | 31:DH:140:LYS:HB2 | 1.83 | 0.60 |
| 25:DA:2262:U:P | 46:D3:19:LYS:NZ | 2.74 | 0.60 |
| 5:CH:152:ARG:NH2 | 8:CK:107:LEU:O | 2.33 | 0.60 |
| 35:BO:83:VAL:CG1 | 35:BO:112:LEU:HD21 | 2.32 | 0.60 |
| 1:CA:1399:C:C2 | 1:CA:1502:A:N6 | 2.70 | 0.60 |
| 23:AD:22:A:C2 | 23:AD:47:G:C8 | 2.90 | 0.60 |
| 25:DA:1771:C:C1' | 25:DA:1786:A:H8 | 2.13 | 0.60 |
| 25:BA:1761:C:N4 | 25:BA:1762:A:H62 | 1.99 | 0.60 |
| 25:DA:669:G:O2' | 25:DA:670:A:P | 2.60 | 0.60 |
| 25:DA:385:C:O2 | 35:DO:71:VAL:HG21 | 2.02 | 0.60 |
| 43:BT:57:LEU:CD1 | 43:BT:78:LYS:HB2 | 2.32 | 0.60 |
| 10:CM:8:LEU:HD22 | 10:CM:20:ALA:HB2 | 1.83 | 0.60 |
| 25:BA:2310:A:H2' | 25:BA:2311:A:H5' | 1.84 | 0.60 |
| 27:BD:31:LYS:HE3 | 27:BD:102:LYS:HD3 | 1.84 | 0.60 |
| 33:BM:46:VAL:HG12 | 33:BM:47:ALA:N | 2.01 | 0.60 |
| 31:DH:153:LYS:O | 31:DH:161:GLY:HA2 | 2.02 | 0.60 |
| 14:AQ:45:ARG:NH1 | 14:AQ:49:HIS:HE1 | 2.00 | 0.60 |
| 33:BM:28:THR:HA | 33:BM:106:MET:HE2 | 1.83 | 0.60 |
| 1:CA:1133:G:H1 | 1:CA:1141:C:H42 | 1.48 | 0.60 |
| 54:B8:52:LYS:N | 54:B8:53:PRO:CD | 2.63 | 0.60 |
| 12:CO:47:LYS:CB | 12:CO:48:PRO:HD2 | 2.31 | 0.60 |
| 25:DA:943:U:OP2 | 35:DO:36:LYS:HE3 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 35:DO:78:PRO:HA | 35:DO:110:TYR:HD2 | 1.67 | 0.60 |
| 1:AA:437:U:H2' | 1:AA:438:G:O4' | 2.02 | 0.60 |
| 2:AE:187:LEU:HA | 2:AE:201:ILE:HB | 1.83 | 0.60 |
| 2:CE:82:ARG:HA | 2:CE:92:TYR:HE1 | 1.67 | 0.60 |
| 38:DQ:59:LYS:CD | 38:DQ:60:GLY:H | 2.15 | 0.60 |
| 38:DQ:61:ASN:O | 38:DQ:65:VAL:HB | 2.02 | 0.60 |
| 4:CG:62:GLN:HE22 | 4:CG:65:ARG:HE | 1.49 | 0.60 |
| 3:CF:75:VAL:O | 3:CF:83:ARG:NE | 2.35 | 0.60 |
| 1:AA:271:C:H2' | 1:AA:272:C:H6 | 1.66 | 0.60 |
| 25:DA:1101:U:H2' | 25:DA:1102:C:H6 | 1.67 | 0.60 |
| 1:CA:965:A:C2 | 1:CA:969:A:C2 | 2.90 | 0.60 |
| 28:BE:167:VAL:CG1 | 28:BE:189:PRO:HD3 | 2.31 | 0.60 |
| 22:CB:31:C:H2' | 22:CB:32:C:H6 | 1.65 | 0.60 |
| 25:DA:1190:G:H2' | 25:DA:1191:G:H8 | 1.67 | 0.60 |
| 25:BA:2898:U:H2' | 25:BA:2899:G:C8 | 2.37 | 0.60 |
| 1:CA:1045:C:H2' | 1:CA:1046:A:O4' | 2.02 | 0.60 |
| 47:BZ:84:GLY:O | 47:BZ:87:PRO:HD3 | 2.01 | 0.60 |
| 1:AA:1159:U:C2 | 1:AA:1182:G:N1 | 2.70 | 0.60 |
| 36:DP:38:GLU:HB2 | 36:DP:127:ILE:HG22 | 1.84 | 0.60 |
| 25:DA:993:G:OP1 | 40:D1:50:ARG:NH2 | 2.34 | 0.60 |
| 28:BE:52:LEU:CD2 | 28:BE:52:LEU:N | 2.58 | 0.60 |
| 35:BO:66:GLY:O | 35:BO:67:MET:C | 2.40 | 0.60 |
| 25:DA:2753:A:H2' | 25:DA:2754:U:H5'' | 1.84 | 0.60 |
| 39:BR:36:GLU:HG3 | 39:BR:41:ARG:CD | 2.25 | 0.60 |
| 25:BA:2416:C:OP1 | 35:BO:64:LYS:O | 2.18 | 0.60 |
| 25:DA:1012:U:O4 | 33:DM:25:ARG:HD3 | 2.02 | 0.60 |
| 1:CA:1127:G:N2 | 1:CA:1145:C:C2 | 2.70 | 0.60 |
| 25:DA:1689:A:N7 | 25:DA:1698:A:N1 | 2.49 | 0.60 |
| 25:BA:1480:G:C2 | 25:BA:1482:U:O2 | 2.54 | 0.60 |
| 2:AE:8:LYS:H | 2:AE:8:LYS:CD | 2.14 | 0.60 |
| 25:DA:2159:G:H2' | 25:DA:2160:G:O4' | 2.02 | 0.60 |
| 45:DV:150:LEU:HD22 | 45:DV:154:ASP:HB2 | 1.82 | 0.60 |
| 29:DF:46:ARG:HG2 | 29:DF:46:ARG:NH1 | 2.11 | 0.60 |
| 25:BA:1204:A:H2 | 25:BA:1241:A:N1 | 2.00 | 0.60 |
| 25:DA:1786:A:C2 | 25:DA:2606:C:H1' | 2.37 | 0.60 |
| 10:AM:40:LEU:HB2 | 10:AM:69:ASN:HB3 | 1.82 | 0.60 |
| 1:AA:737:A:H2' | 1:AA:738:C:H6 | 1.64 | 0.60 |
| 1:CA:690:G:H2' | 1:CA:691:G:O4' | 2.01 | 0.60 |
| 13:AP:60:VAL:HG13 | 13:AP:64:TRP:HE1 | 1.67 | 0.60 |
| 3:CF:157:ILE:HD11 | 3:CF:166:GLU:HB2 | 1.84 | 0.60 |
| 4:AG:3:ARG:HG2 | 4:AG:118:ARG:CZ | 2.32 | 0.60 |
| 25:DA:1858:G:H1' | 25:DA:1884:A:N6 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:270(M):U:H1' | 25:BA:270(N):G:C6 | 2.36 | 0.60 |
| 5:AH:79:GLU:HB3 | 5:AH:92:LYS:HG3 | 1.82 | 0.60 |
| 5:CH:48:ALA:HB1 | 5:CH:49:PRO:HD2 | 1.84 | 0.60 |
| 8:AK:7:ALA:HB2 | 8:AK:85:ARG:HD2 | 1.82 | 0.60 |
| 50:D4:40:HIS:HB3 | 50:D4:45:GLY:HA3 | 1.82 | 0.60 |
| 8:AK:129:VAL:HG23 | 8:AK:130:GLY:H | 1.66 | 0.60 |
| 37:D0:51:LEU:HD22 | 37:D0:66:VAL:HG13 | 1.82 | 0.60 |
| 48:DW:64:LEU:HD23 | 48:DW:64:LEU:O | 2.02 | 0.60 |
| 34:BN:7:TYR:CZ | 34:BN:44:LYS:HG3 | 2.37 | 0.60 |
| 25:DA:733:G:O6 | 25:DA:761:A:C8 | 2.55 | 0.60 |
| 25:BA:1156:A:C8 | 40:B1:51:LYS:HD2 | 2.37 | 0.60 |
| 32:BK:79:ILE:HB | 32:BK:142:VAL:HG12 | 1.84 | 0.60 |
| 1:AA:1157:A:N3 | 1:AA:1157:A:H2' | 2.17 | 0.60 |
| 1:AA:1176:A:H2' | 1:AA:1177:G:H5' | 1.84 | 0.60 |
| 35:BO:16:ARG:HG3 | 35:BO:16:ARG:NH1 | 2.15 | 0.60 |
| 30:BG:63:ILE:HG12 | 30:BG:64:THR:N | 2.15 | 0.60 |
| 52:B6:41:PRO:HD2 | 52:B6:46:HIS:H | 1.66 | 0.60 |
| 4:CG:11:LEU:HD22 | 4:CG:66:ARG:NE | 2.17 | 0.60 |
| 1:AA:1442:G:C6 | 1:AA:1446:A:N6 | 2.70 | 0.60 |
| 48:BW:47:ASN:O | 48:BW:49:LYS:N | 2.34 | 0.60 |
| 1:CA:632:A:C1' | 1:CA:633:G:OP2 | 2.45 | 0.60 |
| 25:DA:530:G:O2' | 25:DA:531:C:OP2 | 2.17 | 0.60 |
| 1:CA:1128:C:N3 | 1:CA:1139:G:N1 | 2.50 | 0.60 |
| 1:AA:235:C:C5' | 17:AT:70:ARG:HG2 | 2.28 | 0.60 |
| 38:BQ:101:LEU:O | 38:BQ:101:LEU:HD12 | 2.02 | 0.60 |
| 19:CV:67:VAL:HG12 | 19:CV:68:GLY:N | 2.15 | 0.60 |
| 25:DA:1252:G:O4' | 40:D1:33:ARG:HD3 | 2.02 | 0.60 |
| 25:BA:141:A:C8 | 25:BA:1408:C:H1' | 2.37 | 0.60 |
| 25:BA:329:G:H4' | 25:BA:330:A:OP2 | 2.00 | 0.60 |
| 40:B1:79:PHE:C | 40:B1:79:PHE:CD2 | 2.73 | 0.60 |
| 40:B1:79:PHE:HE2 | 40:B1:83:LEU:HD21 | 1.66 | 0.60 |
| 32:BK:78:THR:HG23 | 32:BK:141:LYS:HZ3 | 1.65 | 0.60 |
| 35:BO:39:LYS:HG3 | 35:BO:45:LEU:CD2 | 2.32 | 0.60 |
| 25:DA:204:A:HO2' | 25:DA:205:G:P | 2.25 | 0.60 |
| 25:DA:340:A:H2' | 25:DA:341:G:H5' | 1.84 | 0.60 |
| 3:AF:32:LEU:HD13 | 3:AF:59:ARG:HD3 | 1.84 | 0.60 |
| 3:AF:58:GLU:H | 3:AF:65:ALA:HB3 | 1.65 | 0.60 |
| 25:DA:639:U:H2' | 25:DA:640:C:C6 | 2.36 | 0.60 |
| 1:CA:1028(B):C:H3' | 1:CA:1029:G:H5'' | 1.84 | 0.60 |
| 22:AB:23:A:O2' | 22:AB:24:C:OP1 | 2.18 | 0.60 |
| 41:B2:65:GLY:HA3 | 41:B2:91:TYR:CE1 | 2.37 | 0.60 |
| 25:BA:1095:A:N3 | 25:BA:1095:A:H2' | 2.15 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 27:BD:110:GLY:O | 27:BD:112:GLN:HG3 | 2.00 | 0.60 |
| 25:BA:2467:C:C4' | 36:BP:123:HIS:ND1 | 2.65 | 0.59 |
| 25:DA:2419:U:O4 | 54:D8:31:HIS:CG | 2.55 | 0.59 |
| 1:CA:1321:C:C4 | 1:CA:1322:C:H5 | 2.19 | 0.59 |
| 1:AA:1036:G:H5' | 1:AA:1037:C:OP2 | 2.01 | 0.59 |
| 10:AM:48:THR:HG23 | 10:AM:62:HIS:ND1 | 2.16 | 0.59 |
| 1:AA:872:A:C5 | 1:AA:874:G:C8 | 2.90 | 0.59 |
| 13:AP:108:ARG:HH11 | 13:AP:108:ARG:CG | 2.12 | 0.59 |
| 36:BP:20:ALA:CB | 36:BP:99:PRO:HD2 | 2.32 | 0.59 |
| 1:CA:1325:C:OP1 | 21:CX:15:ARG:HD2 | 2.01 | 0.59 |
| 1:AA:167:G:C2' | 1:AA:168:G:H5' | 2.32 | 0.59 |
| 1:AA:933:G:O6 | 7:AJ:3:ARG:NH2 | 2.35 | 0.59 |
| 25:DA:125:G:H4' | 25:DA:126:A:OP2 | 2.02 | 0.59 |
| 4:CG:58:LEU:HD22 | 4:CG:62:GLN:HG3 | 1.84 | 0.59 |
| 38:BQ:48:LEU:CD2 | 38:BQ:82:ILE:HD11 | 2.32 | 0.59 |
| 2:AE:236:TYR:HA | 2:AE:239:VAL:HG21 | 1.83 | 0.59 |
| 25:DA:96:G:H4' | 48:DW:48:HIS:CD2 | 2.37 | 0.59 |
| 31:DH:149:ARG:HG3 | 31:DH:162:ILE:O | 2.01 | 0.59 |
| 31:BH:97:ARG:NH2 | 31:BH:104:GLU:OE2 | 2.35 | 0.59 |
| 34:BN:17:ARG:HE | 34:BN:47:ILE:HD13 | 1.65 | 0.59 |
| 1:CA:842:C:H4' | 1:CA:848:C:O2 | 2.01 | 0.59 |
| 27:BD:132:PRO:HD3 | 27:BD:190:TYR:CZ | 2.37 | 0.59 |
| 26:BB:89:G:OP2 | 26:BB:89:G:H8 | 1.85 | 0.59 |
| 3:CF:21:ARG:NH1 | 3:CF:21:ARG:HB3 | 2.17 | 0.59 |
| 54:B8:13:ARG:O | 54:B8:14:VAL:HG23 | 2.01 | 0.59 |
| 25:BA:2309:A:N6 | 25:BA:2310:A:C6 | 2.70 | 0.59 |
| 28:BE:46:ALA:C | 28:BE:47:VAL:CG2 | 2.70 | 0.59 |
| 23:CC:20:G:H4' | 23:CC:21:U:OP2 | 2.01 | 0.59 |
| 41:D2:76:LYS:CB | 41:D2:79:VAL:CG2 | 2.79 | 0.59 |
| 31:DH:152:ARG:O | 31:DH:153:LYS:CB | 2.33 | 0.59 |
| 26:DB:45:A:H2' | 26:DB:45:A:N3 | 2.16 | 0.59 |
| 28:DE:199:ARG:HG2 | 28:DE:200:GLU:N | 2.16 | 0.59 |
| 25:BA:2336:A:H61 | 46:B3:43:THR:CG2 | 2.15 | 0.59 |
| 1:AA:964:A:N3 | 1:AA:969:A:O2' | 2.33 | 0.59 |
| 37:D0:38:VAL:HG12 | 37:D0:42:LYS:HD2 | 1.84 | 0.59 |
| 25:DA:774:A:H2 | 25:DA:787:U:O2' | 1.82 | 0.59 |
| 25:DA:298:G:O2' | 25:DA:322:A:N1 | 2.29 | 0.59 |
| 41:D2:49:THR:HB | 41:D2:50:PRO:CD | 2.31 | 0.59 |
| 28:DE:111:ARG:HB2 | 28:DE:160:TYR:O | 2.01 | 0.59 |
| 1:AA:96:G:H2' | 1:AA:97:U:H5' | 1.83 | 0.59 |
| 14:AQ:37:PHE:CE1 | 14:AQ:53:LEU:HD13 | 2.37 | 0.59 |
| 1:CA:188:U:O2' | 1:CA:189:U:H5' | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 38:BQ:49:VAL:HG22 | 38:BQ:80:LEU:HD12 | 1.84 | 0.59 |
| 3:AF:189:ALA:O | 3:AF:191:THR:HG23 | 2.00 | 0.59 |
| 35:BO:105:LEU:HD12 | 35:BO:105:LEU:H | 1.67 | 0.59 |
| 25:BA:1790:C:H5'' | 25:BA:1791:A:OP1 | 2.02 | 0.59 |
| 25:DA:2898:U:H2' | 25:DA:2899:G:C8 | 2.38 | 0.59 |
| 25:BA:246:C:C2' | 25:BA:247:G:H5' | 2.32 | 0.59 |
| 11:AN:81:ASP:OD1 | 11:AN:81:ASP:N | 2.35 | 0.59 |
| 33:BM:128:HIS:HD2 | 33:BM:129:PRO:O | 1.85 | 0.59 |
| 12:CO:7:ILE:HA | 12:CO:10:LEU:HD12 | 1.84 | 0.59 |
| 38:BQ:38:GLN:HG3 | 38:BQ:47:THR:HG21 | 1.84 | 0.59 |
| 25:BA:1057:A:O2' | 25:BA:1058:U:O4' | 2.20 | 0.59 |
| 41:D2:69:LYS:CG | 41:D2:86:GLY:HA3 | 2.24 | 0.59 |
| 23:AC:62:C:H2' | 23:AC:63:C:C6 | 2.34 | 0.59 |
| 1:AA:1132:C:O2' | 1:AA:1133:G:H5' | 2.02 | 0.59 |
| 28:DE:3:GLY:HA3 | 28:DE:81:ILE:CD1 | 2.31 | 0.59 |
| 27:DD:28:GLU:HB3 | 27:DD:29:PRO:CD | 2.33 | 0.59 |
| 45:DV:175:VAL:HG13 | 45:DV:176:PRO:HD3 | 1.82 | 0.59 |
| 25:DA:1062:G:N2 | 25:DA:1076:C:N3 | 2.50 | 0.59 |
| 36:DP:75:THR:HG22 | 36:DP:89:ASN:H | 1.67 | 0.59 |
| 48:BW:50:ILE:CD1 | 48:BW:51:ARG:H | 2.08 | 0.59 |
| 23:CD:15:G:H5'' | 23:CD:16:C:OP2 | 2.02 | 0.59 |
| 1:CA:1279:A:H5'' | 1:CA:1280:A:OP1 | 2.02 | 0.59 |
| 25:BA:783:A:H2' | 25:BA:785:G:OP1 | 2.03 | 0.59 |
| 25:BA:847:U:C5 | 25:BA:933:A:C2 | 2.90 | 0.59 |
| 25:BA:2306:C:H3' | 25:BA:2307:G:H5' | 1.84 | 0.59 |
| 38:DQ:20:ARG:O | 38:DQ:20:ARG:HG2 | 2.02 | 0.59 |
| 39:BR:39:ARG:HG2 | 39:BR:40:THR:N | 2.15 | 0.59 |
| 25:BA:1204:A:N1 | 25:BA:1241:A:N1 | 2.51 | 0.59 |
| 25:BA:1678:G:H22 | 25:BA:1989:G:H22 | 1.49 | 0.59 |
| 25:DA:1786:A:H2 | 25:DA:2606:C:H1' | 1.66 | 0.59 |
| 10:CM:4:ILE:HD13 | 10:CM:100:THR:HG21 | 1.84 | 0.59 |
| 1:AA:1240:U:C4 | 7:AJ:32:ARG:HD3 | 2.37 | 0.59 |
| 30:DG:96:ARG:NH1 | 30:DG:96:ARG:HG2 | 2.16 | 0.59 |
| 1:AA:336:C:O2' | 1:AA:337:C:H5' | 2.02 | 0.59 |
| 25:DA:2716:U:O2' | 25:DA:2717:G:H5' | 2.02 | 0.59 |
| 40:D1:81:HIS:CE1 | 40:D1:85:LYS:HD2 | 2.36 | 0.59 |
| 29:BF:132:VAL:HG23 | 29:BF:133:ASN:N | 2.16 | 0.59 |
| 27:BD:148:GLU:HB3 | 27:BD:151:LYS:HD2 | 1.83 | 0.59 |
| 23:AC:66:C:O2' | 23:AC:67:C:H5' | 2.03 | 0.59 |
| 1:CA:56:U:H2' | 1:CA:57:G:C8 | 2.36 | 0.59 |
| 33:DM:71:ILE:O | 33:DM:71:ILE:HD12 | 2.03 | 0.59 |
| 25:BA:2469:A:H61 | 25:BA:2481:G:H1' | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:BA:2309:A:C3' | 25:BA:2310:A:H5' | 2.32 | 0.59 |
| 23:AC:20:G:C4 | 23:AC:58:A:C2 | 2.90 | 0.59 |
| 1:CA:972:C:C4' | 10:CM:57:LYS:HG3 | 2.31 | 0.59 |
| 36:BP:33:GLY:HA2 | 36:BP:105:GLU:HA | 1.84 | 0.59 |
| 44:BU:49:VAL:HG12 | 44:BU:50:ARG:H | 1.66 | 0.59 |
| 31:DH:117:PRO:HB3 | 31:DH:123:PHE:HE1 | 1.64 | 0.59 |
| 46:D3:38:VAL:CG1 | 46:D3:40:GLN:HG2 | 2.33 | 0.59 |
| 25:DA:654(D):G:H1 | 25:DA:654(Q):C:N4 | 2.00 | 0.59 |
| 25:DA:975:G:H1' | 25:DA:990:A:C2 | 2.38 | 0.59 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:H1 | 1.51 | 0.59 |
| 25:BA:873:G:H1 | 25:BA:904:C:N4 | 1.99 | 0.59 |
| 1:AA:673:G:H2' | 1:AA:674:G:C8 | 2.37 | 0.59 |
| 53:B7:48:LYS:O | 53:B7:49:ARG:CB | 2.50 | 0.59 |
| 1:AA:943:U:H1' | 9:AL:124:GLN:HE22 | 1.67 | 0.59 |
| 11:CN:63:LEU:H | 11:CN:63:LEU:HD23 | 1.68 | 0.59 |
| 1:CA:45:U:H2' | 1:CA:46:G:C8 | 2.37 | 0.59 |
| 9:AL:18:PHE:HD1 | 9:AL:62:TYR:HD2 | 1.48 | 0.59 |
| 1:CA:396:G:O2' | 1:CA:398:C:OP1 | 2.17 | 0.59 |
| 25:DA:2790:A:C4' | 25:DA:2791:C:OP2 | 2.50 | 0.59 |
| 25:BA:1336:A:OP2 | 43:BT:64:LYS:HE3 | 2.01 | 0.59 |
| 25:DA:2761:G:H1' | 31:DH:143:GLN:OE1 | 2.02 | 0.59 |
| 28:BE:59:VAL:CG1 | 28:BE:63:LEU:HD13 | 2.32 | 0.59 |
| 28:DE:45:THR:CG2 | 28:DE:45:THR:O | 2.44 | 0.59 |
| 28:DE:36:ARG:NH2 | 28:DE:88:GLY:HA3 | 2.16 | 0.59 |
| 1:CA:973:G:H1' | 10:CM:55:LYS:CE | 2.30 | 0.59 |
| 25:DA:1012:U:H5 | 33:DM:28:THR:HG21 | 1.66 | 0.59 |
| 25:DA:2311:A:O2' | 30:DG:88:ILE:CD1 | 2.50 | 0.59 |
| 25:BA:2439:A:H4' | 25:BA:2440:C:O5' | 2.02 | 0.59 |
| 2:CE:43:ASP:O | 2:CE:47:THR:OG1 | 2.17 | 0.59 |
| 25:BA:774:A:C2 | 25:BA:787:U:O2' | 2.49 | 0.59 |
| 1:AA:923:A:O2' | 1:AA:1399:C:OP2 | 2.16 | 0.59 |
| 23:AD:15:G:H2' | 23:AD:60:A:C2 | 2.37 | 0.59 |
| 49:BX:52:HIS:CD2 | 49:BX:52:HIS:H | 2.21 | 0.59 |
| 36:DP:57:HIS:O | 36:DP:57:HIS:CG | 2.56 | 0.59 |
| 25:BA:2208:U:O2' | 25:BA:2209:C:H5' | 2.02 | 0.59 |
| 25:BA:2483:C:N3 | 36:BP:124:LYS:HE3 | 2.16 | 0.59 |
| 20:AW:23:ARG:O | 20:AW:27:LYS:HB3 | 2.01 | 0.59 |
| 25:BA:2159:G:H2' | 25:BA:2160:G:H8 | 1.66 | 0.59 |
| 36:BP:80:GLU:OE2 | 36:BP:80:GLU:HA | 2.02 | 0.59 |
| 1:CA:1135:U:H4' | 1:CA:1136:U:H5 | 1.67 | 0.59 |
| 1:AA:626:U:C2 | 1:AA:627:G:C8 | 2.91 | 0.59 |
| 52:D6:9:LEU:N | 52:D6:27:LYS:HG3 | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 28:BE:79:ARG:NH2 | 28:BE:164:ARG:NH1 | 2.49 | 0.59 |
| 38:DQ:7:TYR:CZ | 38:DQ:91:PRO:HG3 | 2.38 | 0.59 |
| 28:BE:50:GLY:CA | 28:BE:77:ILE:HA | 2.25 | 0.59 |
| 35:DO:15:ARG:O | 35:DO:16:ARG:O | 2.21 | 0.59 |
| 4:CG:30:LYS:N | 4:CG:30:LYS:HE2 | 2.17 | 0.59 |
| 25:DA:1558:A:H4' | 25:DA:1559:G:O5' | 2.02 | 0.59 |
| 1:AA:824:C:H4' | 8:AK:1:MET:HB2 | 1.83 | 0.59 |
| 25:DA:2131:G:H5' | 25:DA:2132:U:OP1 | 2.02 | 0.59 |
| 28:BE:119:ARG:HH11 | 28:BE:119:ARG:HG3 | 1.68 | 0.59 |
| 25:DA:975:G:N2 | 25:DA:990:A:O4' | 2.36 | 0.59 |
| 54:B8:16:ILE:HD13 | 54:B8:57:ARG:HG2 | 1.84 | 0.59 |
| 25:BA:1188:U:O2' | 25:BA:1189:A:H5' | 2.02 | 0.59 |
| 1:AA:1399:C:H4' | 1:AA:1400:C:O5' | 2.02 | 0.59 |
| 22:CB:44:G:O2' | 22:CB:45:U:H5' | 2.03 | 0.59 |
| 7:CJ:143:ARG:NH1 | 23:CD:42:C:O2' | 2.36 | 0.59 |
| 5:CH:55:VAL:O | 5:CH:58:ALA:HB3 | 2.01 | 0.59 |
| 25:DA:572:A:H5'' | 25:DA:573:G:OP2 | 2.03 | 0.59 |
| 8:CK:35:ILE:O | 8:CK:39:LEU:HB2 | 2.03 | 0.59 |
| 25:DA:2584:U:H5'' | 25:DA:2585:U:OP2 | 2.03 | 0.59 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.38 | 0.59 |
| 1:CA:404:U:H2' | 1:CA:405:U:C6 | 2.37 | 0.59 |
| 44:BU:35:TYR:CE1 | 44:BU:69:ALA:HB3 | 2.37 | 0.59 |
| 25:BA:1102:C:H2' | 25:BA:1103:A:H8 | 1.67 | 0.59 |
| 25:DA:2287:A:C2 | 25:DA:2346:A:N1 | 2.70 | 0.59 |
| 20:AW:10:LEU:HD21 | 20:AW:12:ALA:HB2 | 1.80 | 0.59 |
| 27:DD:35:LYS:CB | 27:DD:64:ILE:H | 2.16 | 0.59 |
| 33:DM:4:TYR:CE2 | 40:D1:100:VAL:HG11 | 2.37 | 0.59 |
| 1:AA:1133:G:H2' | 1:AA:1134:G:H8 | 1.68 | 0.59 |
| 39:DR:56:GLY:O | 39:DR:59:THR:N | 2.35 | 0.59 |
| 1:CA:984:C:H2' | 1:CA:985:C:C6 | 2.38 | 0.59 |
| 35:BO:64:LYS:HB3 | 54:B8:25:MET:HG2 | 1.82 | 0.59 |
| 29:DF:29:ASN:N | 29:DF:112:MET:HE1 | 2.17 | 0.59 |
| 25:DA:2271:G:H5'' | 46:D3:20:ARG:CD | 2.32 | 0.59 |
| 1:CA:1127:G:N2 | 1:CA:1144:G:H22 | 2.01 | 0.59 |
| 30:DG:67:LYS:HB3 | 50:D4:6:HIS:CD2 | 2.37 | 0.59 |
| 45:DV:120:ILE:HB | 45:DV:169:GLU:OE2 | 2.03 | 0.59 |
| 25:DA:2720:U:C4 | 25:DA:2873:A:N1 | 2.70 | 0.59 |
| 51:B5:40:LYS:CG | 51:B5:47:PRO:HD2 | 2.33 | 0.59 |
| 39:BR:26:ASP:O | 39:BR:49:VAL:HG13 | 2.02 | 0.59 |
| 39:BR:16:ARG:NH2 | 39:BR:83:ILE:O | 2.36 | 0.59 |
| 19:CV:31:ILE:CG2 | 19:CV:50:ALA:H | 2.15 | 0.59 |
| 22:AB:50:A:N1 | 22:AB:52:U:H5'' | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 32:DK:77:LEU:HA | 32:DK:141:LYS:H | 1.68 | 0.59 |
| 1:AA:1065:U:O2' | 1:AA:1066:C:OP2 | 2.20 | 0.59 |
| 1:CA:513:C:H42 | 1:CA:538:G:H1 | 1.51 | 0.59 |
| 25:DA:2537:U:H2' | 25:DA:2538:C:C6 | 2.38 | 0.59 |
| 25:DA:2823:A:OP1 | 28:DE:113:PHE:HB2 | 2.03 | 0.59 |
| 1:AA:763:G:H2' | 1:AA:764:C:H6 | 1.68 | 0.59 |
| 25:DA:535:C:O2' | 25:DA:536:A:H5' | 2.02 | 0.59 |
| 27:BD:264:LYS:O | 27:BD:267:SER:HB2 | 2.03 | 0.59 |
| 6:CI:72:VAL:HG13 | 6:CI:73:ASN:H | 1.67 | 0.59 |
| 25:DA:912:C:H2' | 25:DA:912:C:O2 | 2.03 | 0.59 |
| 25:BA:989:G:C8 | 49:BX:13:ILE:HD11 | 2.37 | 0.59 |
| 1:CA:1112:C:N3 | 3:CF:178:LEU:HB2 | 2.18 | 0.59 |
| 43:DT:15:GLU:H | 43:DT:15:GLU:CD | 2.04 | 0.59 |
| 25:BA:2724:C:OP1 | 28:BE:118:LYS:HE3 | 2.02 | 0.59 |
| 29:DF:11:VAL:HG23 | 29:DF:12:LEU:H | 1.66 | 0.59 |
| 25:BA:1980:G:O2' | 25:BA:1982:C:OP2 | 2.17 | 0.59 |
| 25:DA:2284:C:OP2 | 52:D6:27:LYS:HD2 | 2.03 | 0.59 |
| 28:BE:38:THR:O | 28:BE:40:GLU:N | 2.36 | 0.59 |
| 28:BE:61:ARG:O | 28:BE:63:LEU:N | 2.30 | 0.59 |
| 28:DE:38:THR:HG23 | 28:DE:40:GLU:HB2 | 1.84 | 0.59 |
| 1:CA:485:G:O2' | 1:CA:486:U:H6 | 1.86 | 0.59 |
| 19:AV:42:PRO:HD3 | 50:B4:63:TYR:CD1 | 2.37 | 0.59 |
| 25:DA:1064:C:H2' | 25:DA:1065:U:C6 | 2.38 | 0.59 |
| 2:CE:19:HIS:CE1 | 2:CE:204:ASN:HB3 | 2.38 | 0.59 |
| 46:B3:38:VAL:HG12 | 46:B3:40:GLN:HG2 | 1.85 | 0.59 |
| 1:AA:1368:G:OP1 | 9:AL:111:ARG:NH2 | 2.36 | 0.59 |
| 1:CA:1128:C:HO2' | 1:CA:1129:C:P | 2.25 | 0.59 |
| 25:DA:330:A:H2 | 25:DA:1210:A:C2' | 2.16 | 0.59 |
| 25:DA:2192:G:C2' | 25:DA:2193:G:H5' | 2.33 | 0.59 |
| 25:DA:2298:A:H1' | 25:DA:2321:G:H22 | 1.68 | 0.59 |
| 41:B2:44:LYS:CG | 41:B2:45:THR:N | 2.65 | 0.59 |
| 37:D0:24:GLN:HE22 | 37:D0:36:THR:HG21 | 1.68 | 0.59 |
| 25:BA:528:A:C2 | 25:BA:2043:C:H4' | 2.37 | 0.59 |
| 25:DA:2210:G:H3' | 25:DA:2211:G:C4 | 2.38 | 0.59 |
| 23:AD:22:A:H2 | 23:AD:47:G:H2' | 1.67 | 0.59 |
| 25:BA:1827:C:H2' | 25:BA:1828:G:H5' | 1.85 | 0.59 |
| 1:CA:1016:A:H2' | 1:CA:1017:G:O4' | 2.01 | 0.59 |
| 1:CA:77:C:H3' | 1:CA:78:G:H5" | 1.84 | 0.59 |
| 4:AG:162:LEU:O | 4:AG:165:MET:HB2 | 2.03 | 0.59 |
| 25:DA:877:U:O4 | 25:DA:899:A:N6 | 2.34 | 0.59 |
| 1:AA:664:G:H22 | 1:AA:741:G:H1 | 1.50 | 0.59 |
| 25:BA:1494:A:O2' | 25:BA:1495:A:H5' | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:779:U:OP1 | 27:DD:49:ILE:HG23 | 2.03 | 0.59 |
| 25:DA:2681:C:H6 | 25:DA:2683:C:H41 | 1.50 | 0.59 |
| 13:CP:102:ARG:O | 13:CP:107:ALA:HB2 | 2.03 | 0.59 |
| 1:AA:1004:A:C1' | 1:AA:1036:G:H1 | 2.13 | 0.59 |
| 30:DG:83:ARG:O | 30:DG:86:MET:HB2 | 2.02 | 0.59 |
| 25:DA:886:C:H1' | 25:DA:890:A:C2 | 2.37 | 0.59 |
| 25:DA:1863:G:O2' | 25:DA:2411:A:O2' | 2.21 | 0.59 |
| 25:DA:1486:A:H2' | 25:DA:1487:G:H8 | 1.67 | 0.59 |
| 1:CA:413:G:O2' | 1:CA:428:G:N2 | 2.36 | 0.59 |
| 25:DA:2056:G:C2 | 25:DA:2057:A:C8 | 2.90 | 0.59 |
| 26:BB:90:C:H5' | 36:BP:18:LYS:HA | 1.84 | 0.59 |
| 12:CO:69:TYR:CG | 12:CO:90:VAL:HG21 | 2.37 | 0.59 |
| 25:DA:2565:A:H5'' | 25:DA:2566:A:OP2 | 2.02 | 0.59 |
| 4:CG:105:VAL:HG21 | 4:CG:126:ILE:HG13 | 1.83 | 0.59 |
| 25:DA:278:A:O2' | 25:DA:279:C:OP1 | 2.15 | 0.59 |
| 1:CA:1151:A:O2' | 1:CA:1152:A:O5' | 2.18 | 0.59 |
| 31:BH:27:LYS:HG3 | 31:BH:27:LYS:O | 2.03 | 0.59 |
| 27:BD:32:SER:O | 27:BD:33:LEU:HB3 | 2.01 | 0.59 |
| 25:DA:2371:G:H4' | 52:D6:45:LYS:CG | 2.33 | 0.59 |
| 33:BM:46:VAL:O | 33:BM:47:ALA:CB | 2.51 | 0.59 |
| 1:CA:1317:C:OP1 | 14:CQ:16:PHE:HB3 | 2.03 | 0.59 |
| 1:CA:1305:G:C5' | 21:CX:4:GLY:HA3 | 2.32 | 0.59 |
| 25:DA:1109:C:H5'' | 25:DA:1110:G:OP2 | 2.02 | 0.59 |
| 25:DA:330:A:HO2' | 25:DA:331:A:H8 | 1.50 | 0.59 |
| 2:CE:137:ARG:HH12 | 2:CE:140:HIS:CB | 2.11 | 0.59 |
| 25:BA:2173:A:H8 | 25:BA:2173:A:OP1 | 1.86 | 0.59 |
| 31:BH:92:ILE:HD12 | 31:BH:92:ILE:N | 2.16 | 0.59 |
| 35:DO:37:GLY:O | 35:DO:40:SER:OG | 2.21 | 0.59 |
| 33:DM:128:HIS:HE2 | 33:DM:134:ARG:HD2 | 1.68 | 0.59 |
| 37:B0:104:ARG:HH12 | 37:B0:107:ASP:CG | 2.06 | 0.59 |
| 1:AA:438:G:H4' | 4:AG:123:HIS:ND1 | 2.17 | 0.59 |
| 25:BA:592:G:N2 | 54:B8:4:MET:HE1 | 2.17 | 0.59 |
| 36:DP:7:MET:CB | 36:DP:10:ARG:HH22 | 2.15 | 0.59 |
| 25:BA:529:A:H8 | 25:BA:530:G:C6 | 2.21 | 0.59 |
| 50:B4:34:GLU:HG2 | 50:B4:35:VAL:N | 2.17 | 0.59 |
| 1:CA:1072:G:C6 | 1:CA:1073:U:C4 | 2.90 | 0.59 |
| 1:AA:719:C:H5 | 1:AA:720:C:C4 | 2.21 | 0.59 |
| 1:CA:1386:G:C2 | 1:CA:1387:G:N7 | 2.71 | 0.59 |
| 27:DD:48:ARG:HG3 | 27:DD:48:ARG:HH11 | 1.66 | 0.59 |
| 25:DA:277:C:H5'' | 25:DA:278:A:N7 | 2.17 | 0.59 |
| 14:AQ:2:ALA:HB1 | 14:AQ:6:LEU:CD1 | 2.33 | 0.59 |
| 11:CN:69:ALA:HB1 | 11:CN:103:LEU:HD21 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 54:B8:17:THR:OG1 | 54:B8:21:LYS:HB2 | 2.02 | 0.59 |
| 25:BA:2121:G:H1 | 25:BA:2177:C:H42 | 1.51 | 0.59 |
| 25:DA:1676:A:C2 | 25:DA:1993:U:H5' | 2.38 | 0.59 |
| 1:AA:1149:C:P | 9:AL:9:ARG:HH21 | 2.26 | 0.59 |
| 12:CO:23:LYS:HE2 | 12:CO:23:LYS:H | 1.68 | 0.59 |
| 45:DV:52:SER:O | 45:DV:52:SER:OG | 2.14 | 0.59 |
| 25:BA:1147:C:H2' | 25:BA:1148:A:H5'' | 1.85 | 0.59 |
| 20:AW:13:LEU:HD12 | 20:AW:13:LEU:C | 2.23 | 0.59 |
| 31:BH:89:ILE:O | 31:BH:89:ILE:HG12 | 2.02 | 0.59 |
| 34:BN:4:PRO:O | 34:BN:5:GLN:CB | 2.50 | 0.59 |
| 25:DA:1499:C:O2' | 25:DA:1500:G:H5' | 2.03 | 0.59 |
| 17:CT:87:LYS:O | 17:CT:91:ARG:HG3 | 2.03 | 0.59 |
| 25:DA:2638:G:HO2' | 25:DA:2639:A:H8 | 1.48 | 0.58 |
| 27:DD:35:LYS:HD2 | 27:DD:104:TYR:CE1 | 2.33 | 0.58 |
| 40:D1:62:ILE:HG13 | 40:D1:76:TYR:CE1 | 2.37 | 0.58 |
| 40:D1:66:ASN:O | 40:D1:70:ARG:HD2 | 2.03 | 0.58 |
| 52:D6:15:GLU:HG2 | 52:D6:16:CYS:N | 2.17 | 0.58 |
| 1:CA:978:A:H5' | 1:CA:979:C:OP2 | 2.02 | 0.58 |
| 1:CA:980:C:H5' | 1:CA:981:U:OP2 | 2.03 | 0.58 |
| 35:DO:66:GLY:O | 35:DO:67:MET:C | 2.40 | 0.58 |
| 4:CG:31:CYS:O | 4:CG:32:ALA:HB3 | 2.03 | 0.58 |
| 22:CB:22:G:N2 | 22:CB:59:U:H5' | 2.18 | 0.58 |
| 29:BF:178:PRO:HB3 | 29:BF:198:ALA:HB1 | 1.85 | 0.58 |
| 25:BA:890:A:H3' | 25:BA:892:G:H8 | 1.68 | 0.58 |
| 25:DA:2470:G:OP1 | 36:DP:56:ARG:CZ | 2.50 | 0.58 |
| 1:AA:1299:A:H2' | 1:AA:1301:U:H1' | 1.84 | 0.58 |
| 5:CH:91:LEU:HD12 | 5:CH:120:THR:CG2 | 2.28 | 0.58 |
| 31:BH:152:ARG:HE | 31:BH:153:LYS:NZ | 2.00 | 0.58 |
| 51:B5:40:LYS:NZ | 51:B5:46:CYS:HB3 | 2.18 | 0.58 |
| 12:CO:62:SER:HB2 | 12:CO:64:TYR:CD1 | 2.33 | 0.58 |
| 1:CA:1326:C:OP1 | 21:CX:17:THR:OG1 | 2.20 | 0.58 |
| 35:BO:19:VAL:HG22 | 35:BO:20:GLY:H | 1.68 | 0.58 |
| 25:DA:1991:U:C2' | 25:DA:1992:G:H5'' | 2.33 | 0.58 |
| 4:AG:30:LYS:HA | 4:AG:34:GLU:HB2 | 1.85 | 0.58 |
| 25:DA:1283:G:N2 | 25:DA:1286:A:H5' | 2.18 | 0.58 |
| 1:CA:1208:C:H2' | 1:CA:1209:C:H6 | 1.68 | 0.58 |
| 3:CF:113:ALA:HB3 | 3:CF:114:PRO:HD3 | 1.85 | 0.58 |
| 1:AA:93:U:H2' | 1:AA:95:G:C4' | 2.33 | 0.58 |
| 1:CA:1151:A:H5' | 10:CM:41:PRO:HA | 1.85 | 0.58 |
| 25:BA:1668:A:N3 | 25:BA:1670:C:C4 | 2.71 | 0.58 |
| 1:AA:157:G:H2' | 1:AA:158:G:H5' | 1.85 | 0.58 |
| 45:BV:107:THR:HB | 45:BV:108:PRO:HD2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:234:C:H2' | 25:DA:235:U:H6 | 1.67 | 0.58 |
| 25:BA:2795:G:H3' | 25:BA:2797:U:C5' | 2.33 | 0.58 |
| 42:DS:29:LEU:HD21 | 42:DS:33:ARG:CZ | 2.33 | 0.58 |
| 1:AA:78:G:H1 | 1:AA:91:C:H42 | 1.50 | 0.58 |
| 32:DK:27:ARG:HG2 | 47:DZ:71:TYR:CE1 | 2.38 | 0.58 |
| 47:BZ:41:ARG:HG3 | 47:BZ:41:ARG:HH11 | 1.67 | 0.58 |
| 25:DA:1688:U:O2 | 25:DA:1700:A:H5' | 2.03 | 0.58 |
| 40:D1:61:TRP:O | 40:D1:65:ILE:HD13 | 2.04 | 0.58 |
| 27:BD:35:LYS:N | 27:BD:64:ILE:HG23 | 2.18 | 0.58 |
| 25:DA:1070:A:H8 | 25:DA:1096:A:O2' | 1.85 | 0.58 |
| 4:AG:19:LEU:N | 4:AG:19:LEU:HD22 | 2.15 | 0.58 |
| 25:BA:674:G:C1' | 29:BF:74:ARG:HD3 | 2.29 | 0.58 |
| 6:CI:33:TYR:HE1 | 6:CI:78:GLU:HG3 | 1.68 | 0.58 |
| 9:CL:8:GLY:HA3 | 9:CL:79:LEU:HB3 | 1.86 | 0.58 |
| 10:CM:23:ILE:HA | 10:CM:26:ALA:HB3 | 1.85 | 0.58 |
| 25:BA:1678:G:H8 | 25:BA:1678:G:O5' | 1.86 | 0.58 |
| 32:DK:75:LEU:HD23 | 32:DK:76:THR:N | 2.18 | 0.58 |
| 1:AA:310:G:OP1 | 16:AS:27:LYS:NZ | 2.36 | 0.58 |
| 10:CM:69:ASN:O | 10:CM:70:ARG:HG3 | 2.03 | 0.58 |
| 5:CH:107:ARG:HG2 | 5:CH:108:ALA:N | 2.18 | 0.58 |
| 1:CA:1152:A:H2' | 1:CA:1153:C:H6 | 1.68 | 0.58 |
| 1:CA:262:A:H5' | 20:CW:74:LYS:HG3 | 1.84 | 0.58 |
| 35:BO:85:LEU:HA | 35:BO:88:LEU:HD22 | 1.86 | 0.58 |
| 1:CA:1302:U:C5 | 13:CP:17:VAL:HG21 | 2.37 | 0.58 |
| 37:B0:38:VAL:HB | 37:B0:39:PRO:HD3 | 1.85 | 0.58 |
| 25:DA:1250:G:N7 | 35:DO:18:ARG:NH2 | 2.51 | 0.58 |
| 33:BM:24:GLY:HA2 | 33:BM:27:ALA:HB3 | 1.85 | 0.58 |
| 25:DA:1392:A:N6 | 25:DA:1393:A:N6 | 2.51 | 0.58 |
| 27:DD:31:LYS:O | 27:DD:31:LYS:HG3 | 2.03 | 0.58 |
| 25:BA:1544:C:H2' | 25:BA:1544:C:O2 | 2.02 | 0.58 |
| 23:CD:35:C:H2' | 23:CD:35:C:O2 | 2.02 | 0.58 |
| 1:AA:1405:G:O4' | 1:AA:1519:A:H4' | 2.03 | 0.58 |
| 25:BA:1242:A:H5'' | 25:BA:1243:G:OP2 | 2.03 | 0.58 |
| 25:DA:846:C:C2 | 25:DA:847:U:H5 | 2.20 | 0.58 |
| 28:BE:79:ARG:NE | 28:BE:197:ILE:HG22 | 2.19 | 0.58 |
| 1:AA:1156:G:H2' | 1:AA:1157:A:H5'' | 1.85 | 0.58 |
| 28:BE:35:GLN:CD | 28:BE:37:ARG:NH1 | 2.57 | 0.58 |
| 33:BM:42:TRP:CD1 | 40:B1:63:VAL:HG11 | 2.38 | 0.58 |
| 25:DA:2062:A:H62 | 25:DA:2503:A:N6 | 2.01 | 0.58 |
| 54:B8:36:LYS:HD3 | 54:B8:40:GLU:CD | 2.23 | 0.58 |
| 31:DH:6:ARG:HB2 | 31:DH:66:GLY:HA2 | 1.85 | 0.58 |
| 25:BA:1142(A):A:C4 | 25:BA:1144:G:C8 | 2.91 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 40:B1:90:VAL:O | 40:B1:92:ARG:N | 2.36 | 0.58 |
| 37:D0:86:ARG:HG2 | 37:D0:118:GLU:OE2 | 2.03 | 0.58 |
| 41:D2:43:GLU:O | 41:D2:44:LYS:HG2 | 2.03 | 0.58 |
| 35:DO:80:TYR:CD1 | 35:DO:111:ARG:HB3 | 2.38 | 0.58 |
| 15:AR:25:THR:HG21 | 15:AR:70:LEU:HB2 | 1.84 | 0.58 |
| 1:CA:1503:A:C8 | 1:CA:1531:A:N3 | 2.71 | 0.58 |
| 25:BA:1329:U:H5'' | 25:BA:1330:C:C5 | 2.38 | 0.58 |
| 25:DA:172:C:H2' | 25:DA:173:G:H8 | 1.67 | 0.58 |
| 25:BA:2314:C:H2' | 25:BA:2315:G:H8 | 1.68 | 0.58 |
| 46:B3:42:GLY:C | 46:B3:57:PHE:HD1 | 2.07 | 0.58 |
| 19:CV:41:VAL:O | 19:CV:44:MET:HB2 | 2.03 | 0.58 |
| 27:BD:123:ALA:CB | 27:BD:131:LEU:HG | 2.33 | 0.58 |
| 1:AA:116:A:H61 | 1:AA:313:A:H1' | 1.68 | 0.58 |
| 1:AA:93:U:H2' | 1:AA:95:G:O4' | 2.03 | 0.58 |
| 27:BD:70:TRP:CD1 | 27:BD:70:TRP:C | 2.76 | 0.58 |
| 25:BA:1442:G:C2 | 25:BA:1550:C:O2 | 2.56 | 0.58 |
| 42:BS:3:ALA:HB2 | 42:BS:64:MET:HE3 | 1.85 | 0.58 |
| 31:DH:111:HIS:ND1 | 31:DH:112:PRO:HD2 | 2.17 | 0.58 |
| 25:DA:1926:U:H2' | 25:DA:1928:A:OP2 | 2.03 | 0.58 |
| 8:CK:103:VAL:HG21 | 8:CK:110:ALA:HB2 | 1.84 | 0.58 |
| 25:DA:1388:G:C2' | 25:DA:1389:G:H5' | 2.33 | 0.58 |
| 4:AG:146:ILE:N | 4:AG:146:ILE:HD12 | 2.18 | 0.58 |
| 33:BM:45:ASN:CG | 33:BM:45:ASN:O | 2.41 | 0.58 |
| 9:AL:93:ARG:HB2 | 9:AL:93:ARG:HH11 | 1.67 | 0.58 |
| 38:DQ:24:LEU:HD23 | 38:DQ:84:GLN:O | 2.03 | 0.58 |
| 25:BA:2811:G:C2' | 25:BA:2812:G:H5' | 2.33 | 0.58 |
| 45:DV:145:GLU:O | 45:DV:145:GLU:HG3 | 2.03 | 0.58 |
| 22:CB:70:G:H3' | 22:CB:71:U:C6 | 2.38 | 0.58 |
| 47:DZ:92:LYS:O | 47:DZ:95:LEU:N | 2.27 | 0.58 |
| 1:AA:1004:A:H8 | 1:AA:1036:G:N2 | 2.01 | 0.58 |
| 25:BA:442:G:H21 | 29:BF:48:THR:HG23 | 1.67 | 0.58 |
| 25:DA:1142(A):A:C8 | 25:DA:1144:G:N7 | 2.71 | 0.58 |
| 25:DA:1826:G:C2' | 25:DA:1827:C:O5' | 2.51 | 0.58 |
| 10:AM:48:THR:HG23 | 10:AM:62:HIS:CB | 2.33 | 0.58 |
| 34:DN:47:ILE:CG1 | 34:DN:48:PRO:HD2 | 2.29 | 0.58 |
| 26:DB:40:U:H1' | 26:DB:46:A:C2 | 2.37 | 0.58 |
| 25:DA:1677:A:H2' | 25:DA:1678:G:C8 | 2.38 | 0.58 |
| 40:B1:92:ARG:HD2 | 41:B2:11:GLN:HB2 | 1.86 | 0.58 |
| 2:AE:204:ASN:HD22 | 2:AE:205:ASP:N | 2.00 | 0.58 |
| 25:BA:780:G:N2 | 25:BA:783:A:N6 | 2.43 | 0.58 |
| 1:CA:1333:A:H2' | 1:CA:1334:G:O4' | 2.04 | 0.58 |
| 35:DO:47:ASP:O | 35:DO:49:ARG:N | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 2:CE:144:ARG:HD2 | 2:CE:148:TYR:CE2 | 2.38 | 0.58 |
| 25:BA:1771:C:C1' | 25:BA:1786:A:H8 | 2.16 | 0.58 |
| 25:BA:2473:U:N3 | 25:BA:2474:C:C6 | 2.71 | 0.58 |
| 1:CA:1186:G:N2 | 1:CA:1187:G:H1' | 2.18 | 0.58 |
| 25:DA:2015:A:C2 | 51:D5:6:VAL:CG2 | 2.86 | 0.58 |
| 1:AA:244:U:H4' | 1:AA:245:C:C5' | 2.33 | 0.58 |
| 1:AA:200:G:N2 | 1:AA:218:C:C2 | 2.71 | 0.58 |
| 1:CA:1503:A:H1' | 1:CA:1504:G:OP1 | 2.02 | 0.58 |
| 1:CA:827:U:H3 | 1:CA:872:A:N6 | 2.00 | 0.58 |
| 23:CD:21:U:C2' | 23:CD:22:A:H5'' | 2.33 | 0.58 |
| 25:DA:2818:G:O2' | 25:DA:2819:G:H5' | 2.03 | 0.58 |
| 28:DE:128:SER:OG | 28:DE:129:HIS:N | 2.35 | 0.58 |
| 1:CA:1084:G:H2' | 1:CA:1085:U:H6 | 1.67 | 0.58 |
| 32:BK:73:GLU:HG3 | 32:BK:137:PRO:HD2 | 1.84 | 0.58 |
| 27:BD:145:VAL:HG12 | 27:BD:146:GLU:O | 2.03 | 0.58 |
| 35:DO:71:VAL:HG13 | 35:DO:72:PRO:HD3 | 1.85 | 0.58 |
| 32:BK:13:GLY:HA3 | 32:BK:17:GLN:OE1 | 2.02 | 0.58 |
| 25:BA:363(B):G:H2' | 25:BA:363(C):G:H8 | 1.68 | 0.58 |
| 1:CA:640:A:C2' | 1:CA:641:U:H5' | 2.33 | 0.58 |
| 25:DA:579:G:H2' | 25:DA:580:C:C6 | 2.38 | 0.58 |
| 25:DA:2142:C:H2' | 25:DA:2143:C:C6 | 2.38 | 0.58 |
| 1:AA:1086:U:H3 | 1:AA:1099:G:H22 | 1.51 | 0.58 |
| 28:BE:52:LEU:CB | 28:BE:75:VAL:HG22 | 2.25 | 0.58 |
| 35:BO:15:ARG:O | 35:BO:16:ARG:O | 2.21 | 0.58 |
| 25:DA:747:U:O2 | 25:DA:2014:A:H1' | 2.04 | 0.58 |
| 36:DP:79:LEU:HD13 | 36:DP:80:GLU:OE2 | 2.04 | 0.58 |
| 25:DA:2314:C:C2' | 25:DA:2315:G:H5' | 2.33 | 0.58 |
| 44:DU:17:SER:OG | 44:DU:18:GLY:N | 2.34 | 0.58 |
| 4:CG:22:LYS:HG3 | 4:CG:26:CYS:SG | 2.44 | 0.58 |
| 28:BE:119:ARG:HH12 | 28:BE:158:GLY:CA | 2.16 | 0.58 |
| 1:CA:1190:G:H5' | 3:CF:176:HIS:NE2 | 2.18 | 0.58 |
| 32:BK:10:GLU:O | 32:BK:11:ASN:HB2 | 2.03 | 0.58 |
| 25:BA:606:U:H4' | 25:BA:658:C:H4' | 1.85 | 0.58 |
| 25:BA:1179:C:C2' | 25:BA:1180:C:H5'' | 2.31 | 0.58 |
| 30:BG:114:ILE:HB | 30:BG:117:PHE:HB2 | 1.86 | 0.58 |
| 1:AA:200:G:H1 | 1:AA:217:C:H42 | 1.50 | 0.58 |
| 1:CA:1392:G:O2' | 1:CA:1393:U:H5' | 2.03 | 0.58 |
| 25:DA:2150:U:H2' | 25:DA:2151:G:C8 | 2.38 | 0.58 |
| 26:DB:56:G:H4' | 26:DB:57:A:H8 | 1.69 | 0.58 |
| 39:DR:98:LYS:HB3 | 39:DR:100:TYR:CE1 | 2.38 | 0.58 |
| 25:DA:2364:C:O2' | 25:DA:2365:G:H5' | 2.03 | 0.58 |
| 25:BA:1316:U:H2' | 25:BA:1317:A:C8 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 29:BF:20:LEU:HD12 | 29:BF:21:ALA:H | 1.69 | 0.58 |
| 33:BM:73:THR:HB | 33:BM:82:LEU:HD11 | 1.86 | 0.58 |
| 1:CA:1510:U:H2' | 1:CA:1511:G:C8 | 2.38 | 0.58 |
| 25:DA:601:C:O2 | 25:DA:605:C:H4' | 2.04 | 0.58 |
| 10:AM:16:LEU:HD11 | 10:AM:70:ARG:HB2 | 1.84 | 0.58 |
| 19:AV:15:LEU:O | 19:AV:19:VAL:HG23 | 2.03 | 0.58 |
| 30:DG:42:GLY:O | 30:DG:43:LEU:HD13 | 2.03 | 0.58 |
| 25:BA:1278:A:O2' | 37:B0:34:ILE:HD11 | 2.03 | 0.58 |
| 25:DA:2389:G:H5'' | 25:DA:2390:U:H5' | 1.85 | 0.58 |
| 1:CA:552:U:C2' | 1:CA:553:A:H5' | 2.33 | 0.58 |
| 1:AA:1312:G:C2' | 1:AA:1313:U:H5' | 2.34 | 0.58 |
| 1:CA:390:C:H2' | 1:CA:391:G:C8 | 2.37 | 0.58 |
| 25:BA:1038:C:H2' | 25:BA:1039:G:O4' | 2.03 | 0.58 |
| 33:DM:18:ALA:HA | 33:DM:21:LYS:HD2 | 1.84 | 0.58 |
| 12:AO:62:SER:HB2 | 12:AO:64:TYR:HD1 | 1.68 | 0.58 |
| 25:BA:1069:A:H4' | 25:BA:1070:A:O5' | 2.02 | 0.58 |
| 35:BO:68:GLN:HG2 | 54:B8:12:LYS:HD3 | 1.84 | 0.58 |
| 33:BM:115:ARG:H | 33:BM:118:LYS:HE3 | 1.69 | 0.58 |
| 28:DE:38:THR:HG23 | 28:DE:40:GLU:N | 2.15 | 0.58 |
| 27:DD:25:THR:HG23 | 27:DD:26:LYS:N | 2.18 | 0.58 |
| 1:CA:1316:G:H2' | 1:CA:1317:C:H5'' | 1.85 | 0.58 |
| 1:AA:559:A:OP1 | 5:AH:126:ARG:NH2 | 2.37 | 0.58 |
| 1:CA:973:G:C1' | 10:CM:55:LYS:HE2 | 2.31 | 0.58 |
| 1:CA:1159:U:O2 | 1:CA:1181:G:O6 | 2.22 | 0.58 |
| 1:AA:1301:U:O4 | 1:AA:1303:C:H1' | 2.04 | 0.58 |
| 25:BA:2572:A:N7 | 28:BE:145:LYS:HB2 | 2.19 | 0.58 |
| 2:CE:141:GLU:O | 2:CE:145:LEU:HB2 | 2.04 | 0.58 |
| 38:DQ:69:VAL:HG13 | 38:DQ:101:LEU:HD22 | 1.86 | 0.58 |
| 25:DA:1384:A:N3 | 25:DA:1405:U:H1' | 2.18 | 0.58 |
| 12:CO:41:ARG:HD2 | 12:CO:42:THR:H | 1.68 | 0.58 |
| 25:BA:1405:U:H2' | 25:BA:1406:U:C6 | 2.38 | 0.58 |
| 4:CG:24:GLU:HG2 | 4:CG:25:ARG:H | 1.67 | 0.58 |
| 45:DV:157:LEU:HB3 | 45:DV:161:VAL:HG12 | 1.85 | 0.58 |
| 25:BA:270(L):U:O2 | 32:BK:50:ARG:HD2 | 2.03 | 0.58 |
| 8:CK:82:HIS:HD2 | 8:CK:82:HIS:O | 1.87 | 0.58 |
| 10:CM:4:ILE:HA | 10:CM:100:THR:HG22 | 1.86 | 0.58 |
| 25:DA:905:U:H3' | 25:DA:906:G:H5'' | 1.85 | 0.58 |
| 27:DD:267:SER:C | 27:DD:269:PHE:H | 2.06 | 0.58 |
| 11:CN:59:TYR:CE1 | 11:CN:63:LEU:HD21 | 2.38 | 0.58 |
| 31:DH:143:GLN:HE21 | 31:DH:143:GLN:HA | 1.68 | 0.58 |
| 51:D5:31:VAL:HG13 | 51:D5:42:PRO:HG3 | 1.85 | 0.58 |
| 1:AA:753:A:H4' | 1:AA:754:C:H5'' | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:711:G:O2' | 1:CA:712:A:H5' | 2.03 | 0.58 |
| 1:CA:811:C:H4' | 1:CA:900:A:N6 | 2.19 | 0.58 |
| 25:DA:637:A:P | 35:DO:116:GLY:HA2 | 2.44 | 0.58 |
| 25:DA:854:G:H2' | 25:DA:855:G:H8 | 1.68 | 0.58 |
| 1:AA:859:A:H2' | 1:AA:860:A:H8 | 1.68 | 0.58 |
| 23:CD:9:G:O2' | 23:CD:10:G:C8 | 2.53 | 0.58 |
| 25:BA:2248:C:C2' | 25:BA:2249:U:H5' | 2.34 | 0.58 |
| 25:BA:2098:U:H2' | 25:BA:2099:U:O4' | 2.04 | 0.58 |
| 25:DA:1378:A:OP1 | 53:D7:10:ARG:NH2 | 2.36 | 0.58 |
| 8:AK:14:ARG:O | 8:AK:18:ARG:HD3 | 2.04 | 0.58 |
| 30:DG:145:THR:HG23 | 50:D4:28:LYS:HE2 | 1.85 | 0.58 |
| 52:D6:28:ARG:HB3 | 52:D6:30:THR:O | 2.03 | 0.58 |
| 38:BQ:85:VAL:CG2 | 38:BQ:112:PHE:CZ | 2.85 | 0.58 |
| 38:DQ:87:PHE:C | 38:DQ:87:PHE:CD2 | 2.77 | 0.58 |
| 39:BR:61:PHE:HD2 | 39:BR:61:PHE:H | 1.52 | 0.58 |
| 25:DA:2303:G:O2' | 25:DA:2304:G:H5' | 2.04 | 0.58 |
| 25:DA:91:A:H2' | 25:DA:92:G:O4' | 2.03 | 0.58 |
| 25:BA:1482:U:O4 | 25:BA:1510:A:C8 | 2.56 | 0.58 |
| 25:BA:2126:A:N6 | 25:BA:2163:C:H1' | 2.19 | 0.58 |
| 50:B4:57:GLU:HA | 50:B4:60:GLN:HB2 | 1.86 | 0.58 |
| 25:BA:1593:G:H2' | 25:BA:1594:G:C8 | 2.39 | 0.58 |
| 25:DA:2439:A:C5' | 25:DA:2439:A:C8 | 2.86 | 0.58 |
| 1:AA:1096:C:H2' | 1:AA:1097:C:C6 | 2.37 | 0.58 |
| 25:DA:11:G:H2' | 25:DA:12:U:H5' | 1.86 | 0.58 |
| 45:BV:150:LEU:CD2 | 45:BV:154:ASP:HB2 | 2.32 | 0.58 |
| 45:BV:111:VAL:O | 45:BV:111:VAL:HG23 | 2.03 | 0.58 |
| 25:BA:414:C:H2' | 25:BA:415:A:H8 | 1.67 | 0.58 |
| 1:AA:87:A:OP1 | 1:AA:87:A:H4' | 2.03 | 0.58 |
| 29:BF:64:ILE:O | 29:BF:65:TRP:CD1 | 2.57 | 0.58 |
| 49:DX:46:ASN:O | 49:DX:50:VAL:HG22 | 2.04 | 0.58 |
| 42:DS:54:ALA:HB1 | 42:DS:107:LEU:HD22 | 1.86 | 0.58 |
| 25:BA:64:A:O3' | 43:BT:71:GLY:HA3 | 2.04 | 0.58 |
| 35:DO:131:SER:HB3 | 35:DO:134:ALA:H | 1.67 | 0.58 |
| 1:CA:731:G:H5' | 1:CA:766:A:H4' | 1.85 | 0.58 |
| 43:BT:70:LEU:HD23 | 43:BT:70:LEU:N | 2.19 | 0.58 |
| 25:BA:1792:G:H5' | 27:BD:205:VAL:HG13 | 1.86 | 0.58 |
| 25:BA:1477:A:C2 | 25:BA:1517:G:C2 | 2.91 | 0.58 |
| 30:BG:83:ARG:HG3 | 30:BG:86:MET:SD | 2.44 | 0.58 |
| 25:DA:1568:G:OP2 | 27:DD:63:ARG:NH2 | 2.36 | 0.58 |
| 29:DF:63:LYS:HE2 | 29:DF:67:GLN:HB3 | 1.84 | 0.58 |
| 50:B4:4:GLY:O | 50:B4:5:ILE:HG22 | 2.03 | 0.58 |
| 51:D5:40:LYS:HE2 | 51:D5:44:THR:O | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 13:CP:33:ALA:HA | 13:CP:59:TYR:HE2 | 1.68 | 0.58 |
| 25:DA:531:C:OP1 | 25:DA:561:G:C2 | 2.56 | 0.58 |
| 2:AE:7:VAL:HG23 | 2:AE:8:LYS:HE2 | 1.84 | 0.58 |
| 25:BA:2790:A:H2 | 25:BA:2894:G:H5' | 1.67 | 0.58 |
| 1:CA:210:U:OP1 | 1:CA:210:U:O4' | 2.22 | 0.58 |
| 31:BH:154:PRO:HB3 | 31:BH:163:TYR:CZ | 2.39 | 0.58 |
| 33:BM:130:HIS:HD2 | 33:BM:134:ARG:HH12 | 1.50 | 0.58 |
| 2:AE:165:VAL:HG23 | 2:AE:166:ASP:N | 2.18 | 0.58 |
| 29:DF:118:ALA:HB2 | 29:DF:123:LEU:CD2 | 2.34 | 0.58 |
| 1:CA:413:G:HO2' | 1:CA:414:A:P | 2.25 | 0.58 |
| 36:DP:137:TYR:HE1 | 45:DV:83:PRO:HG3 | 1.69 | 0.58 |
| 25:BA:1310:G:OP2 | 53:B7:9:ARG:NH1 | 2.23 | 0.58 |
| 25:DA:2292:C:O2' | 25:DA:2293:C:H5' | 2.03 | 0.58 |
| 1:AA:66:G:O4' | 1:AA:173:U:C4 | 2.56 | 0.58 |
| 25:DA:2542:A:H5' | 25:DA:2543:G:OP1 | 2.03 | 0.58 |
| 25:DA:535:C:C2' | 25:DA:536:A:H5' | 2.34 | 0.58 |
| 46:D3:27:GLU:HG3 | 46:D3:68:GLU:HA | 1.84 | 0.58 |
| 1:CA:425:G:O3' | 4:CG:45:GLN:NE2 | 2.36 | 0.58 |
| 31:DH:107:VAL:HG12 | 31:DH:107:VAL:O | 2.03 | 0.58 |
| 1:AA:1234:C:H1' | 1:AA:1364:U:O2 | 2.04 | 0.58 |
| 45:BV:44:PHE:CZ | 45:BV:86:VAL:HG11 | 2.39 | 0.58 |
| 22:AB:58:U:O2 | 22:AB:58:U:H2' | 2.02 | 0.58 |
| 1:CA:542:G:OP1 | 4:CG:10:ARG:NH2 | 2.37 | 0.58 |
| 48:BW:64:LEU:HD21 | 48:BW:68:ARG:NH1 | 2.19 | 0.58 |
| 20:AW:10:LEU:CD2 | 20:AW:12:ALA:H | 2.16 | 0.58 |
| 36:DP:36:ALA:HB1 | 36:DP:127:ILE:HD12 | 1.86 | 0.58 |
| 38:DQ:106:ARG:HB3 | 38:DQ:110:LEU:HD11 | 1.84 | 0.58 |
| 53:D7:8:ASN:HD22 | 53:D7:11:LYS:N | 1.97 | 0.58 |
| 27:DD:27:THR:CG2 | 27:DD:83:GLU:HG2 | 2.22 | 0.58 |
| 54:D8:25:MET:C | 54:D8:48:PHE:HE1 | 2.06 | 0.58 |
| 25:DA:2404:C:O3' | 35:DO:77:ARG:NH2 | 2.36 | 0.58 |
| 25:BA:442:G:H4' | 29:BF:46:ARG:HD3 | 1.86 | 0.58 |
| 25:DA:1558:A:H1' | 25:DA:1559:G:OP2 | 2.04 | 0.58 |
| 2:AE:6:THR:OG1 | 2:AE:7:VAL:N | 2.36 | 0.58 |
| 5:CH:80:ILE:HD11 | 5:CH:138:ALA:CB | 2.31 | 0.58 |
| 27:BD:28:GLU:HB3 | 27:BD:29:PRO:CD | 2.33 | 0.58 |
| 31:BH:153:LYS:HG3 | 31:BH:162:ILE:N | 2.18 | 0.58 |
| 12:CO:27:LEU:HB3 | 12:CO:33:ARG:HD3 | 1.86 | 0.58 |
| 19:CV:28:LYS:HG2 | 19:CV:29:ARG:H | 1.69 | 0.58 |
| 23:CD:31:G:H2' | 23:CD:32:G:H8 | 1.68 | 0.58 |
| 51:B5:31:VAL:HG13 | 51:B5:42:PRO:HG3 | 1.84 | 0.58 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:C6 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:BA:2104:G:C2 | 25:BA:2186:G:C2 | 2.92 | 0.58 |
| 5:CH:33:VAL:HG12 | 5:CH:34:VAL:H | 1.68 | 0.58 |
| 25:BA:945:A:C4 | 25:BA:2448:A:C2 | 2.92 | 0.58 |
| 14:CQ:4:LYS:O | 14:CQ:7:ILE:HG12 | 2.04 | 0.58 |
| 25:BA:1955:U:O3' | 25:BA:1956:U:H6 | 1.87 | 0.58 |
| 30:DG:77:ILE:O | 30:DG:81:LYS:O | 2.21 | 0.58 |
| 25:DA:247:G:H4' | 25:DA:386:G:C5 | 2.39 | 0.58 |
| 11:CN:34:ASP:HB2 | 11:CN:35:PRO:CD | 2.33 | 0.58 |
| 17:AT:17:LYS:HG3 | 17:AT:47:PRO:HA | 1.86 | 0.58 |
| 25:BA:990:A:OP2 | 25:BA:991:C:OP2 | 2.21 | 0.58 |
| 20:AW:12:ALA:O | 20:AW:15:ARG:HB2 | 2.03 | 0.58 |
| 23:AC:62:C:C6 | 23:AC:63:C:H5 | 2.22 | 0.58 |
| 25:DA:2059:A:H5'' | 25:DA:2060:A:OP2 | 2.04 | 0.58 |
| 52:B6:44:ARG:HH11 | 52:B6:44:ARG:HG2 | 1.68 | 0.58 |
| 20:AW:71:THR:CG2 | 20:AW:72:LEU:H | 2.12 | 0.58 |
| 25:DA:329:G:H4' | 25:DA:330:A:OP2 | 2.03 | 0.58 |
| 1:AA:5:U:O2' | 1:AA:6:G:C4 | 2.57 | 0.58 |
| 25:BA:2779:U:O4' | 25:BA:2779:U:O2 | 2.19 | 0.58 |
| 3:AF:58:GLU:HB2 | 3:AF:65:ALA:HB2 | 1.84 | 0.58 |
| 39:DR:8:LYS:HZ3 | 39:DR:8:LYS:HB3 | 1.67 | 0.58 |
| 1:CA:279:A:H2' | 1:CA:279:A:N3 | 2.19 | 0.58 |
| 1:AA:1237:C:O2 | 1:AA:1334:G:O2' | 2.20 | 0.58 |
| 1:AA:1072:G:C5 | 1:AA:1073:U:C4 | 2.92 | 0.58 |
| 27:BD:134:ARG:HG3 | 27:BD:135:PHE:CD2 | 2.38 | 0.58 |
| 5:CH:36:ASP:CG | 5:CH:38:GLN:HB2 | 2.24 | 0.58 |
| 25:BA:643:A:C2' | 25:BA:644:A:O5' | 2.52 | 0.58 |
| 1:AA:967:C:H6 | 1:AA:967:C:O5' | 1.86 | 0.58 |
| 25:BA:1060:U:H4' | 25:BA:1061:U:O5' | 2.03 | 0.57 |
| 27:DD:35:LYS:CD | 27:DD:64:ILE:N | 2.67 | 0.57 |
| 28:BE:53:PRO:HA | 28:BE:74:PRO:CB | 2.34 | 0.57 |
| 23:AC:63:C:O2 | 23:AC:64:G:C8 | 2.56 | 0.57 |
| 28:DE:47:VAL:CG1 | 28:DE:49:LEU:HD23 | 2.33 | 0.57 |
| 25:DA:1331:A:O2' | 25:DA:1332:G:H8 | 1.87 | 0.57 |
| 13:CP:5:ALA:HB2 | 13:CP:22:ILE:HD13 | 1.84 | 0.57 |
| 1:CA:253:U:H2' | 1:CA:254:G:H8 | 1.69 | 0.57 |
| 25:BA:1359:A:N1 | 25:BA:1372:U:C4 | 2.72 | 0.57 |
| 25:DA:2571:C:H5' | 25:DA:2572:A:C5' | 2.29 | 0.57 |
| 1:AA:17:U:O4' | 1:AA:1080:A:H1' | 2.04 | 0.57 |
| 1:AA:16:A:H2' | 1:AA:17:U:H5' | 1.84 | 0.57 |
| 25:DA:39:C:H2' | 25:DA:40:C:C6 | 2.39 | 0.57 |
| 12:CO:27:LEU:HD21 | 12:CO:60:LEU:HB3 | 1.84 | 0.57 |
| 25:DA:2335:A:O2' | 25:DA:2336:A:H2' | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 32:BK:78:THR:HG23 | 32:BK:141:LYS:HZ2 | 1.68 | 0.57 |
| 25:BA:527:C:OP2 | 25:BA:2779:U:C5 | 2.57 | 0.57 |
| 30:BG:109:VAL:CG1 | 50:B4:33:VAL:HG21 | 2.34 | 0.57 |
| 25:DA:1771:C:C1' | 25:DA:1786:A:C8 | 2.87 | 0.57 |
| 1:AA:1106:G:H2' | 1:AA:1107:C:H6 | 1.69 | 0.57 |
| 1:AA:1186:G:H21 | 14:AQ:61:TRP:C | 2.07 | 0.57 |
| 25:BA:815:C:H2' | 25:BA:816:C:H6 | 1.69 | 0.57 |
| 1:AA:881:G:P | 12:AO:12:ARG:HH22 | 2.27 | 0.57 |
| 25:BA:2037:G:H2' | 25:BA:2038:G:C8 | 2.38 | 0.57 |
| 27:BD:17:THR:HG22 | 27:BD:204:ILE:HA | 1.86 | 0.57 |
| 35:BO:122:PRO:HB3 | 35:BO:141:ALA:HB1 | 1.85 | 0.57 |
| 25:BA:1230:C:H2' | 25:BA:1231:G:C8 | 2.39 | 0.57 |
| 51:B5:57:VAL:O | 51:B5:57:VAL:HG13 | 2.03 | 0.57 |
| 1:CA:1490:C:H2' | 1:CA:1491:G:O4' | 2.03 | 0.57 |
| 25:DA:78:A:H2' | 25:DA:79:G:C8 | 2.39 | 0.57 |
| 14:CQ:12:ARG:C | 14:CQ:14:PRO:HD3 | 2.24 | 0.57 |
| 14:CQ:12:ARG:HB3 | 14:CQ:14:PRO:HD3 | 1.85 | 0.57 |
| 28:BE:14:ILE:O | 28:BE:15:PHE:CD2 | 2.56 | 0.57 |
| 1:AA:1053:G:C6 | 1:AA:1199:U:C2 | 2.92 | 0.57 |
| 28:DE:84:PHE:CZ | 28:DE:86:PRO:HB3 | 2.39 | 0.57 |
| 25:DA:1342:A:C6 | 25:DA:1397:U:C6 | 2.92 | 0.57 |
| 2:AE:21:ARG:HB2 | 2:AE:39:ILE:HA | 1.85 | 0.57 |
| 1:CA:1128:C:O2' | 1:CA:1129:C:OP1 | 2.22 | 0.57 |
| 25:DA:1210:A:H5' | 25:DA:1212:G:O4' | 2.04 | 0.57 |
| 25:DA:2170:A:H5'' | 25:DA:2171:A:OP2 | 2.03 | 0.57 |
| 35:BO:21:ARG:HA | 35:BO:21:ARG:HE | 1.69 | 0.57 |
| 19:CV:65:ASN:HB2 | 19:CV:66:MET:HE1 | 1.85 | 0.57 |
| 25:DA:2872:G:O2' | 25:DA:2873:A:H5' | 2.04 | 0.57 |
| 25:DA:2875:C:C4' | 39:DR:5:ALA:HB2 | 2.31 | 0.57 |
| 1:CA:765:G:N2 | 1:CA:813:U:OP2 | 2.35 | 0.57 |
| 41:D2:44:LYS:HG3 | 41:D2:45:THR:N | 2.19 | 0.57 |
| 27:DD:186:HIS:CD2 | 27:DD:187:GLY:N | 2.72 | 0.57 |
| 1:AA:606:G:N2 | 1:AA:631:G:H8 | 2.01 | 0.57 |
| 3:CF:11:ARG:O | 3:CF:14:ILE:O | 2.22 | 0.57 |
| 49:DX:19:GLN:NE2 | 49:DX:52:HIS:CE1 | 2.72 | 0.57 |
| 35:BO:29:LYS:HD2 | 35:BO:30:THR:HG22 | 1.85 | 0.57 |
| 25:DA:239:U:H6 | 25:DA:239:U:C5' | 2.17 | 0.57 |
| 20:CW:53:LEU:HD13 | 20:CW:104:LEU:HD13 | 1.85 | 0.57 |
| 44:DU:20:TYR:HD1 | 44:DU:20:TYR:N | 2.01 | 0.57 |
| 34:DN:68:GLU:HA | 34:DN:78:ARG:HB3 | 1.85 | 0.57 |
| 25:BA:2283:C:H2' | 25:BA:2284:C:O4' | 2.04 | 0.57 |
| 7:AJ:36:LYS:HB2 | 7:AJ:36:LYS:HZ2 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:1053:C:H3' | 25:DA:1054:A:H5'' | 1.85 | 0.57 |
| 27:DD:108:PRO:HB3 | 27:DD:143:HIS:HE1 | 1.68 | 0.57 |
| 25:DA:2366:A:H2' | 25:DA:2367:G:O4' | 2.04 | 0.57 |
| 44:DU:90:LEU:HD23 | 44:DU:90:LEU:H | 1.69 | 0.57 |
| 25:BA:287:C:H2' | 25:BA:288:C:H6 | 1.69 | 0.57 |
| 11:CN:82:VAL:HB | 11:CN:108:ILE:HG12 | 1.86 | 0.57 |
| 25:DA:1472:A:H2' | 25:DA:1473:G:H5' | 1.86 | 0.57 |
| 27:BD:30:GLU:CG | 27:BD:63:ARG:NH2 | 2.64 | 0.57 |
| 27:BD:65:ILE:HD11 | 27:BD:67:PHE:CZ | 2.40 | 0.57 |
| 28:BE:52:LEU:O | 28:BE:75:VAL:N | 2.29 | 0.57 |
| 28:DE:25:VAL:HG12 | 28:DE:26:ILE:N | 2.15 | 0.57 |
| 31:DH:89:ILE:O | 31:DH:161:GLY:O | 2.22 | 0.57 |
| 36:DP:62:GLY:O | 36:DP:63:LYS:HB2 | 2.04 | 0.57 |
| 25:DA:1653:G:H4' | 25:DA:1654:A:O5' | 2.04 | 0.57 |
| 25:BA:2401:U:H2' | 25:BA:2402:C:C6 | 2.39 | 0.57 |
| 2:AE:217:ARG:HB2 | 2:AE:217:ARG:CZ | 2.34 | 0.57 |
| 27:BD:270:ILE:O | 27:BD:271:ILE:CG1 | 2.49 | 0.57 |
| 25:BA:229:A:C1' | 25:BA:230:U:OP2 | 2.51 | 0.57 |
| 31:BH:151:ILE:O | 31:BH:153:LYS:HD3 | 2.03 | 0.57 |
| 31:BH:153:LYS:HB3 | 31:BH:154:PRO:HD3 | 1.85 | 0.57 |
| 9:CL:95:LYS:HZ2 | 9:CL:96:LEU:HD12 | 1.68 | 0.57 |
| 25:BA:527:C:OP2 | 25:BA:2779:U:H5 | 1.86 | 0.57 |
| 25:BA:1799:G:H5' | 25:BA:1819:A:N6 | 2.19 | 0.57 |
| 1:CA:652:U:O2' | 1:CA:653:A:C2 | 2.56 | 0.57 |
| 25:DA:2197:U:H1' | 25:DA:2198:A:C8 | 2.39 | 0.57 |
| 1:AA:49:U:C2 | 1:AA:361:G:N2 | 2.72 | 0.57 |
| 25:BA:1317:A:O2' | 25:BA:1318:C:H5' | 2.03 | 0.57 |
| 5:AH:33:VAL:HG11 | 5:AH:109:ILE:HA | 1.86 | 0.57 |
| 32:DK:69:LYS:O | 32:DK:73:GLU:HB2 | 2.04 | 0.57 |
| 3:CF:56:ASP:HB2 | 3:CF:69:HIS:HE1 | 1.69 | 0.57 |
| 25:DA:1146:C:C2' | 25:DA:1147:C:H5' | 2.34 | 0.57 |
| 13:AP:81:LEU:O | 13:AP:89:GLY:HA3 | 2.04 | 0.57 |
| 2:CE:128:GLU:HA | 2:CE:128:GLU:OE2 | 2.04 | 0.57 |
| 25:BA:280:C:H2' | 25:BA:281:G:H5' | 1.86 | 0.57 |
| 43:BT:41:ASN:O | 43:BT:45:THR:HG23 | 2.04 | 0.57 |
| 26:DB:17:C:H2' | 26:DB:18:G:O4' | 2.04 | 0.57 |
| 32:DK:62:LYS:O | 32:DK:62:LYS:HD2 | 2.03 | 0.57 |
| 29:BF:152:GLU:HG3 | 29:BF:191:ARG:HD2 | 1.86 | 0.57 |
| 45:BV:117:LEU:HD13 | 45:BV:118:GLN:N | 2.18 | 0.57 |
| 25:BA:614:U:O4 | 29:BF:168:ARG:HG2 | 2.05 | 0.57 |
| 36:DP:26:TYR:CE1 | 36:DP:139:GLU:CG | 2.73 | 0.57 |
| 1:AA:1053:G:N7 | 1:AA:1199:U:C6 | 2.72 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 26:BB:15:A:OP1 | 26:BB:15:A:C4' | 2.52 | 0.57 |
| 25:BA:2286:A:H4' | 25:BA:2287:A:O5' | 2.04 | 0.57 |
| 4:CG:13:ARG:CG | 4:CG:14:ARG:N | 2.63 | 0.57 |
| 1:AA:1004:A:N9 | 1:AA:1025:U:O2 | 2.37 | 0.57 |
| 39:DR:88:ILE:HD11 | 39:DR:91:ARG:HG2 | 1.86 | 0.57 |
| 1:CA:1178:G:H5' | 9:CL:93:ARG:NH2 | 2.19 | 0.57 |
| 1:CA:1256:A:N6 | 1:CA:1278:U:OP2 | 2.37 | 0.57 |
| 25:BA:443:A:C5 | 29:BF:45:ARG:HD2 | 2.39 | 0.57 |
| 19:CV:40:ILE:HD11 | 19:CV:71:LEU:HD23 | 1.86 | 0.57 |
| 2:CE:71:VAL:CG1 | 2:CE:97:TRP:HD1 | 2.17 | 0.57 |
| 1:CA:452:A:H2' | 1:CA:453:A:C8 | 2.38 | 0.57 |
| 29:BF:32:LEU:HD13 | 29:BF:105:VAL:CG1 | 2.31 | 0.57 |
| 25:BA:528:A:N1 | 25:BA:2043:C:C5' | 2.67 | 0.57 |
| 25:DA:587:C:C2 | 35:DO:33:ARG:NH1 | 2.73 | 0.57 |
| 45:DV:3:TYR:O | 45:DV:58:VAL:HB | 2.04 | 0.57 |
| 1:CA:554:C:H2' | 1:CA:555:C:C6 | 2.38 | 0.57 |
| 36:DP:57:HIS:CE1 | 36:DP:116:GLU:HB3 | 2.40 | 0.57 |
| 25:DA:2517:C:C2 | 25:DA:2542:A:N6 | 2.72 | 0.57 |
| 25:BA:856:C:C2' | 25:BA:857:C:O5' | 2.53 | 0.57 |
| 22:AB:12:G:H1 | 22:AB:24:C:N4 | 2.03 | 0.57 |
| 1:AA:78:G:H1 | 1:AA:91:C:N4 | 2.03 | 0.57 |
| 4:AG:134:ASP:O | 4:AG:136:PRO:HD3 | 2.05 | 0.57 |
| 36:BP:110:THR:HG23 | 36:BP:113:GLN:OE1 | 2.03 | 0.57 |
| 25:DA:708:C:H42 | 25:DA:723:G:H1 | 1.51 | 0.57 |
| 1:CA:909:A:H2' | 1:CA:910:C:O4' | 2.03 | 0.57 |
| 28:DE:132:HIS:O | 28:DE:133:LYS:HB2 | 2.05 | 0.57 |
| 25:BA:1412:A:H2' | 25:BA:1413:G:C8 | 2.40 | 0.57 |
| 3:AF:34:LEU:HD21 | 3:AF:38:ARG:HH11 | 1.69 | 0.57 |
| 25:BA:795:C:H2' | 25:BA:796:C:H6 | 1.68 | 0.57 |
| 10:CM:35:SER:OG | 10:CM:73:ASP:HB2 | 2.03 | 0.57 |
| 20:CW:50:GLU:HA | 20:CW:100:ILE:HB | 1.87 | 0.57 |
| 30:BG:78:SER:O | 30:BG:80:PHE:N | 2.37 | 0.57 |
| 28:BE:47:VAL:HG21 | 28:BE:84:PHE:O | 2.05 | 0.57 |
| 35:DO:64:LYS:CG | 54:D8:25:MET:SD | 2.92 | 0.57 |
| 36:DP:31:ASP:H | 36:DP:107:ALA:HB2 | 1.70 | 0.57 |
| 25:DA:1057:A:C2 | 25:DA:1081:U:N3 | 2.68 | 0.57 |
| 1:CA:706:A:O4' | 11:CN:29:ILE:HD11 | 2.05 | 0.57 |
| 1:AA:1301:U:C2' | 1:AA:1302:U:H5' | 2.34 | 0.57 |
| 42:DS:59:VAL:HG23 | 42:DS:65:LEU:H | 1.70 | 0.57 |
| 12:CO:24:VAL:HG12 | 12:CO:26:ALA:HB2 | 1.87 | 0.57 |
| 25:BA:139:G:N3 | 25:BA:141:A:N1 | 2.52 | 0.57 |
| 31:BH:86:GLU:O | 31:BH:131:VAL:O | 2.22 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 3:CF:15:THR:HG22 | 3:CF:16:ARG:N | 2.19 | 0.57 |
| 3:CF:9:GLY:HA3 | 14:CQ:49:HIS:HA | 1.85 | 0.57 |
| 45:DV:8:TYR:HA | 45:DV:62:PRO:CD | 2.35 | 0.57 |
| 25:DA:2057:A:C2' | 25:DA:2058:A:H5' | 2.33 | 0.57 |
| 25:BA:1204:A:N1 | 25:BA:1241:A:C2 | 2.73 | 0.57 |
| 3:CF:58:GLU:HB2 | 3:CF:65:ALA:CB | 2.34 | 0.57 |
| 32:DK:104:GLN:HG2 | 32:DK:105:HIS:CD2 | 2.40 | 0.57 |
| 35:DO:71:VAL:CG1 | 35:DO:72:PRO:HD3 | 2.34 | 0.57 |
| 25:DA:389:G:N1 | 35:DO:71:VAL:HG12 | 2.20 | 0.57 |
| 23:AC:66:C:C2' | 23:AC:67:C:H5' | 2.35 | 0.57 |
| 14:AQ:2:ALA:HB1 | 14:AQ:6:LEU:HD11 | 1.86 | 0.57 |
| 42:DS:29:LEU:HG | 42:DS:29:LEU:O | 2.03 | 0.57 |
| 1:AA:89:U:O2' | 1:AA:90:C:O4' | 2.23 | 0.57 |
| 43:DT:26:TYR:CD1 | 43:DT:89:ILE:HD12 | 2.39 | 0.57 |
| 36:BP:133:ARG:O | 36:BP:134:ARG:HB2 | 2.04 | 0.57 |
| 25:BA:394:A:O2' | 25:BA:395:U:H5' | 2.03 | 0.57 |
| 1:CA:7:G:H5' | 1:CA:298:A:O4' | 2.05 | 0.57 |
| 25:DA:395:U:H2' | 25:DA:396:G:N7 | 2.19 | 0.57 |
| 49:BX:10:LYS:NZ | 49:BX:15:TYR:OH | 2.27 | 0.57 |
| 26:BB:59:A:H2' | 26:BB:60:C:H6 | 1.68 | 0.57 |
| 1:CA:570:G:C6 | 1:CA:873:A:C2 | 2.92 | 0.57 |
| 45:DV:112:ARG:H | 45:DV:112:ARG:HE | 1.53 | 0.57 |
| 25:DA:2637:U:H2' | 25:DA:2638:G:O4' | 2.05 | 0.57 |
| 20:AW:10:LEU:HD23 | 20:AW:12:ALA:CB | 2.34 | 0.57 |
| 28:BE:35:GLN:HB3 | 28:BE:48:GLN:HB2 | 1.86 | 0.57 |
| 23:CC:20:G:N1 | 23:CC:58:A:C2 | 2.73 | 0.57 |
| 39:DR:54:ARG:CG | 39:DR:54:ARG:NH1 | 2.50 | 0.57 |
| 1:CA:1320:C:O2 | 19:CV:36:ARG:NH2 | 2.37 | 0.57 |
| 19:AV:40:ILE:HD11 | 19:AV:62:ILE:HG23 | 1.87 | 0.57 |
| 25:DA:2275:C:H5' | 25:DA:2275:C:C6 | 2.39 | 0.57 |
| 1:AA:1060:C:O2' | 10:AM:56:HIS:CD2 | 2.57 | 0.57 |
| 13:CP:37:THR:HG21 | 13:CP:56:LEU:HD23 | 1.85 | 0.57 |
| 10:CM:84:GLN:O | 10:CM:88:LEU:HB3 | 2.05 | 0.57 |
| 25:BA:483:A:H4' | 44:BU:49:VAL:CA | 2.28 | 0.57 |
| 2:CE:142:LEU:HD23 | 2:CE:142:LEU:O | 2.05 | 0.57 |
| 25:DA:2720:U:C2 | 25:DA:2873:A:C2 | 2.92 | 0.57 |
| 38:DQ:3:ARG:HG3 | 38:DQ:4:LEU:N | 2.19 | 0.57 |
| 25:BA:2712:U:H1' | 25:BA:2712(A):A:C8 | 2.39 | 0.57 |
| 1:AA:920:U:H2' | 1:AA:921:U:C6 | 2.39 | 0.57 |
| 3:CF:14:ILE:CG1 | 3:CF:15:THR:N | 2.68 | 0.57 |
| 10:AM:40:LEU:HB2 | 10:AM:69:ASN:HB2 | 1.86 | 0.57 |
| 28:DE:111:ARG:HD2 | 28:DE:160:TYR:CD1 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 40:B1:8:VAL:HG23 | 40:B1:11:ARG:NH2 | 2.19 | 0.57 |
| 47:BZ:53:VAL:CG2 | 47:BZ:74:VAL:HG22 | 2.35 | 0.57 |
| 1:CA:628:G:O2' | 1:CA:629:G:H5' | 2.04 | 0.57 |
| 1:AA:73:G:C2 | 1:AA:74:C:C5 | 2.92 | 0.57 |
| 27:BD:70:TRP:CH2 | 27:BD:150:LYS:HA | 2.39 | 0.57 |
| 25:BA:1230:C:H2' | 25:BA:1231:G:H8 | 1.70 | 0.57 |
| 25:BA:540:G:H5' | 25:BA:541:C:OP2 | 2.04 | 0.57 |
| 1:AA:1486:G:H2' | 1:AA:1487:G:O4' | 2.04 | 0.57 |
| 25:DA:343:C:O2' | 25:DA:344:G:H5' | 2.04 | 0.57 |
| 25:BA:1845:G:C2' | 25:BA:1846:G:H5' | 2.34 | 0.57 |
| 4:AG:190:ASP:O | 4:AG:193:ASP:HB2 | 2.03 | 0.57 |
| 3:CF:28:GLN:HB3 | 3:CF:32:LEU:HD12 | 1.86 | 0.57 |
| 25:BA:2393:A:O3' | 35:BO:62:LEU:HA | 2.03 | 0.57 |
| 28:BE:61:ARG:H | 28:BE:62:PRO:CD | 2.17 | 0.57 |
| 39:DR:74:ARG:HH11 | 39:DR:74:ARG:CG | 1.97 | 0.57 |
| 1:CA:1321:C:C4 | 1:CA:1322:C:C5 | 2.93 | 0.57 |
| 54:D8:24:ALA:O | 54:D8:48:PHE:CE1 | 2.57 | 0.57 |
| 10:CM:61:GLU:OE1 | 14:CQ:58:LYS:HE2 | 2.05 | 0.57 |
| 22:CB:16:U:O4' | 22:CB:70:G:N2 | 2.37 | 0.57 |
| 1:AA:791:G:O5' | 1:AA:791:G:H8 | 1.86 | 0.57 |
| 25:DA:1534:G:H5' | 25:DA:1535:U:OP2 | 2.04 | 0.57 |
| 30:DG:36:LYS:HE3 | 30:DG:38:VAL:CG2 | 2.34 | 0.57 |
| 44:DU:17:SER:HB2 | 44:DU:71:LYS:HE2 | 1.87 | 0.57 |
| 28:BE:119:ARG:HB3 | 28:BE:120:TRP:CD1 | 2.39 | 0.57 |
| 7:CJ:26:PHE:CD2 | 7:CJ:30:ILE:HD11 | 2.39 | 0.57 |
| 25:BA:528:A:N1 | 25:BA:2042:A:H2' | 2.20 | 0.57 |
| 1:AA:1450:U:O2' | 1:AA:1451:A:C8 | 2.54 | 0.57 |
| 15:AR:55:GLY:HA2 | 15:AR:58:MET:CE | 2.32 | 0.57 |
| 25:DA:27:G:N2 | 25:DA:512:G:H1' | 2.19 | 0.57 |
| 23:CD:22:A:H2' | 23:CD:47:G:C6 | 2.38 | 0.57 |
| 11:AN:62:GLN:O | 11:AN:66:LEU:HG | 2.05 | 0.57 |
| 17:AT:88:TYR:CD2 | 17:AT:89:LEU:HD23 | 2.38 | 0.57 |
| 25:BA:1310:G:OP2 | 53:B7:9:ARG:HD2 | 2.05 | 0.57 |
| 25:BA:581:C:H2' | 25:BA:582:G:C8 | 2.40 | 0.57 |
| 11:CN:105:VAL:O | 11:CN:105:VAL:HG23 | 2.04 | 0.57 |
| 25:BA:153:C:O2' | 25:BA:154:G:H5' | 2.04 | 0.57 |
| 9:AL:70:LYS:O | 9:AL:74:ILE:HG13 | 2.05 | 0.57 |
| 25:BA:246:C:H2' | 25:BA:247:G:H5' | 1.87 | 0.57 |
| 25:BA:1494:A:H2' | 25:BA:1495:A:C8 | 2.39 | 0.57 |
| 25:BA:795:C:H2' | 25:BA:796:C:C6 | 2.40 | 0.57 |
| 1:CA:1337:G:H5'' | 1:CA:1338:G:OP1 | 2.05 | 0.57 |
| 25:DA:1810:A:H2' | 25:DA:1811:G:O4' | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:CC:38:A:H2' | 23:CC:39:A:O4' | 2.05 | 0.57 |
| 25:DA:375:C:H2' | 25:DA:376:C:C6 | 2.40 | 0.57 |
| 27:BD:72:LYS:HB3 | 27:BD:75:ILE:HD12 | 1.85 | 0.57 |
| 1:CA:791:G:C6 | 1:CA:792:A:N7 | 2.73 | 0.57 |
| 35:DO:61:ARG:HA | 54:D8:27:THR:HG21 | 1.86 | 0.57 |
| 40:D1:97:ASP:OD2 | 40:D1:98:LEU:N | 2.38 | 0.57 |
| 41:D2:6:LYS:H | 41:D2:37:VAL:HG12 | 1.69 | 0.57 |
| 29:BF:29:ASN:N | 29:BF:112:MET:HE1 | 2.19 | 0.57 |
| 14:AQ:22:THR:HB | 14:AQ:33:VAL:HG11 | 1.87 | 0.57 |
| 25:BA:654(M):C:H2' | 25:BA:654(N):G:H8 | 1.62 | 0.57 |
| 9:CL:63:ILE:HD13 | 9:CL:77:ILE:HG23 | 1.86 | 0.57 |
| 4:AG:114:ARG:HG3 | 4:AG:114:ARG:HH11 | 1.69 | 0.57 |
| 27:BD:236:GLY:O | 27:BD:237:GLU:O | 2.23 | 0.57 |
| 1:CA:1122:U:O4 | 1:CA:1123:A:N6 | 2.36 | 0.57 |
| 1:AA:599:C:H2' | 1:AA:600:C:H6 | 1.68 | 0.57 |
| 25:BA:2001:A:H2' | 25:BA:2002:G:C8 | 2.39 | 0.57 |
| 25:BA:389:G:H22 | 35:BO:72:PRO:CD | 2.17 | 0.57 |
| 25:BA:1843:C:H5' | 27:BD:253:GLN:OE1 | 2.04 | 0.57 |
| 25:DA:636:G:N7 | 35:DO:113:LYS:HE2 | 2.18 | 0.57 |
| 1:CA:745:C:H2' | 1:CA:746:A:H8 | 1.70 | 0.57 |
| 1:AA:1084:G:C5 | 1:AA:1085:U:C4 | 2.93 | 0.57 |
| 25:BA:1162:G:H21 | 41:B2:89:GLN:HE22 | 1.52 | 0.57 |
| 25:BA:1085:A:H4' | 25:BA:1086:A:OP1 | 2.03 | 0.57 |
| 28:BE:6:GLY:HA2 | 28:BE:51:PHE:CZ | 2.40 | 0.57 |
| 23:AC:63:C:O2 | 23:AC:63:C:H2' | 2.05 | 0.57 |
| 1:CA:485:G:O2' | 1:CA:486:U:C6 | 2.58 | 0.57 |
| 1:AA:1002:G:H2' | 1:AA:1003:G:H8 | 1.69 | 0.57 |
| 22:CB:40:G:H2' | 22:CB:41:G:C8 | 2.40 | 0.57 |
| 25:DA:2270:G:C2' | 25:DA:2271:G:H5' | 2.34 | 0.57 |
| 13:CP:39:ILE:HG22 | 13:CP:40:ASN:H | 1.70 | 0.57 |
| 1:AA:560:U:H4' | 1:AA:561:U:O5' | 2.03 | 0.57 |
| 25:BA:2701:C:C2' | 25:BA:2702:U:OP1 | 2.53 | 0.57 |
| 29:DF:148:LEU:HD23 | 29:DF:191:ARG:NH1 | 2.19 | 0.57 |
| 1:AA:1309:G:C6 | 1:AA:1329:A:C2 | 2.93 | 0.57 |
| 2:CE:8:LYS:O | 2:CE:9:GLU:HB3 | 2.04 | 0.57 |
| 22:CB:45:U:C2' | 22:CB:46:G:H5'' | 2.35 | 0.57 |
| 25:BA:660:G:H21 | 35:BO:12:ALA:HA | 1.69 | 0.57 |
| 44:DU:60:PHE:N | 44:DU:60:PHE:CD2 | 2.72 | 0.57 |
| 1:AA:1269:A:H2 | 1:AA:1312:G:N3 | 2.02 | 0.57 |
| 38:BQ:5:THR:OG1 | 38:BQ:8:GLU:HG3 | 2.05 | 0.57 |
| 48:BW:28:LYS:HD2 | 48:BW:56:GLN:NE2 | 2.20 | 0.57 |
| 10:AM:4:ILE:HD13 | 10:AM:100:THR:HG23 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 32:BK:64:GLU:HG3 | 32:BK:67:ARG:NH2 | 2.20 | 0.57 |
| 25:DA:2420:C:P | 54:D8:34:TRP:HB3 | 2.45 | 0.57 |
| 1:CA:1037:C:H2' | 1:CA:1038:C:C6 | 2.40 | 0.57 |
| 25:DA:672:C:H2' | 25:DA:673:C:C5' | 2.15 | 0.57 |
| 23:CC:62:C:C2 | 23:CC:63:C:C5 | 2.92 | 0.57 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C6 | 2.40 | 0.57 |
| 43:DT:50:LYS:H | 43:DT:87:GLN:NE2 | 2.03 | 0.57 |
| 25:BA:747:U:OP2 | 51:B5:3:LYS:HD3 | 2.05 | 0.57 |
| 25:BA:768:G:O2' | 25:BA:1379:A:N6 | 2.37 | 0.57 |
| 33:BM:28:THR:HG22 | 33:BM:29:LYS:N | 2.19 | 0.57 |
| 9:CL:5:TYR:OH | 9:CL:16:ARG:HG2 | 2.05 | 0.57 |
| 9:CL:26:VAL:HG13 | 9:CL:61:ALA:HB3 | 1.87 | 0.57 |
| 22:AB:59:U:H4' | 22:AB:60:A:H5' | 1.86 | 0.57 |
| 19:CV:9:VAL:HG12 | 19:CV:10:PHE:H | 1.70 | 0.57 |
| 35:DO:101:VAL:HG23 | 35:DO:106:LEU:HB3 | 1.87 | 0.57 |
| 35:DO:146:VAL:HG22 | 35:DO:147:LEU:HD12 | 1.86 | 0.57 |
| 1:CA:957:U:H1' | 1:CA:960:U:C5 | 2.39 | 0.57 |
| 5:AH:45:PHE:CD2 | 5:AH:47:LYS:HD2 | 2.39 | 0.57 |
| 1:AA:1091:U:H1' | 1:AA:1095:U:O2 | 2.04 | 0.57 |
| 25:DA:2657:A:O2' | 31:DH:160:LYS:HE3 | 2.05 | 0.57 |
| 23:CC:35:C:H2' | 23:CC:35:C:O2 | 2.04 | 0.57 |
| 1:AA:163:C:H2' | 1:AA:164:U:C6 | 2.40 | 0.57 |
| 23:CD:52:C:N3 | 23:CD:64:G:N2 | 2.46 | 0.57 |
| 1:AA:619:U:O2 | 4:AG:135:LEU:HD22 | 2.05 | 0.57 |
| 25:DA:959:A:C6 | 25:DA:960:A:N1 | 2.72 | 0.57 |
| 25:BA:1760:A:C2' | 25:BA:1761:C:H5' | 2.35 | 0.57 |
| 1:AA:157:G:C2' | 1:AA:158:G:H5' | 2.34 | 0.57 |
| 34:BN:122:LEU:HD13 | 39:BR:72:VAL:HG11 | 1.87 | 0.57 |
| 30:BG:105:LYS:HE3 | 30:BG:143:GLU:OE1 | 2.04 | 0.57 |
| 1:AA:1190:G:H5' | 3:AF:176:HIS:CE1 | 2.40 | 0.57 |
| 31:BH:40:GLU:OE1 | 31:BH:61:HIS:NE2 | 2.38 | 0.57 |
| 40:B1:34:LYS:HZ1 | 40:B1:37:GLU:CD | 2.08 | 0.57 |
| 22:CB:34:U:H2' | 22:CB:36:A:OP2 | 2.04 | 0.57 |
| 25:BA:302:C:H2' | 25:BA:303:U:C6 | 2.40 | 0.57 |
| 1:CA:777:A:H2 | 11:CN:119:CYS:HB3 | 1.70 | 0.57 |
| 39:DR:18:ASP:N | 39:DR:18:ASP:OD1 | 2.32 | 0.57 |
| 25:BA:1042:G:H2' | 25:BA:1043:C:O4' | 2.05 | 0.57 |
| 27:BD:12:SER:O | 27:BD:16:MET:HB2 | 2.05 | 0.57 |
| 25:DA:2638:G:O2' | 25:DA:2639:A:C8 | 2.58 | 0.56 |
| 1:AA:1160:G:H22 | 1:AA:1177:G:H21 | 1.52 | 0.56 |
| 31:DH:153:LYS:HB3 | 31:DH:161:GLY:HA2 | 1.87 | 0.56 |
| 1:CA:984:C:H2' | 1:CA:985:C:H6 | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 13:AP:23:TYR:HB3 | 13:AP:67:GLU:HA | 1.87 | 0.56 |
| 25:BA:2287:A:N1 | 25:BA:2346:A:C2 | 2.73 | 0.56 |
| 36:DP:30:GLY:HA2 | 36:DP:107:ALA:HB2 | 1.88 | 0.56 |
| 22:CB:18:G:H1 | 22:CB:71:U:H3 | 1.52 | 0.56 |
| 11:AN:79:SER:C | 11:AN:80:VAL:HG13 | 2.24 | 0.56 |
| 25:BA:897:C:H2' | 25:BA:898:C:O4' | 2.05 | 0.56 |
| 29:DF:28:ILE:HD11 | 29:DF:119:ARG:HD3 | 1.86 | 0.56 |
| 1:AA:1060:C:C5 | 3:AF:2:GLY:HA2 | 2.40 | 0.56 |
| 44:DU:84:ARG:NH2 | 44:DU:97:ARG:HB2 | 2.20 | 0.56 |
| 25:DA:2310:A:H5' | 25:DA:2311:A:OP2 | 2.05 | 0.56 |
| 1:AA:1321:C:C5 | 1:AA:1322:C:C2 | 2.92 | 0.56 |
| 25:DA:2192:G:H2' | 25:DA:2193:G:H5' | 1.86 | 0.56 |
| 36:DP:59:ARG:HH21 | 36:DP:59:ARG:CG | 2.12 | 0.56 |
| 13:CP:84:ILE:HG21 | 19:CV:63:THR:HG21 | 1.86 | 0.56 |
| 25:DA:140:A:H8 | 25:DA:1408:C:HO2' | 1.43 | 0.56 |
| 30:DG:109:VAL:O | 30:DG:113:ARG:HG3 | 2.05 | 0.56 |
| 1:CA:619:U:H3 | 4:CG:134:ASP:HB2 | 1.69 | 0.56 |
| 25:DA:99:U:H4' | 25:DA:102:G:H1' | 1.87 | 0.56 |
| 25:DA:1278:A:H5'' | 37:D0:36:THR:HG22 | 1.86 | 0.56 |
| 41:B2:76:LYS:HG3 | 41:B2:81:TYR:CD1 | 2.39 | 0.56 |
| 1:CA:156:G:H1 | 1:CA:165:C:H42 | 1.53 | 0.56 |
| 36:DP:21:THR:HB | 36:DP:99:PRO:O | 2.05 | 0.56 |
| 28:DE:111:ARG:HD2 | 28:DE:160:TYR:CE1 | 2.40 | 0.56 |
| 7:AJ:15:ASP:O | 7:AJ:19:GLY:HA2 | 2.05 | 0.56 |
| 1:AA:1490:C:C2' | 1:AA:1491:G:H5' | 2.34 | 0.56 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:C8 | 2.39 | 0.56 |
| 1:AA:1074:G:N3 | 1:AA:1102:A:C2 | 2.73 | 0.56 |
| 17:AT:29:HIS:CE1 | 17:AT:32:TYR:CD1 | 2.93 | 0.56 |
| 22:AB:12:G:H1 | 22:AB:24:C:H42 | 1.53 | 0.56 |
| 28:BE:118:LYS:HG2 | 28:BE:118:LYS:O | 2.06 | 0.56 |
| 25:DA:185:U:H4' | 25:DA:218:A:H4' | 1.86 | 0.56 |
| 14:CQ:13:THR:N | 14:CQ:14:PRO:HD3 | 2.20 | 0.56 |
| 30:DG:125:PHE:CE2 | 30:DG:131:TYR:HB2 | 2.40 | 0.56 |
| 1:CA:818:G:O2' | 1:CA:819:A:H5' | 2.05 | 0.56 |
| 25:BA:638:G:C5 | 25:BA:651:G:C2 | 2.92 | 0.56 |
| 25:DA:571:A:H5' | 25:DA:2030:A:N7 | 2.20 | 0.56 |
| 25:BA:495:G:H1' | 42:BS:57:ASN:ND2 | 2.20 | 0.56 |
| 1:AA:1047:G:C2' | 1:AA:1048:G:H5' | 2.35 | 0.56 |
| 25:BA:2427:C:H5'' | 25:BA:2428:G:OP1 | 2.06 | 0.56 |
| 32:BK:81:VAL:HG11 | 32:BK:88:ILE:HD13 | 1.87 | 0.56 |
| 25:DA:226:G:H21 | 25:DA:228:A:H61 | 0.57 | 0.56 |
| 25:DA:2420:C:OP1 | 54:D8:34:TRP:CB | 2.43 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:2799:A:H2' | 25:DA:2801:A:C4 | 2.39 | 0.56 |
| 36:DP:66:ILE:HA | 36:DP:104:PHE:HA | 1.87 | 0.56 |
| 38:DQ:14:VAL:HG21 | 38:DQ:89:ARG:HG2 | 1.86 | 0.56 |
| 28:DE:33:VAL:HA | 28:DE:49:LEU:HA | 1.86 | 0.56 |
| 1:CA:1321:C:H4' | 13:CP:87:TYR:CE2 | 2.39 | 0.56 |
| 52:B6:38:LYS:HG3 | 52:B6:47:THR:O | 2.05 | 0.56 |
| 25:DA:1018:C:O2' | 25:DA:1019:U:H5' | 2.04 | 0.56 |
| 44:DU:98:VAL:HG13 | 44:DU:99:CYS:N | 2.20 | 0.56 |
| 1:CA:1129:C:H4' | 1:CA:1130:A:C5' | 2.32 | 0.56 |
| 36:DP:79:LEU:O | 36:DP:81:VAL:HG13 | 2.05 | 0.56 |
| 30:DG:36:LYS:HB2 | 30:DG:95:ARG:NH1 | 2.19 | 0.56 |
| 25:DA:1300:U:H4' | 25:DA:1301:A:H5' | 1.85 | 0.56 |
| 1:AA:686:U:H1' | 11:AN:42:TRP:NE1 | 2.13 | 0.56 |
| 33:BM:137:LYS:HG3 | 33:BM:138:LEU:N | 2.15 | 0.56 |
| 2:CE:97:TRP:CZ3 | 2:CE:98:LEU:O | 2.57 | 0.56 |
| 35:DO:83:VAL:CG1 | 35:DO:112:LEU:HD21 | 2.35 | 0.56 |
| 45:DV:105:VAL:HG22 | 45:DV:106:GLY:N | 2.17 | 0.56 |
| 12:AO:116:SER:O | 12:AO:120:TYR:HD1 | 1.87 | 0.56 |
| 1:CA:1071:C:O2' | 1:CA:1072:G:H5' | 2.06 | 0.56 |
| 35:DO:55:ARG:O | 35:DO:57:THR:N | 2.38 | 0.56 |
| 1:CA:1085:U:H3' | 1:CA:1086:U:C6 | 2.40 | 0.56 |
| 1:CA:1032:A:N7 | 1:CA:1032(A):G:H1' | 2.20 | 0.56 |
| 2:CE:17:PHE:HE2 | 2:CE:44:LEU:HA | 1.69 | 0.56 |
| 42:BS:61:ASN:HB3 | 42:BS:62:HIS:ND1 | 2.19 | 0.56 |
| 23:CD:71:G:C2 | 23:CD:72:C:C6 | 2.94 | 0.56 |
| 12:CO:17:LYS:HD3 | 12:CO:18:VAL:H | 1.70 | 0.56 |
| 25:DA:2232:U:P | 47:DZ:40:ARG:HH12 | 2.28 | 0.56 |
| 1:AA:403:C:OP1 | 4:AG:137:SER:OG | 2.11 | 0.56 |
| 18:CU:29:PHE:HD1 | 18:CU:39:VAL:HG11 | 1.70 | 0.56 |
| 32:BK:38:LEU:HD12 | 32:BK:38:LEU:H | 1.70 | 0.56 |
| 25:DA:362:U:H6 | 25:DA:362:U:H3' | 1.70 | 0.56 |
| 4:CG:139:ARG:HG3 | 4:CG:139:ARG:HH11 | 1.70 | 0.56 |
| 32:BK:71:ILE:O | 32:BK:71:ILE:HG12 | 2.06 | 0.56 |
| 25:BA:1085:A:H2 | 25:BA:1086:A:N7 | 2.02 | 0.56 |
| 25:DA:848:G:H2' | 25:DA:849:A:H8 | 1.67 | 0.56 |
| 38:DQ:84:GLN:HA | 38:DQ:110:LEU:H | 1.70 | 0.56 |
| 16:AS:22:THR:HG23 | 16:AS:23:ASP:H | 1.70 | 0.56 |
| 28:BE:53:PRO:O | 28:BE:54:GLN:C | 2.42 | 0.56 |
| 28:BE:75:VAL:HG23 | 28:BE:76:ARG:N | 2.16 | 0.56 |
| 28:BE:38:THR:HB | 28:BE:39:PRO:CD | 2.22 | 0.56 |
| 25:DA:1257:C:C2' | 29:DF:84:VAL:CG1 | 2.81 | 0.56 |
| 33:BM:40:PRO:O | 40:B1:64:ARG:HG2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:963:G:N2 | 10:CM:55:LYS:CD | 2.65 | 0.56 |
| 1:AA:1004:A:O5' | 1:AA:1025:U:N3 | 2.39 | 0.56 |
| 2:AE:21:ARG:C | 2:AE:23:ARG:H | 2.09 | 0.56 |
| 45:BV:7:ALA:HB2 | 45:BV:59:LEU:CD1 | 2.32 | 0.56 |
| 4:AG:26:CYS:HA | 4:AG:31:CYS:HA | 1.88 | 0.56 |
| 25:DA:1045:A:O2' | 25:DA:1047:G:O4' | 2.23 | 0.56 |
| 1:CA:182:U:C5 | 1:CA:183:G:C4 | 2.92 | 0.56 |
| 1:CA:1127:G:O2' | 1:CA:1128:C:H5' | 2.06 | 0.56 |
| 9:CL:78:LYS:HZ3 | 9:CL:78:LYS:HB2 | 1.70 | 0.56 |
| 25:BA:2112:G:O2' | 25:BA:2113:U:O2 | 2.23 | 0.56 |
| 25:BA:2173:A:C8 | 25:BA:2173:A:OP1 | 2.59 | 0.56 |
| 13:CP:80:ARG:NH1 | 19:CV:66:MET:SD | 2.78 | 0.56 |
| 45:DV:129:SER:HB2 | 45:DV:131:ARG:HD3 | 1.86 | 0.56 |
| 25:DA:2319:G:O6 | 38:DQ:4:LEU:HB3 | 2.05 | 0.56 |
| 25:BA:1537:C:H2' | 25:BA:1538:G:O4' | 2.05 | 0.56 |
| 37:B0:104:ARG:NH1 | 37:B0:104:ARG:HG2 | 2.21 | 0.56 |
| 3:CF:184:TYR:HA | 3:CF:200:ALA:O | 2.05 | 0.56 |
| 25:DA:910:A:H62 | 36:DP:12:GLN:HA | 1.69 | 0.56 |
| 25:BA:1771:C:C1' | 25:BA:1786:A:C8 | 2.88 | 0.56 |
| 21:CX:5:ASP:O | 21:CX:11:GLY:HA3 | 2.05 | 0.56 |
| 25:DA:2335:A:HO2' | 25:DA:2336:A:P | 2.29 | 0.56 |
| 25:BA:1408:C:C2 | 25:BA:1595:G:N2 | 2.74 | 0.56 |
| 37:D0:37:THR:HG22 | 37:D0:40:LYS:H | 1.68 | 0.56 |
| 25:DA:1006:C:H1' | 33:DM:106:MET:HE3 | 1.88 | 0.56 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:C6 | 2.36 | 0.56 |
| 35:BO:39:LYS:CG | 35:BO:45:LEU:HD22 | 2.35 | 0.56 |
| 3:CF:181:ASN:HB3 | 3:CF:205:GLY:O | 2.05 | 0.56 |
| 3:CF:8:ILE:HB | 14:CQ:49:HIS:O | 2.06 | 0.56 |
| 2:CE:8:LYS:C | 2:CE:10:LEU:H | 2.08 | 0.56 |
| 41:B2:66:ARG:CZ | 41:B2:88:ARG:HD3 | 2.34 | 0.56 |
| 23:AD:21:U:H3' | 23:AD:22:A:H5'' | 1.88 | 0.56 |
| 25:DA:300:A:H2' | 25:DA:334:C:H1' | 1.88 | 0.56 |
| 28:BE:13:ARG:HH11 | 28:BE:13:ARG:CB | 2.17 | 0.56 |
| 32:DK:77:LEU:HG | 32:DK:78:THR:N | 2.20 | 0.56 |
| 30:DG:15:VAL:HG13 | 30:DG:175:LEU:CB | 2.35 | 0.56 |
| 1:AA:1374:A:O2' | 7:AJ:28:ASN:HB3 | 2.05 | 0.56 |
| 49:BX:19:GLN:NE2 | 49:BX:52:HIS:HE1 | 2.02 | 0.56 |
| 19:AV:53:ASN:O | 19:AV:77:THR:HG22 | 2.06 | 0.56 |
| 35:BO:55:ARG:O | 35:BO:57:THR:N | 2.38 | 0.56 |
| 14:CQ:29:ARG:O | 14:CQ:30:ALA:HB3 | 2.05 | 0.56 |
| 1:CA:1244:C:OP2 | 21:CX:9:ARG:HG2 | 2.05 | 0.56 |
| 1:AA:652:U:O2' | 1:AA:653:A:H5'' | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 37:B0:44:LEU:O | 37:B0:48:VAL:HG23 | 2.05 | 0.56 |
| 25:BA:1761:C:C4 | 25:BA:1762:A:N7 | 2.74 | 0.56 |
| 13:CP:7:VAL:O | 13:CP:8:GLU:HG2 | 2.05 | 0.56 |
| 52:B6:34:LEU:HD22 | 52:B6:34:LEU:H | 1.70 | 0.56 |
| 25:BA:974(A):C:H4' | 25:BA:975:G:C5' | 2.35 | 0.56 |
| 25:BA:644:A:C2 | 25:BA:646:A:C4 | 2.93 | 0.56 |
| 25:BA:813:U:H2' | 25:BA:814:C:C6 | 2.40 | 0.56 |
| 25:BA:1354:A:OP1 | 27:BD:38:LYS:NZ | 2.35 | 0.56 |
| 5:CH:39:GLY:HA2 | 5:CH:113:ALA:O | 2.06 | 0.56 |
| 25:DA:2646:C:H2' | 25:DA:2647:U:O4' | 2.06 | 0.56 |
| 6:AI:97:PHE:HD2 | 18:AU:31:LEU:HD21 | 1.69 | 0.56 |
| 30:BG:118:ARG:O | 30:BG:181:ARG:HG3 | 2.05 | 0.56 |
| 25:DA:445:C:O2' | 25:DA:446:G:H5' | 2.05 | 0.56 |
| 2:CE:5:ILE:HD11 | 2:CE:221:LEU:HD21 | 1.87 | 0.56 |
| 25:DA:2074:U:H2' | 25:DA:2075:U:C6 | 2.41 | 0.56 |
| 29:BF:116:ASP:OD2 | 35:BO:1:MET:HB2 | 2.05 | 0.56 |
| 2:AE:146:GLN:O | 2:AE:150:SER:HB3 | 2.05 | 0.56 |
| 1:AA:928:G:O2' | 1:AA:1533:C:OP1 | 2.23 | 0.56 |
| 1:AA:292:G:N7 | 1:AA:293:G:H1' | 2.21 | 0.56 |
| 25:DA:979:G:H3' | 25:DA:980:A:C5' | 2.35 | 0.56 |
| 25:BA:1830:C:O2' | 25:BA:1831:G:H5' | 2.05 | 0.56 |
| 12:AO:32:PHE:HE1 | 12:AO:86:ARG:HG3 | 1.70 | 0.56 |
| 28:DE:120:TRP:CE3 | 28:DE:155:LYS:HD3 | 2.41 | 0.56 |
| 45:BV:132:ASN:H | 45:BV:132:ASN:ND2 | 2.02 | 0.56 |
| 25:BA:2319:G:H4' | 25:BA:2319:G:OP2 | 2.04 | 0.56 |
| 1:AA:342:C:H2' | 1:AA:343:U:O4' | 2.04 | 0.56 |
| 25:DA:2233:U:H2' | 25:DA:2234:G:C8 | 2.40 | 0.56 |
| 1:AA:1261:A:H1' | 1:AA:1283:G:H5'' | 1.87 | 0.56 |
| 39:DR:127:ALA:O | 39:DR:131:ALA:HB3 | 2.05 | 0.56 |
| 10:CM:63:PHE:HD1 | 14:CQ:57:ARG:O | 1.88 | 0.56 |
| 25:BA:1061:U:H4' | 25:BA:1070:A:H1' | 1.88 | 0.56 |
| 38:BQ:110:LEU:HA | 38:BQ:112:PHE:CZ | 2.41 | 0.56 |
| 27:DD:30:GLU:CG | 27:DD:63:ARG:HH21 | 2.18 | 0.56 |
| 39:DR:57:PHE:HA | 39:DR:79:HIS:ND1 | 2.21 | 0.56 |
| 25:BA:444:C:H4' | 29:BF:49:ALA:HB2 | 1.87 | 0.56 |
| 25:BA:883:G:C6 | 25:BA:884:C:O2 | 2.58 | 0.56 |
| 29:DF:3:GLU:HA | 29:DF:24:LEU:HD23 | 1.87 | 0.56 |
| 25:DA:273(C):C:H5' | 25:DA:273(D):C:OP2 | 2.06 | 0.56 |
| 30:DG:67:LYS:HB3 | 50:D4:6:HIS:HD2 | 1.69 | 0.56 |
| 38:BQ:14:VAL:HG11 | 38:BQ:90:GLY:O | 2.04 | 0.56 |
| 25:BA:2165:G:H2' | 25:BA:2165:G:N3 | 2.19 | 0.56 |
| 22:AB:60:A:H5'' | 22:AB:61:C:OP2 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:2610:C:C4' | 25:BA:2611:U:OP2 | 2.51 | 0.56 |
| 25:BA:1771:C:O2' | 25:BA:1786:A:H8 | 1.88 | 0.56 |
| 43:DT:55:ASN:O | 43:DT:79:ALA:HA | 2.06 | 0.56 |
| 25:BA:1210:A:H8 | 25:BA:1210:A:C5' | 2.19 | 0.56 |
| 2:CE:85:ALA:HB3 | 2:CE:92:TYR:HD1 | 1.70 | 0.56 |
| 45:BV:110:GLY:O | 45:BV:111:VAL:HG22 | 2.06 | 0.56 |
| 14:CQ:36:PHE:HD1 | 14:CQ:37:PHE:CD2 | 2.22 | 0.56 |
| 25:DA:2543:G:H2' | 25:DA:2544:G:C8 | 2.39 | 0.56 |
| 25:BA:1668:A:H4' | 25:BA:1669:A:O5' | 2.05 | 0.56 |
| 11:CN:66:LEU:HD22 | 11:CN:101:SER:HB3 | 1.87 | 0.56 |
| 1:CA:986:A:H1' | 19:CV:54:GLY:O | 2.04 | 0.56 |
| 30:DG:173:LEU:O | 30:DG:178:PHE:HB2 | 2.05 | 0.56 |
| 6:CI:24:GLU:HG2 | 6:CI:28:ARG:NH1 | 2.19 | 0.56 |
| 25:BA:2751:G:O2' | 25:BA:2752:C:O5' | 2.23 | 0.56 |
| 25:DA:1666:G:C2' | 25:DA:1667:G:H5' | 2.34 | 0.56 |
| 13:CP:108:ARG:HD3 | 13:CP:114:ARG:HG2 | 1.86 | 0.56 |
| 25:BA:2:G:H2' | 25:BA:3:U:C6 | 2.41 | 0.56 |
| 42:BS:89:ALA:O | 42:BS:90:ARG:HB2 | 2.05 | 0.56 |
| 18:AU:52:PRO:HB2 | 18:AU:54:ARG:HG2 | 1.87 | 0.56 |
| 25:BA:2139:C:H2' | 25:BA:2140:C:H5' | 1.86 | 0.56 |
| 18:CU:37:VAL:CG1 | 18:CU:78:LEU:HB3 | 2.35 | 0.56 |
| 28:BE:78:LEU:HD12 | 28:BE:79:ARG:CG | 2.34 | 0.56 |
| 28:BE:56:PRO:O | 28:BE:57:LYS:CB | 2.35 | 0.56 |
| 31:DH:153:LYS:H | 31:DH:154:PRO:HD2 | 1.68 | 0.56 |
| 52:B6:14:THR:O | 52:B6:49:HIS:HA | 2.05 | 0.56 |
| 19:AV:41:VAL:HG12 | 19:AV:45:VAL:N | 2.21 | 0.56 |
| 45:BV:62:PRO:O | 45:BV:63:ASP:CB | 2.54 | 0.56 |
| 1:AA:1351:U:O4' | 7:AJ:33:ASP:HB3 | 2.05 | 0.56 |
| 26:DB:13:A:H2' | 26:DB:70:C:O2' | 2.05 | 0.56 |
| 25:DA:2688:U:C5 | 25:DA:2720:U:OP2 | 2.57 | 0.56 |
| 25:BA:34:C:HO2' | 25:BA:35:G:P | 2.23 | 0.56 |
| 25:BA:1385:G:O6 | 25:BA:1403:C:N4 | 2.38 | 0.56 |
| 4:AG:155:LEU:O | 4:AG:157:LEU:N | 2.39 | 0.56 |
| 1:CA:1092:A:C2 | 1:CA:1183:A:C2 | 2.94 | 0.56 |
| 1:CA:673:G:O3' | 6:CI:87:ARG:NH2 | 2.39 | 0.56 |
| 5:AH:11:ILE:H | 5:AH:11:ILE:HD13 | 1.71 | 0.56 |
| 1:CA:382:A:H2' | 1:CA:383:A:H8 | 1.67 | 0.56 |
| 25:BA:627:A:H4' | 25:BA:628:G:OP1 | 2.06 | 0.56 |
| 13:AP:3:ARG:HG2 | 13:AP:9:ILE:HG13 | 1.87 | 0.56 |
| 19:CV:78:ARG:HD3 | 19:CV:79:THR:N | 2.19 | 0.56 |
| 1:CA:192:U:C4' | 20:CW:103:GLY:HA3 | 2.35 | 0.56 |
| 43:DT:11:PRO:HB3 | 43:DT:92:LEU:HD21 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:1761:C:N3 | 25:BA:1762:A:N6 | 2.52 | 0.56 |
| 1:CA:186:C:H1' | 20:CW:81:LYS:NZ | 2.21 | 0.56 |
| 1:CA:1154:G:H2' | 1:CA:1155:G:H8 | 1.71 | 0.56 |
| 25:BA:2751:G:O2' | 25:BA:2752:C:P | 2.64 | 0.56 |
| 16:AS:45:THR:HG22 | 16:AS:47:ASP:H | 1.71 | 0.56 |
| 53:D7:35:ARG:HG2 | 53:D7:42:LEU:HD11 | 1.87 | 0.56 |
| 1:AA:1141:C:O2' | 1:AA:1142:G:H5' | 2.04 | 0.56 |
| 20:CW:37:SER:O | 20:CW:41:ILE:HG13 | 2.04 | 0.56 |
| 15:AR:18:PHE:CE1 | 15:AR:21:ASP:HB2 | 2.40 | 0.56 |
| 1:AA:811:C:H4' | 1:AA:900:A:N6 | 2.21 | 0.56 |
| 28:BE:38:THR:HA | 28:BE:44:TYR:O | 2.06 | 0.56 |
| 23:AC:19:G:C4 | 23:AC:59:A:C2 | 2.94 | 0.56 |
| 23:CC:20:G:N2 | 23:CC:58:A:N3 | 2.53 | 0.56 |
| 1:CA:981:U:H5'' | 1:CA:982:U:O5' | 2.06 | 0.56 |
| 45:DV:144:LEU:CD1 | 45:DV:144:LEU:O | 2.47 | 0.56 |
| 1:CA:973:G:O3' | 14:CQ:41:ARG:NH2 | 2.32 | 0.56 |
| 47:DZ:92:LYS:O | 47:DZ:93:GLU:C | 2.44 | 0.56 |
| 11:AN:79:SER:CB | 11:AN:106:LYS:HD2 | 2.35 | 0.56 |
| 1:CA:1160:G:N2 | 1:CA:1161:C:C6 | 2.74 | 0.56 |
| 25:BA:1143:A:OP1 | 33:BM:25:ARG:NH2 | 2.37 | 0.56 |
| 1:CA:1275:A:H2' | 1:CA:1276:G:O4' | 2.05 | 0.56 |
| 42:BS:92:ARG:HD3 | 42:BS:93:ALA:H | 1.69 | 0.56 |
| 2:AE:8:LYS:H | 2:AE:8:LYS:HE2 | 1.71 | 0.56 |
| 25:BA:2118:U:H5'' | 25:BA:2119:A:OP1 | 2.05 | 0.56 |
| 45:DV:108:PRO:CA | 45:DV:143:GLY:N | 2.68 | 0.56 |
| 35:DO:85:LEU:CA | 35:DO:88:LEU:HB3 | 2.33 | 0.56 |
| 35:DO:11:GLY:C | 35:DO:13:ASN:N | 2.59 | 0.56 |
| 27:BD:25:THR:OG1 | 27:BD:113:VAL:HG21 | 2.05 | 0.56 |
| 27:BD:28:GLU:HB3 | 27:BD:29:PRO:HD3 | 1.88 | 0.56 |
| 25:DA:598:G:H1' | 35:DO:12:ALA:CB | 2.35 | 0.56 |
| 25:DA:2523:G:H5' | 25:DA:2523:G:C8 | 2.40 | 0.56 |
| 25:BA:1869:G:C5' | 25:BA:1869:G:H8 | 2.19 | 0.56 |
| 52:B6:27:LYS:HB2 | 52:B6:27:LYS:NZ | 2.20 | 0.56 |
| 45:BV:157:LEU:HD11 | 45:BV:163:LEU:CD2 | 2.36 | 0.56 |
| 25:DA:1181:C:O2' | 25:DA:1182:A:H5' | 2.06 | 0.56 |
| 27:BD:70:TRP:HZ3 | 27:BD:146:GLU:OE2 | 1.89 | 0.56 |
| 29:BF:160:ASN:OD1 | 29:BF:163:VAL:HG23 | 2.06 | 0.56 |
| 25:BA:320:A:H2' | 29:BF:136:THR:HG21 | 1.88 | 0.56 |
| 32:DK:14:ASP:N | 32:DK:17:GLN:OE1 | 2.34 | 0.56 |
| 8:CK:42:GLU:OE2 | 8:CK:122:ARG:NH2 | 2.39 | 0.56 |
| 7:CJ:95:ARG:HH21 | 7:CJ:99:LEU:HD11 | 1.71 | 0.56 |
| 1:CA:577:G:C8 | 1:CA:816:A:C6 | 2.93 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 45:BV:53:ILE:HA | 45:BV:71:VAL:HG13 | 1.87 | 0.56 |
| 25:DA:1544:C:H2' | 25:DA:1544:C:O2 | 2.04 | 0.56 |
| 45:BV:128:VAL:CG2 | 45:BV:160:GLY:HA3 | 2.36 | 0.56 |
| 27:DD:30:GLU:CG | 27:DD:63:ARG:NH2 | 2.69 | 0.56 |
| 25:BA:1813:G:H1' | 27:BD:50:THR:OG1 | 2.05 | 0.56 |
| 1:CA:1004:A:OP1 | 1:CA:1025:U:O4 | 2.23 | 0.56 |
| 28:DE:3:GLY:O | 28:DE:4:ILE:HG23 | 2.05 | 0.56 |
| 25:BA:259:G:N2 | 25:BA:621:A:C8 | 2.73 | 0.56 |
| 34:DN:102:VAL:HB | 34:DN:106:LEU:HD12 | 1.88 | 0.56 |
| 30:DG:101:ILE:HB | 30:DG:105:LYS:NZ | 2.19 | 0.56 |
| 30:BG:166:ASP:HA | 30:BG:169:ALA:CB | 2.36 | 0.56 |
| 25:BA:482:A:H8 | 25:BA:482:A:OP2 | 1.89 | 0.56 |
| 2:AE:8:LYS:HE3 | 2:AE:11:LEU:CB | 2.32 | 0.56 |
| 1:AA:192:U:C4' | 20:AW:103:GLY:HA2 | 2.35 | 0.56 |
| 41:D2:28:GLU:HB3 | 41:D2:29:PRO:CD | 2.35 | 0.56 |
| 16:CS:8:ARG:HG3 | 16:CS:8:ARG:HH11 | 1.67 | 0.56 |
| 37:B0:55:ALA:HB2 | 37:B0:79:LEU:HD13 | 1.86 | 0.56 |
| 27:DD:70:TRP:CH2 | 27:DD:150:LYS:HA | 2.40 | 0.56 |
| 23:AD:49:C:H6 | 23:AD:49:C:OP2 | 1.88 | 0.56 |
| 28:DE:154:LYS:HA | 28:DE:154:LYS:HE3 | 1.86 | 0.56 |
| 1:CA:1015:A:C5 | 1:CA:1016:A:C5 | 2.94 | 0.56 |
| 45:DV:149:SER:CB | 45:DV:172:ALA:O | 2.54 | 0.56 |
| 25:DA:1000:A:C6 | 25:DA:1001:A:N1 | 2.73 | 0.56 |
| 34:DN:1:MET:HE3 | 34:DN:67:LYS:HG2 | 1.87 | 0.56 |
| 4:CG:9:CYS:HA | 4:CG:12:CYS:CB | 2.36 | 0.56 |
| 1:AA:33:A:H2' | 1:AA:34:C:C6 | 2.41 | 0.56 |
| 1:AA:983:A:H5'' | 1:AA:984:C:OP2 | 2.05 | 0.56 |
| 10:CM:24:VAL:O | 10:CM:28:ARG:HB2 | 2.06 | 0.56 |
| 9:AL:48:GLU:N | 9:AL:49:PRO:HD2 | 2.21 | 0.56 |
| 51:D5:51:TYR:HB2 | 51:D5:54:GLY:HA3 | 1.88 | 0.56 |
| 5:AH:139:LEU:HA | 5:AH:142:LEU:HD12 | 1.87 | 0.56 |
| 46:B3:11:ARG:O | 46:B3:14:ARG:NH2 | 2.38 | 0.56 |
| 4:CG:78:LEU:HD22 | 4:CG:96:LEU:HB3 | 1.86 | 0.56 |
| 39:DR:107:ASP:N | 39:DR:107:ASP:OD1 | 2.39 | 0.56 |
| 30:BG:17:PRO:HA | 30:BG:20:ILE:HG13 | 1.88 | 0.56 |
| 38:BQ:106:ARG:HB2 | 38:BQ:106:ARG:NH1 | 2.20 | 0.56 |
| 33:DM:36:GLY:H | 33:DM:42:TRP:HZ3 | 1.54 | 0.56 |
| 28:BE:41:LYS:O | 28:BE:42:ASP:CG | 2.43 | 0.56 |
| 33:BM:35:ARG:O | 33:BM:35:ARG:HG3 | 2.05 | 0.56 |
| 1:CA:1320:C:OP1 | 19:CV:70:LYS:HE3 | 2.06 | 0.56 |
| 1:CA:1189:C:OP1 | 10:CM:51:ARG:NH2 | 2.33 | 0.56 |
| 1:AA:1004:A:O4' | 1:AA:1025:U:N3 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:1019:U:H2' | 25:DA:1020:A:H8 | 1.71 | 0.56 |
| 14:AQ:45:ARG:HH11 | 14:AQ:49:HIS:HE1 | 1.54 | 0.56 |
| 31:BH:59:ARG:NH1 | 31:BH:59:ARG:CG | 2.57 | 0.56 |
| 1:CA:1127:G:H8 | 1:CA:1127:G:OP2 | 1.88 | 0.56 |
| 1:CA:1133:G:H1 | 1:CA:1141:C:N4 | 2.02 | 0.56 |
| 30:DG:60:LEU:O | 30:DG:60:LEU:HD23 | 2.06 | 0.56 |
| 33:BM:97:ARG:HA | 33:BM:100:GLU:HB2 | 1.88 | 0.56 |
| 25:DA:2387:U:H1' | 46:D3:41:ARG:CD | 2.36 | 0.56 |
| 32:BK:9:LEU:O | 32:BK:10:GLU:HB3 | 2.06 | 0.56 |
| 41:B2:44:LYS:O | 41:B2:46:VAL:N | 2.39 | 0.56 |
| 29:BF:185:ASP:HA | 29:BF:188:ARG:HD3 | 1.86 | 0.56 |
| 41:B2:34:GLU:O | 41:B2:36:PRO:HD3 | 2.05 | 0.56 |
| 6:AI:67:MET:SD | 6:AI:75:LEU:HD12 | 2.46 | 0.56 |
| 25:BA:805:G:OP2 | 35:BO:41:ARG:HG2 | 2.05 | 0.56 |
| 9:AL:8:GLY:HA2 | 9:AL:79:LEU:HD13 | 1.87 | 0.56 |
| 1:CA:838:G:H2' | 1:CA:841:U:H5' | 1.87 | 0.56 |
| 25:DA:877:U:H4' | 25:DA:878:A:OP1 | 2.04 | 0.56 |
| 1:AA:1312:G:O2' | 1:AA:1313:U:H5' | 2.05 | 0.56 |
| 30:DG:145:THR:O | 30:DG:146:TYR:HB3 | 2.06 | 0.56 |
| 25:BA:637:A:O5' | 35:BO:116:GLY:HA3 | 2.06 | 0.56 |
| 39:DR:107:ASP:OD2 | 39:DR:109:GLU:HB2 | 2.06 | 0.56 |
| 25:DA:2808:U:H2' | 25:DA:2809:A:H8 | 1.71 | 0.56 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.41 | 0.56 |
| 7:AJ:23:VAL:CG1 | 7:AJ:43:PHE:HE2 | 2.18 | 0.56 |
| 7:AJ:87:VAL:HG11 | 7:AJ:155:ARG:HA | 1.88 | 0.56 |
| 27:DD:235:GLY:O | 27:DD:237:GLU:OE1 | 2.24 | 0.56 |
| 23:AD:67:C:N3 | 23:AD:68:C:N4 | 2.53 | 0.56 |
| 25:BA:1769:G:O2' | 25:BA:1958:C:OP1 | 2.16 | 0.56 |
| 34:BN:35:VAL:HG22 | 34:BN:69:ILE:HG12 | 1.87 | 0.56 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:H6 | 1.71 | 0.56 |
| 11:AN:87:THR:HG22 | 11:AN:88:GLY:H | 1.70 | 0.56 |
| 25:BA:1060:U:H5' | 25:BA:1061:U:H5 | 1.71 | 0.56 |
| 28:BE:27:LEU:CD2 | 28:BE:51:PHE:HZ | 2.19 | 0.56 |
| 28:BE:55:ASN:HD22 | 28:BE:59:VAL:HG23 | 1.71 | 0.56 |
| 25:BA:1794:U:H2' | 25:BA:1795:C:H6 | 1.69 | 0.56 |
| 22:CB:70:G:H3' | 22:CB:71:U:C5 | 2.40 | 0.56 |
| 1:AA:1004:A:P | 1:AA:1025:U:O4 | 2.63 | 0.56 |
| 19:AV:41:VAL:CG1 | 19:AV:44:MET:HB2 | 2.36 | 0.56 |
| 19:AV:68:GLY:HA2 | 50:B4:59:PHE:CD1 | 2.41 | 0.56 |
| 25:DA:529:A:H2' | 25:DA:529:A:N3 | 2.21 | 0.56 |
| 1:AA:201:C:N4 | 1:AA:209:U:O2 | 2.39 | 0.56 |
| 25:BA:2119:A:N6 | 25:BA:2170:A:N6 | 2.52 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 15:AR:56:LEU:HD21 | 25:BA:715:G:C2 | 2.41 | 0.56 |
| 19:CV:68:GLY:HA3 | 50:D4:59:PHE:HE1 | 1.70 | 0.56 |
| 25:BA:2131:G:OP1 | 25:BA:2132:U:H3' | 2.06 | 0.56 |
| 44:DU:39:VAL:HG23 | 44:DU:40:GLU:N | 2.19 | 0.56 |
| 25:BA:242:G:H5'' | 54:B8:62:LEU:HD13 | 1.88 | 0.56 |
| 25:BA:956:G:OP2 | 36:BP:14:ARG:NH2 | 2.39 | 0.56 |
| 41:B2:76:LYS:O | 41:B2:79:VAL:HG12 | 2.06 | 0.56 |
| 1:AA:1392:G:O2' | 1:AA:1393:U:H5' | 2.06 | 0.56 |
| 1:AA:1329:A:N7 | 21:AX:7:ARG:NH2 | 2.54 | 0.56 |
| 45:DV:8:TYR:HA | 45:DV:62:PRO:HD3 | 1.87 | 0.56 |
| 23:AD:13:C:HO2' | 23:AD:14:A:P | 2.29 | 0.56 |
| 30:BG:113:ARG:HH21 | 50:B4:34:GLU:HB3 | 1.71 | 0.56 |
| 39:BR:107:ASP:H | 39:BR:110:ILE:CG2 | 2.19 | 0.56 |
| 25:DA:2111:C:C2 | 25:DA:2118:U:O2' | 2.57 | 0.56 |
| 53:D7:5:TRP:NE1 | 53:D7:7:PRO:HG3 | 2.20 | 0.56 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:H8 | 1.84 | 0.56 |
| 25:BA:581:C:OP1 | 40:B1:33:ARG:HG3 | 2.06 | 0.56 |
| 1:CA:920:U:H2' | 1:CA:921:U:H6 | 1.70 | 0.56 |
| 25:BA:1216:G:OP2 | 40:B1:12:ARG:NH2 | 2.37 | 0.56 |
| 1:AA:943:U:C1' | 9:AL:124:GLN:HE22 | 2.18 | 0.56 |
| 22:AB:27:G:O6 | 22:AB:45:U:C2 | 2.59 | 0.56 |
| 1:CA:570:G:H1' | 1:CA:820:U:C4 | 2.40 | 0.56 |
| 11:CN:109:VAL:HG22 | 18:CU:86:VAL:HG13 | 1.87 | 0.56 |
| 25:DA:1794:U:O2' | 25:DA:1795:C:H5' | 2.06 | 0.56 |
| 34:BN:12:ASP:CG | 34:BN:14:THR:HG23 | 2.26 | 0.56 |
| 25:DA:176:G:O2' | 25:DA:177:G:H5' | 2.06 | 0.56 |
| 33:BM:120:LEU:HD22 | 33:BM:121:LYS:N | 2.20 | 0.56 |
| 25:BA:305:U:H2' | 25:BA:306:U:C6 | 2.40 | 0.56 |
| 25:DA:2037:G:H2' | 25:DA:2038:G:C8 | 2.41 | 0.56 |
| 39:BR:78:LEU:O | 39:BR:78:LEU:HD13 | 2.05 | 0.56 |
| 22:CB:61:C:H42 | 22:CB:75:G:H1 | 1.53 | 0.56 |
| 25:DA:2307:G:O2' | 25:DA:2308:G:C8 | 2.58 | 0.56 |
| 30:BG:61:ALA:HA | 30:BG:66:GLN:O | 2.06 | 0.56 |
| 36:DP:63:LYS:HB3 | 36:DP:107:ALA:O | 2.05 | 0.56 |
| 25:DA:1085:A:HO2' | 25:DA:1086:A:H8 | 1.50 | 0.56 |
| 32:DK:82:ARG:NH1 | 32:DK:146:ALA:HA | 2.21 | 0.56 |
| 23:CD:7:G:C3' | 23:CD:8:U:H5' | 2.35 | 0.56 |
| 25:DA:528:A:C2 | 25:DA:2043:C:C5' | 2.85 | 0.56 |
| 3:AF:40:ARG:HG3 | 3:AF:40:ARG:NH1 | 2.21 | 0.56 |
| 30:BG:133:LEU:O | 30:BG:133:LEU:HD23 | 2.06 | 0.56 |
| 25:BA:475:U:C4 | 25:BA:481:G:O6 | 2.59 | 0.56 |
| 26:DB:7:G:H3' | 26:DB:8:U:H5'' | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:2191:G:O2' | 25:DA:2192:G:P | 2.63 | 0.56 |
| 25:BA:2790:A:C2 | 25:BA:2894:G:H5'' | 2.41 | 0.56 |
| 2:CE:98:LEU:O | 2:CE:101:MET:HG2 | 2.06 | 0.56 |
| 25:DA:2355:C:H5' | 46:D3:36:ILE:CD1 | 2.36 | 0.56 |
| 25:DA:2068:U:N3 | 25:DA:2430:A:C2 | 2.60 | 0.56 |
| 12:CO:26:ALA:O | 12:CO:27:LEU:CD1 | 2.53 | 0.56 |
| 1:AA:1392:G:O2' | 1:AA:1502:A:H5'' | 2.06 | 0.56 |
| 1:CA:411:A:H62 | 1:CA:413:G:H21 | 1.54 | 0.56 |
| 22:CB:26:C:C5 | 22:CB:27:G:N2 | 2.73 | 0.56 |
| 25:DA:288:C:O2 | 25:DA:288:C:H2' | 2.06 | 0.56 |
| 38:DQ:60:GLY:O | 38:DQ:61:ASN:HB2 | 2.05 | 0.56 |
| 3:AF:95:THR:HG22 | 3:AF:96:GLY:N | 2.21 | 0.56 |
| 6:AI:44:GLY:O | 6:AI:59:TYR:HA | 2.04 | 0.56 |
| 25:BA:2593:U:H2' | 25:BA:2594:C:C6 | 2.41 | 0.56 |
| 25:BA:517:C:OP1 | 51:B5:16:ARG:NH2 | 2.39 | 0.56 |
| 3:CF:68:VAL:HG12 | 3:CF:70:VAL:HG23 | 1.87 | 0.56 |
| 1:AA:96:G:C2' | 1:AA:97:U:H5' | 2.36 | 0.56 |
| 50:B4:13:ARG:H | 50:B4:30:GLU:H | 1.54 | 0.56 |
| 44:DU:47:LYS:HG2 | 44:DU:60:PHE:HD1 | 1.71 | 0.56 |
| 25:BA:753:C:O5' | 25:BA:753:C:H6 | 1.88 | 0.56 |
| 2:CE:5:ILE:O | 2:CE:5:ILE:HG23 | 2.05 | 0.56 |
| 6:AI:61:LEU:HB3 | 6:AI:63:TYR:HE2 | 1.69 | 0.56 |
| 35:BO:91:PHE:O | 35:BO:121:LYS:NZ | 2.32 | 0.56 |
| 12:AO:53:ARG:HH11 | 12:AO:53:ARG:HG3 | 1.71 | 0.56 |
| 1:CA:656:C:H42 | 1:CA:750:G:H1 | 1.53 | 0.56 |
| 31:BH:15:VAL:HG12 | 31:BH:29:PRO:HD2 | 1.88 | 0.56 |
| 1:AA:1238:A:N3 | 1:AA:1241:G:O2' | 2.39 | 0.56 |
| 15:AR:27:VAL:O | 15:AR:31:LEU:HB2 | 2.06 | 0.56 |
| 1:AA:636:U:H2' | 1:AA:637:G:C8 | 2.40 | 0.56 |
| 25:DA:2527:C:C4 | 25:DA:2528:U:C5 | 2.94 | 0.56 |
| 38:DQ:110:LEU:HD22 | 38:DQ:111:GLU:N | 2.21 | 0.55 |
| 25:DA:994:C:OP1 | 40:D1:53:ARG:NH2 | 2.39 | 0.55 |
| 27:BD:44:ASN:ND2 | 27:BD:44:ASN:H | 2.04 | 0.55 |
| 25:DA:673:C:H6 | 25:DA:673:C:C5' | 2.18 | 0.55 |
| 28:DE:51:PHE:O | 28:DE:74:PRO:HB3 | 2.06 | 0.55 |
| 31:DH:150:ALA:C | 31:DH:152:ARG:N | 2.60 | 0.55 |
| 26:BB:42:C:O2 | 30:BG:93:THR:N | 2.34 | 0.55 |
| 29:DF:25:PRO:C | 29:DF:27:GLU:H | 2.08 | 0.55 |
| 25:DA:2470:G:OP2 | 36:DP:56:ARG:CZ | 2.54 | 0.55 |
| 39:BR:52:ILE:CD1 | 39:BR:61:PHE:HB3 | 2.26 | 0.55 |
| 37:D0:87:TYR:HD1 | 37:D0:90:ARG:HD2 | 1.70 | 0.55 |
| 25:DA:1358:G:N2 | 25:DA:1372:U:C5 | 2.74 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 52:B6:10:LEU:HD23 | 54:B8:34:TRP:CE2 | 2.40 | 0.55 |
| 25:BA:1396:U:H2' | 25:BA:1396:U:O2 | 2.05 | 0.55 |
| 41:B2:43:GLU:HA | 41:B2:43:GLU:OE2 | 2.05 | 0.55 |
| 29:DF:148:LEU:HD23 | 29:DF:191:ARG:HH12 | 1.70 | 0.55 |
| 45:BV:152:ALA:O | 45:BV:155:LEU:HB2 | 2.06 | 0.55 |
| 11:AN:66:LEU:CD2 | 11:AN:97:ALA:HB1 | 2.35 | 0.55 |
| 1:CA:16:A:N1 | 1:CA:919:A:H2 | 2.04 | 0.55 |
| 27:DD:268:ARG:HG2 | 27:DD:268:ARG:HH11 | 1.72 | 0.55 |
| 25:BA:270(M):U:H1' | 25:BA:270(N):G:C5 | 2.41 | 0.55 |
| 1:AA:1149:C:OP2 | 9:AL:9:ARG:NH2 | 2.39 | 0.55 |
| 34:BN:4:PRO:O | 34:BN:5:GLN:HB2 | 2.05 | 0.55 |
| 27:BD:17:THR:CG2 | 27:BD:204:ILE:HA | 2.37 | 0.55 |
| 31:BH:43:VAL:HG12 | 31:BH:52:VAL:HG22 | 1.89 | 0.55 |
| 52:D6:14:THR:OG1 | 52:D6:19:ARG:HG2 | 2.06 | 0.55 |
| 1:AA:832:C:O2 | 1:AA:855:G:C2 | 2.58 | 0.55 |
| 25:DA:2547:U:O2' | 25:DA:2548:G:H5' | 2.06 | 0.55 |
| 1:CA:35:G:C2 | 1:CA:550:G:N3 | 2.75 | 0.55 |
| 25:BA:852:G:H2' | 25:BA:853:G:H8 | 1.70 | 0.55 |
| 5:CH:75:THR:HG23 | 5:CH:76:ILE:N | 2.21 | 0.55 |
| 1:CA:892:A:O2' | 1:CA:1415:G:H4' | 2.06 | 0.55 |
| 25:BA:546:C:H6 | 25:BA:546:C:OP1 | 1.89 | 0.55 |
| 1:AA:1339:A:H2' | 1:AA:1340:A:O4' | 2.06 | 0.55 |
| 27:BD:124:PRO:HG2 | 27:BD:129:ASN:ND2 | 2.21 | 0.55 |
| 25:BA:1069:A:H4' | 25:BA:1070:A:C5' | 2.36 | 0.55 |
| 44:BU:76:CYS:CB | 44:BU:96:ILE:HD13 | 2.36 | 0.55 |
| 1:CA:517:G:N2 | 1:CA:530:G:OP1 | 2.29 | 0.55 |
| 28:BE:203:LYS:O | 28:BE:203:LYS:HD2 | 2.07 | 0.55 |
| 1:AA:793:U:H3' | 1:AA:794:A:H5'' | 1.89 | 0.55 |
| 25:DA:1728:G:C2 | 25:DA:1730:U:OP2 | 2.59 | 0.55 |
| 25:BA:1496:A:H2' | 25:BA:1577:C:O2' | 2.06 | 0.55 |
| 23:AD:55:U:C4 | 23:AD:56:U:C5 | 2.94 | 0.55 |
| 1:AA:1077:G:N1 | 1:AA:1081:G:C6 | 2.75 | 0.55 |
| 7:CJ:26:PHE:CE2 | 7:CJ:30:ILE:HD11 | 2.42 | 0.55 |
| 25:DA:101:G:C2' | 25:DA:102:G:OP1 | 2.55 | 0.55 |
| 29:DF:125:LEU:HD23 | 29:DF:125:LEU:H | 1.71 | 0.55 |
| 6:CI:33:TYR:CZ | 6:CI:78:GLU:HG3 | 2.40 | 0.55 |
| 37:B0:33:ARG:NH2 | 51:B5:55:ARG:HG2 | 2.21 | 0.55 |
| 1:CA:1346:A:C1' | 1:CA:1347:G:OP2 | 2.54 | 0.55 |
| 22:AB:52:U:C6 | 22:AB:53:A:C8 | 2.95 | 0.55 |
| 22:AB:55:G:H2' | 22:AB:56:G:C8 | 2.41 | 0.55 |
| 32:DK:77:LEU:CG | 32:DK:78:THR:H | 2.19 | 0.55 |
| 1:AA:1106:G:C5 | 1:AA:1107:C:C5 | 2.94 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:2148:G:H2' | 25:DA:2149:G:C8 | 2.41 | 0.55 |
| 5:CH:57:LYS:O | 5:CH:61:TYR:HD2 | 1.88 | 0.55 |
| 39:BR:112:ARG:O | 39:BR:112:ARG:HG3 | 2.06 | 0.55 |
| 1:CA:1206:G:C6 | 1:CA:1207:G:C5 | 2.94 | 0.55 |
| 34:DN:101:PRO:HG3 | 39:DR:67:SER:OG | 2.06 | 0.55 |
| 1:AA:74:C:H2' | 1:AA:75:C:O4' | 2.05 | 0.55 |
| 25:BA:2875:C:O2' | 39:BR:5:ALA:HB3 | 2.06 | 0.55 |
| 27:BD:148:GLU:CB | 27:BD:151:LYS:HD2 | 2.37 | 0.55 |
| 25:BA:2795:G:H3' | 25:BA:2797:U:H5'' | 1.88 | 0.55 |
| 23:AD:71:G:O2' | 23:AD:72:C:H5' | 2.06 | 0.55 |
| 25:BA:270(Y):G:C2 | 25:BA:270(Z):U:O4 | 2.60 | 0.55 |
| 1:AA:1293:G:H2' | 1:AA:1294:G:O4' | 2.05 | 0.55 |
| 1:AA:368:U:P | 32:DK:91:SER:HG | 2.29 | 0.55 |
| 1:AA:989:C:H42 | 1:AA:1216:G:H1 | 1.53 | 0.55 |
| 1:CA:954:G:H2' | 1:CA:955:U:C6 | 2.42 | 0.55 |
| 25:DA:2494:G:H2' | 25:DA:2495:G:H8 | 1.71 | 0.55 |
| 25:DA:1476:C:C2' | 25:DA:1477:A:H5' | 2.36 | 0.55 |
| 25:BA:1409:C:O2' | 25:BA:1410:G:H5' | 2.05 | 0.55 |
| 35:BO:101:VAL:HG22 | 35:BO:106:LEU:HB3 | 1.86 | 0.55 |
| 25:DA:228:A:C8 | 25:DA:228:A:C3' | 2.89 | 0.55 |
| 25:BA:1805:U:O2 | 27:BD:50:THR:HB | 2.06 | 0.55 |
| 16:AS:20:VAL:HG22 | 16:AS:32:TYR:CG | 2.37 | 0.55 |
| 23:AC:20:G:C6 | 23:AC:58:A:C2 | 2.95 | 0.55 |
| 40:B1:60:LEU:HD21 | 40:B1:64:ARG:HH21 | 1.70 | 0.55 |
| 1:AA:542:G:H5' | 4:AG:41:GLY:HA3 | 1.88 | 0.55 |
| 23:AD:5:G:H22 | 23:AD:69:C:N4 | 2.04 | 0.55 |
| 2:CE:19:HIS:HD2 | 2:CE:20:GLU:OE1 | 1.90 | 0.55 |
| 13:CP:25:ILE:HG22 | 13:CP:26:GLY:N | 2.20 | 0.55 |
| 25:DA:1048:A:H5' | 25:DA:1049:C:OP2 | 2.07 | 0.55 |
| 11:AN:41:THR:HG21 | 11:AN:71:LYS:HB2 | 1.88 | 0.55 |
| 25:DA:2157:G:H2' | 25:DA:2158:A:H8 | 1.72 | 0.55 |
| 25:DA:39:C:H2' | 25:DA:40:C:H6 | 1.71 | 0.55 |
| 12:CO:26:ALA:O | 12:CO:27:LEU:HD13 | 2.06 | 0.55 |
| 19:CV:28:LYS:HE3 | 19:CV:29:ARG:N | 2.19 | 0.55 |
| 9:AL:4:TYR:CD1 | 9:AL:88:TYR:HB2 | 2.42 | 0.55 |
| 14:CQ:45:ARG:O | 14:CQ:49:HIS:HD2 | 1.89 | 0.55 |
| 25:BA:2734:A:C5' | 25:BA:2734:A:H8 | 2.19 | 0.55 |
| 1:AA:250:A:C4' | 1:AA:251:G:H5'' | 2.37 | 0.55 |
| 25:BA:1239:G:H2' | 25:BA:1240:U:O4' | 2.06 | 0.55 |
| 45:DV:157:LEU:HD11 | 45:DV:163:LEU:HD23 | 1.89 | 0.55 |
| 22:AB:52:U:C2' | 22:AB:53:A:H5' | 2.36 | 0.55 |
| 3:AF:195:VAL:C | 3:AF:196:LEU:HD23 | 2.27 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 44:DU:50:ARG:O | 44:DU:53:PRO:HD3 | 2.05 | 0.55 |
| 25:BA:756:C:H2' | 25:BA:757:U:O5' | 2.06 | 0.55 |
| 1:AA:1149:C:H2' | 1:AA:1150:U:C6 | 2.41 | 0.55 |
| 25:DA:1499:C:H2' | 25:DA:1500:G:H8 | 1.71 | 0.55 |
| 25:DA:2817:G:P | 37:D0:99:LYS:HZ3 | 2.30 | 0.55 |
| 30:DG:53:LEU:HD21 | 30:DG:90:LEU:HD11 | 1.87 | 0.55 |
| 25:BA:2574:G:O2' | 28:BE:143:ASN:HB3 | 2.06 | 0.55 |
| 17:AT:7:THR:OG1 | 17:AT:58:GLU:HG2 | 2.07 | 0.55 |
| 30:BG:27:ASN:HB3 | 30:BG:30:GLU:HG3 | 1.89 | 0.55 |
| 25:DA:2483:C:H5' | 25:DA:2484:G:OP2 | 2.06 | 0.55 |
| 25:DA:1543:A:H1' | 25:DA:1545:A:H1' | 1.89 | 0.55 |
| 34:DN:10:VAL:HG21 | 34:DN:16:ALA:O | 2.06 | 0.55 |
| 9:AL:99:LEU:HB3 | 9:AL:101:PHE:CE1 | 2.41 | 0.55 |
| 25:DA:270(Y):G:C2 | 25:DA:270(Z):U:O4 | 2.59 | 0.55 |
| 25:BA:1694:C:H6 | 25:BA:1694:C:H5' | 1.71 | 0.55 |
| 8:CK:111:ILE:HG22 | 8:CK:112:LEU:H | 1.71 | 0.55 |
| 27:BD:125:ILE:O | 27:BD:125:ILE:HG22 | 2.06 | 0.55 |
| 28:DE:87:GLU:HG3 | 28:DE:87:GLU:O | 2.06 | 0.55 |
| 1:AA:258:G:H2' | 1:AA:259:G:H8 | 1.72 | 0.55 |
| 25:DA:847:U:C4 | 25:DA:933:A:C6 | 2.90 | 0.55 |
| 27:DD:35:LYS:HA | 27:DD:64:ILE:CG2 | 2.33 | 0.55 |
| 25:DA:996:A:C2 | 25:DA:997:G:C8 | 2.95 | 0.55 |
| 28:BE:41:LYS:C | 28:BE:42:ASP:CG | 2.65 | 0.55 |
| 1:CA:1004:A:O4' | 1:CA:1025:U:N3 | 2.38 | 0.55 |
| 1:AA:1054:C:H2' | 1:AA:1054:C:O2 | 2.07 | 0.55 |
| 23:CC:48:U:H1' | 23:CC:49:C:O5' | 2.06 | 0.55 |
| 39:DR:56:GLY:C | 39:DR:58:ASN:N | 2.58 | 0.55 |
| 51:B5:4:HIS:O | 51:B5:5:PRO:C | 2.43 | 0.55 |
| 26:DB:116:G:H2' | 26:DB:117:G:O4' | 2.07 | 0.55 |
| 25:BA:2373:G:N2 | 25:BA:2380:C:N3 | 2.49 | 0.55 |
| 2:CE:137:ARG:O | 2:CE:137:ARG:HD3 | 2.06 | 0.55 |
| 23:CD:44:A:C2 | 23:CD:45:A:C6 | 2.93 | 0.55 |
| 1:CA:1298:C:N4 | 7:CJ:114:ARG:HB3 | 2.15 | 0.55 |
| 20:AW:100:ILE:CG1 | 20:AW:101:GLY:N | 2.69 | 0.55 |
| 25:BA:1024:G:C3' | 25:BA:1025:G:H5'' | 2.31 | 0.55 |
| 15:AR:87:ILE:HG22 | 15:AR:88:ARG:HG2 | 1.87 | 0.55 |
| 25:BA:229:A:HO2' | 25:BA:230:U:P | 2.29 | 0.55 |
| 25:BA:787:U:H5'' | 25:BA:788:A:H5' | 1.88 | 0.55 |
| 25:BA:2723:C:OP1 | 37:B0:3:HIS:CD2 | 2.54 | 0.55 |
| 2:AE:120:ALA:O | 2:AE:121:LEU:CB | 2.52 | 0.55 |
| 22:AB:16:U:OP2 | 22:AB:16:U:H2' | 2.06 | 0.55 |
| 30:BG:107:LEU:HD11 | 30:BG:178:PHE:CD1 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:603:A:H4' | 25:BA:604:G:O5' | 2.06 | 0.55 |
| 1:CA:1077:G:N1 | 1:CA:1081:G:C6 | 2.75 | 0.55 |
| 12:AO:40:VAL:CG2 | 12:AO:78:GLN:O | 2.54 | 0.55 |
| 42:BS:64:MET:O | 42:BS:65:LEU:HB2 | 2.07 | 0.55 |
| 25:BA:645:C:H2' | 25:BA:646:A:OP1 | 2.06 | 0.55 |
| 7:AJ:23:VAL:CG1 | 7:AJ:43:PHE:CE2 | 2.89 | 0.55 |
| 20:CW:33:ILE:HD13 | 20:CW:62:LEU:HB3 | 1.88 | 0.55 |
| 25:BA:176:G:O2' | 25:BA:177:G:H5' | 2.06 | 0.55 |
| 25:DA:1314:C:C2 | 25:DA:1339:G:N2 | 2.74 | 0.55 |
| 25:BA:1257:C:H4' | 29:BF:83:PHE:CD2 | 2.41 | 0.55 |
| 39:BR:45:PHE:CE1 | 39:BR:65:LYS:HE3 | 2.41 | 0.55 |
| 25:DA:2860:A:N7 | 25:DA:2861:G:H1' | 2.21 | 0.55 |
| 15:AR:38:ARG:HH11 | 15:AR:38:ARG:HG2 | 1.72 | 0.55 |
| 52:D6:28:ARG:HB3 | 52:D6:30:THR:C | 2.27 | 0.55 |
| 27:DD:34:VAL:CG1 | 27:DD:34:VAL:O | 2.55 | 0.55 |
| 25:BA:2310:A:O2' | 25:BA:2311:A:C5' | 2.51 | 0.55 |
| 39:DR:74:ARG:HD3 | 39:DR:76:PHE:CZ | 2.42 | 0.55 |
| 23:CC:15:G:H2' | 23:CC:60:A:N1 | 2.22 | 0.55 |
| 31:DH:89:ILE:HG21 | 31:DH:129:THR:HA | 1.88 | 0.55 |
| 54:D8:47:LYS:C | 54:D8:48:PHE:HD1 | 2.09 | 0.55 |
| 1:CA:1367:C:H5'' | 9:CL:114:TYR:HB3 | 1.87 | 0.55 |
| 11:AN:77:MET:HE3 | 11:AN:80:VAL:HG12 | 1.87 | 0.55 |
| 28:BE:101:ARG:C | 28:BE:201:THR:HG1 | 2.10 | 0.55 |
| 30:BG:129:GLY:HA2 | 30:BG:166:ASP:HB3 | 1.87 | 0.55 |
| 25:DA:888:C:H4' | 25:DA:889:C:O5' | 2.03 | 0.55 |
| 9:CL:48:GLU:N | 9:CL:49:PRO:HD2 | 2.21 | 0.55 |
| 25:BA:1291:C:H5' | 25:BA:1536:A:H5' | 1.87 | 0.55 |
| 25:BA:2712:U:O2 | 25:BA:2712:U:C5' | 2.51 | 0.55 |
| 25:BA:1473:G:H2' | 25:BA:1474:C:H5' | 1.89 | 0.55 |
| 20:CW:25:ARG:NH1 | 20:CW:25:ARG:HG3 | 2.19 | 0.55 |
| 1:CA:1311:G:N2 | 1:CA:1327:C:C2 | 2.74 | 0.55 |
| 1:CA:192:U:H2' | 1:CA:193:C:H6 | 1.71 | 0.55 |
| 1:AA:1320:C:OP1 | 19:AV:70:LYS:HE3 | 2.05 | 0.55 |
| 25:BA:234:C:H2' | 25:BA:235:U:C6 | 2.41 | 0.55 |
| 25:DA:2473:U:O2 | 25:DA:2473:U:C2' | 2.54 | 0.55 |
| 39:BR:85:LYS:HE3 | 39:BR:87:ASP:OD2 | 2.07 | 0.55 |
| 25:DA:479:A:HO2' | 25:DA:481:G:H8 | 1.55 | 0.55 |
| 1:AA:1362(A):C:H5' | 1:AA:1363:A:O5' | 2.06 | 0.55 |
| 25:DA:824:A:H1' | 25:DA:2358:G:N7 | 2.22 | 0.55 |
| 10:AM:15:THR:O | 10:AM:19:SER:N | 2.38 | 0.55 |
| 1:CA:20:U:C2' | 1:CA:21:G:H5' | 2.35 | 0.55 |
| 25:DA:755:C:H2' | 25:DA:756:C:C6 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:2475:C:H5' | 25:DA:2476:A:OP2 | 2.05 | 0.55 |
| 25:BA:213:A:H2' | 25:BA:214:G:O4' | 2.05 | 0.55 |
| 49:DX:17:LYS:HD3 | 49:DX:17:LYS:O | 2.07 | 0.55 |
| 1:AA:1156:G:C3' | 1:AA:1157:A:H5'' | 2.37 | 0.55 |
| 25:DA:2371:G:H4' | 52:D6:45:LYS:CE | 2.35 | 0.55 |
| 52:B6:15:GLU:OE2 | 52:B6:44:ARG:NH1 | 2.39 | 0.55 |
| 1:CA:963:G:N3 | 10:CM:55:LYS:NZ | 2.50 | 0.55 |
| 4:CG:13:ARG:N | 4:CG:13:ARG:HD3 | 2.21 | 0.55 |
| 32:DK:143:SER:O | 32:DK:144:VAL:HB | 2.06 | 0.55 |
| 14:AQ:58:LYS:HB3 | 14:AQ:58:LYS:NZ | 2.21 | 0.55 |
| 23:CD:15:G:N2 | 23:CD:60:A:H1' | 2.21 | 0.55 |
| 43:BT:49:VAL:HG12 | 43:BT:50:LYS:H | 1.68 | 0.55 |
| 25:DA:2127:G:N2 | 25:DA:2173:A:C8 | 2.74 | 0.55 |
| 45:DV:168:GLU:HG3 | 45:DV:169:GLU:N | 2.21 | 0.55 |
| 2:CE:84:GLU:HB3 | 2:CE:219:VAL:HG11 | 1.89 | 0.55 |
| 9:CL:85:LEU:HD13 | 9:CL:92:TYR:CD2 | 2.40 | 0.55 |
| 7:CJ:23:VAL:O | 7:CJ:27:ILE:HG13 | 2.06 | 0.55 |
| 46:B3:53:MET:HA | 46:B3:58:THR:O | 2.06 | 0.55 |
| 25:BA:2292:C:OP2 | 38:BQ:17:ARG:NH2 | 2.38 | 0.55 |
| 49:DX:52:HIS:CD2 | 49:DX:52:HIS:H | 2.24 | 0.55 |
| 25:DA:288:C:H2' | 25:DA:289:A:C8 | 2.42 | 0.55 |
| 37:B0:74:LYS:C | 37:B0:76:VAL:N | 2.59 | 0.55 |
| 50:B4:61:ARG:HE | 50:B4:61:ARG:HA | 1.70 | 0.55 |
| 1:CA:8:A:C6 | 4:CG:209:ARG:HB2 | 2.41 | 0.55 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:H6 | 1.71 | 0.55 |
| 41:B2:64:HIS:ND1 | 41:B2:92:THR:HG22 | 2.21 | 0.55 |
| 25:DA:756:C:C2' | 25:DA:757:U:H5' | 2.37 | 0.55 |
| 37:B0:21:TYR:OH | 37:B0:43:GLU:HG2 | 2.06 | 0.55 |
| 25:BA:2275:C:O2 | 36:BP:83:MET:HG2 | 2.07 | 0.55 |
| 8:AK:27:PRO:HG3 | 8:AK:58:TYR:CE2 | 2.42 | 0.55 |
| 43:BT:36:LYS:HE2 | 43:BT:54:VAL:O | 2.05 | 0.55 |
| 25:BA:1952:A:C5 | 34:BN:22:ILE:HD11 | 2.41 | 0.55 |
| 25:BA:2511:U:O4 | 25:BA:2575:C:N3 | 2.39 | 0.55 |
| 1:CA:668:G:O2' | 1:CA:669:U:H5' | 2.07 | 0.55 |
| 37:D0:23:ASN:HD22 | 37:D0:23:ASN:N | 2.03 | 0.55 |
| 1:CA:1250:A:H4' | 9:CL:68:GLY:N | 2.21 | 0.55 |
| 7:CJ:69:VAL:HG12 | 7:CJ:69:VAL:O | 2.06 | 0.55 |
| 3:AF:141:VAL:O | 3:AF:141:VAL:HG12 | 2.05 | 0.55 |
| 25:DA:1774:C:H4' | 25:DA:1979:C:O2 | 2.07 | 0.55 |
| 38:DQ:108:GLY:O | 38:DQ:110:LEU:HB3 | 2.07 | 0.55 |
| 28:DE:29:GLY:H | 28:DE:51:PHE:HE1 | 1.53 | 0.55 |
| 28:DE:38:THR:O | 28:DE:42:ASP:HB2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 28:DE:50:GLY:O | 28:DE:51:PHE:HB2 | 2.07 | 0.55 |
| 1:CA:979:C:C5 | 1:CA:980:C:C6 | 2.95 | 0.55 |
| 52:B6:39:TYR:O | 52:B6:47:THR:N | 2.39 | 0.55 |
| 52:B6:40:CYS:SG | 52:B6:45:LYS:HE2 | 2.47 | 0.55 |
| 35:BO:11:GLY:C | 35:BO:13:ASN:N | 2.60 | 0.55 |
| 21:AX:15:ARG:HG2 | 21:AX:15:ARG:NH1 | 1.99 | 0.55 |
| 50:B4:50:VAL:O | 50:B4:50:VAL:HG12 | 2.06 | 0.55 |
| 25:BA:1798:U:C5' | 27:BD:259:THR:HG22 | 2.27 | 0.55 |
| 26:BB:32:C:C2 | 26:BB:51:G:N2 | 2.75 | 0.55 |
| 19:CV:23:ASN:HA | 19:CV:27:GLU:CG | 2.36 | 0.55 |
| 19:CV:31:ILE:CG2 | 19:CV:33:THR:HG22 | 2.37 | 0.55 |
| 1:AA:985:C:C2 | 1:AA:1221:G:N2 | 2.75 | 0.55 |
| 1:AA:1278:U:H5' | 1:AA:1279:A:O4' | 2.06 | 0.55 |
| 22:AB:45:U:H3' | 22:AB:45:U:H6 | 1.71 | 0.55 |
| 1:CA:792:A:H4' | 1:CA:793:U:O5' | 2.07 | 0.55 |
| 2:AE:82:ARG:HG2 | 2:AE:92:TYR:CZ | 2.42 | 0.55 |
| 7:CJ:72:ARG:NH2 | 7:CJ:96:GLN:HE22 | 2.05 | 0.55 |
| 25:DA:244:A:C2 | 25:DA:255:A:C4 | 2.95 | 0.55 |
| 25:DA:107:C:H2' | 25:DA:108:U:H6 | 1.72 | 0.55 |
| 25:DA:1520:U:H2' | 25:DA:1521:G:O4' | 2.06 | 0.55 |
| 38:DQ:34:HIS:ND1 | 38:DQ:53:SER:HB3 | 2.22 | 0.55 |
| 27:BD:108:PRO:HD2 | 27:BD:111:LEU:HG | 1.88 | 0.55 |
| 25:BA:1111:A:O2' | 25:BA:1112:G:H4' | 2.06 | 0.55 |
| 3:AF:84:ILE:O | 3:AF:88:ARG:HG3 | 2.07 | 0.55 |
| 25:BA:1430:C:H2' | 25:BA:1431:U:C6 | 2.42 | 0.55 |
| 54:D8:35:GLN:C | 54:D8:36:LYS:CG | 2.76 | 0.55 |
| 54:D8:52:LYS:O | 54:D8:54:GLU:N | 2.32 | 0.55 |
| 38:DQ:87:PHE:HD2 | 38:DQ:87:PHE:C | 2.10 | 0.55 |
| 25:DA:1226:G:H5' | 41:D2:85:LYS:H | 1.72 | 0.55 |
| 27:BD:71:ASP:HB3 | 27:BD:103:ARG:NH2 | 2.21 | 0.55 |
| 25:BA:2404:C:O3' | 35:BO:77:ARG:NH2 | 2.39 | 0.55 |
| 28:DE:48:GLN:O | 28:DE:49:LEU:CD1 | 2.55 | 0.55 |
| 28:DE:79:ARG:O | 28:DE:80:GLU:CG | 2.54 | 0.55 |
| 39:DR:91:ARG:O | 39:DR:116:ALA:HA | 2.07 | 0.55 |
| 26:DB:3:C:H5' | 26:DB:4:C:OP2 | 2.05 | 0.55 |
| 1:CA:1301:U:H2' | 1:CA:1301:U:O2 | 2.05 | 0.55 |
| 5:CH:135:THR:O | 5:CH:138:ALA:HB3 | 2.07 | 0.55 |
| 27:BD:26:LYS:O | 27:BD:27:THR:OG1 | 2.25 | 0.55 |
| 25:BA:1533:C:H42 | 25:BA:1538:G:H1 | 1.55 | 0.55 |
| 31:BH:152:ARG:NH2 | 31:BH:153:LYS:HE2 | 2.22 | 0.55 |
| 32:BK:5:LEU:HD22 | 32:BK:9:LEU:HD21 | 1.89 | 0.55 |
| 25:BA:1169:G:N2 | 25:BA:1181:C:C2 | 2.74 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:AO:6:THR:N | 12:AO:9:GLN:HE21 | 2.02 | 0.55 |
| 48:DW:9:GLN:NE2 | 48:DW:56:GLN:HG2 | 2.18 | 0.55 |
| 1:AA:475:G:H2' | 1:AA:476:G:O4' | 2.07 | 0.55 |
| 3:CF:16:ARG:HH11 | 3:CF:16:ARG:HA | 1.72 | 0.55 |
| 35:DO:136:GLU:O | 35:DO:139:LYS:N | 2.34 | 0.55 |
| 22:CB:46:G:H2' | 22:CB:47:C:C6 | 2.42 | 0.55 |
| 23:CD:21:U:C3' | 23:CD:22:A:H5'' | 2.36 | 0.55 |
| 32:DK:97:ILE:O | 32:DK:100:ALA:HB3 | 2.06 | 0.55 |
| 25:BA:2593:U:H2' | 25:BA:2594:C:H6 | 1.70 | 0.55 |
| 1:CA:93:U:H2' | 1:CA:95:G:H5'' | 1.89 | 0.55 |
| 25:DA:872:A:C4 | 25:DA:906:G:N2 | 2.74 | 0.55 |
| 1:AA:171:A:N6 | 1:AA:172:A:N6 | 2.54 | 0.55 |
| 39:DR:53:ARG:CG | 39:DR:53:ARG:O | 2.54 | 0.55 |
| 6:CI:69:GLU:O | 6:CI:72:VAL:HG12 | 2.07 | 0.55 |
| 34:BN:90:GLN:O | 34:BN:91:LEU:HB2 | 2.07 | 0.55 |
| 21:AX:12:LYS:HB3 | 21:AX:22:ARG:HD2 | 1.89 | 0.55 |
| 46:B3:51:VAL:HG21 | 46:B3:79:VAL:HG12 | 1.87 | 0.55 |
| 25:BA:2648:C:H2' | 25:BA:2649:U:C6 | 2.41 | 0.55 |
| 54:B8:10:ALA:C | 54:B8:12:LYS:H | 2.11 | 0.55 |
| 23:AC:17:C:C2' | 23:AC:18:C:H5'' | 2.37 | 0.55 |
| 23:AC:62:C:O2' | 23:AC:63:C:H5' | 2.06 | 0.55 |
| 1:CA:1022:G:H2' | 1:CA:1023:G:O4' | 2.07 | 0.55 |
| 25:BA:1899:G:HO2' | 25:BA:1900:A:P | 2.30 | 0.55 |
| 28:DE:36:ARG:HH11 | 28:DE:36:ARG:CG | 2.19 | 0.55 |
| 30:BG:64:THR:CG2 | 30:BG:66:GLN:H | 2.19 | 0.55 |
| 19:CV:80:TYR:CE1 | 19:CV:82:GLY:HA2 | 2.42 | 0.55 |
| 46:D3:18:ALA:CB | 46:D3:20:ARG:HE | 2.17 | 0.55 |
| 4:AG:31:CYS:HB3 | 4:AG:33:MET:HB2 | 1.88 | 0.55 |
| 30:DG:7:LEU:HB2 | 30:DG:104:GLU:OE1 | 2.06 | 0.55 |
| 17:CT:66:SER:O | 17:CT:70:ARG:NH1 | 2.40 | 0.55 |
| 25:BA:482:A:H4' | 44:BU:47:LYS:HD3 | 1.89 | 0.55 |
| 25:BA:507:A:C5' | 25:BA:508:G:H5' | 2.37 | 0.55 |
| 25:DA:2131:G:N2 | 25:DA:2158:A:H2' | 2.22 | 0.55 |
| 25:DA:654(D):G:N2 | 25:DA:654(Q):C:N3 | 2.52 | 0.55 |
| 34:DN:49:ARG:HD3 | 34:DN:49:ARG:N | 2.19 | 0.55 |
| 1:CA:168:G:C2' | 1:CA:169:C:H5'' | 2.37 | 0.55 |
| 35:BO:19:VAL:HG23 | 35:BO:27:HIS:HB3 | 1.87 | 0.55 |
| 24:A1:14:U:O2' | 24:A1:15:U:O4' | 2.24 | 0.55 |
| 25:BA:1600:C:O2' | 53:B7:49:ARG:HG2 | 2.07 | 0.55 |
| 25:DA:1246:A:O2' | 29:DF:45:ARG:NH2 | 2.39 | 0.55 |
| 3:CF:70:VAL:O | 3:CF:106:VAL:N | 2.38 | 0.55 |
| 25:DA:128:C:H2' | 25:DA:129:C:C6 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:AB:45:U:H2' | 22:AB:46:G:H5'' | 1.88 | 0.55 |
| 8:AK:95:VAL:HG21 | 8:AK:133:LEU:HD12 | 1.88 | 0.55 |
| 45:DV:112:ARG:HE | 45:DV:112:ARG:N | 2.04 | 0.55 |
| 1:CA:518:C:H4' | 1:CA:519:C:O5' | 2.07 | 0.55 |
| 1:CA:1438:G:H2' | 1:CA:1439:C:C6 | 2.42 | 0.55 |
| 1:CA:1075:C:OP1 | 2:CE:179:LYS:HE2 | 2.06 | 0.55 |
| 15:CR:44:LYS:O | 15:CR:47:LYS:HE2 | 2.06 | 0.55 |
| 25:DA:2591:C:H2' | 25:DA:2592:G:C8 | 2.42 | 0.55 |
| 25:DA:845:G:OP2 | 25:DA:845:G:H8 | 1.90 | 0.55 |
| 38:BQ:67:ARG:HB2 | 38:BQ:67:ARG:NH1 | 2.22 | 0.55 |
| 48:BW:16:LEU:HG | 48:BW:16:LEU:O | 2.07 | 0.55 |
| 52:D6:27:LYS:CB | 52:D6:27:LYS:HZ3 | 2.19 | 0.55 |
| 1:AA:1178:G:N2 | 1:AA:1181:G:N7 | 2.42 | 0.55 |
| 28:DE:37:ARG:HD2 | 28:DE:80:GLU:OE2 | 2.07 | 0.55 |
| 3:CF:146:ALA:HB1 | 3:CF:203:PHE:O | 2.07 | 0.55 |
| 25:DA:1342:A:C2 | 25:DA:1602:U:C4 | 2.94 | 0.55 |
| 1:CA:997:U:H2' | 1:CA:998:G:C8 | 2.41 | 0.55 |
| 26:DB:38:C:N3 | 26:DB:44:G:N2 | 2.48 | 0.55 |
| 27:DD:164:GLN:HG2 | 27:DD:166:GLN:NE2 | 2.22 | 0.55 |
| 26:DB:111:U:H2' | 26:DB:112:G:H8 | 1.70 | 0.55 |
| 5:CH:103:GLY:H | 5:CH:106:PRO:HG2 | 1.70 | 0.55 |
| 25:BA:2894:G:H2' | 25:BA:2895:U:OP2 | 2.07 | 0.55 |
| 36:DP:7:MET:HB3 | 36:DP:10:ARG:CZ | 2.37 | 0.55 |
| 25:DA:340:A:C2' | 25:DA:341:G:H5' | 2.36 | 0.55 |
| 22:AB:52:U:H2' | 22:AB:53:A:C5' | 2.37 | 0.55 |
| 30:BG:36:LYS:HG2 | 30:BG:38:VAL:HG23 | 1.89 | 0.55 |
| 1:AA:1237:C:C5 | 1:AA:1336:C:C5 | 2.95 | 0.55 |
| 4:CG:162:LEU:HD12 | 4:CG:181:MET:CE | 2.37 | 0.55 |
| 6:AI:3:ARG:HA | 6:AI:65:VAL:O | 2.07 | 0.55 |
| 30:DG:11:TYR:CZ | 30:DG:16:ARG:HD2 | 2.43 | 0.55 |
| 8:AK:9:MET:HG3 | 8:AK:26:VAL:HG21 | 1.89 | 0.55 |
| 32:DK:92:VAL:HB | 32:DK:120:ILE:HB | 1.88 | 0.55 |
| 25:BA:547:A:H2' | 25:BA:548:A:C8 | 2.42 | 0.55 |
| 1:CA:1350:A:C6 | 1:CA:1351:U:N3 | 2.75 | 0.55 |
| 25:DA:620:G:H5' | 25:DA:620:G:N3 | 2.22 | 0.55 |
| 25:DA:1443:G:H2' | 25:DA:1444:G:H5' | 1.89 | 0.55 |
| 3:CF:82:GLU:HA | 3:CF:85:ARG:HB2 | 1.87 | 0.55 |
| 39:BR:20:PRO:HG2 | 39:BR:86:ILE:O | 2.06 | 0.55 |
| 25:BA:1783:A:H5' | 25:BA:2608:G:H4' | 1.89 | 0.55 |
| 25:BA:1028:A:N6 | 25:BA:1125:G:H2' | 2.21 | 0.55 |
| 18:AU:73:ALA:HB3 | 18:AU:79:LEU:HD12 | 1.89 | 0.55 |
| 54:B8:11:LYS:HG2 | 54:B8:11:LYS:O | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 26:DB:53:A:H2' | 26:DB:54:G:O4' | 2.07 | 0.55 |
| 8:CK:66:GLY:O | 8:CK:76:PRO:HB3 | 2.07 | 0.55 |
| 25:DA:1956:U:H2' | 25:DA:1957:C:H5' | 1.89 | 0.55 |
| 41:D2:75:PHE:HD2 | 41:D2:81:TYR:CD1 | 2.25 | 0.54 |
| 25:DA:997:G:H2' | 25:DA:998:C:H5' | 1.89 | 0.54 |
| 23:AC:17:C:C3' | 23:AC:18:C:C5' | 2.68 | 0.54 |
| 25:BA:1900:A:C8 | 25:BA:1900:A:H5' | 2.38 | 0.54 |
| 35:BO:65:ARG:NH2 | 54:B8:15:LYS:HB2 | 2.11 | 0.54 |
| 29:BF:198:ALA:HA | 29:BF:201:VAL:CG1 | 2.28 | 0.54 |
| 19:AV:40:ILE:HD11 | 19:AV:62:ILE:HG21 | 1.89 | 0.54 |
| 50:B4:59:PHE:O | 50:B4:63:TYR:HB2 | 2.06 | 0.54 |
| 25:DA:882:G:N1 | 25:DA:894:C:N4 | 2.40 | 0.54 |
| 4:AG:31:CYS:C | 4:AG:33:MET:H | 2.10 | 0.54 |
| 26:DB:38:C:N4 | 26:DB:44:G:H1 | 2.02 | 0.54 |
| 38:BQ:14:VAL:O | 38:BQ:18:ILE:HD13 | 2.08 | 0.54 |
| 25:BA:1557:C:H5'' | 25:BA:1558:A:OP2 | 2.07 | 0.54 |
| 25:DA:607:U:O2 | 25:DA:621:A:N1 | 2.40 | 0.54 |
| 1:AA:827:U:O2 | 1:AA:827:U:O5' | 2.25 | 0.54 |
| 23:CD:27:G:C2' | 23:CD:28:U:H5' | 2.37 | 0.54 |
| 35:DO:34:GLY:O | 35:DO:35:HIS:C | 2.45 | 0.54 |
| 25:BA:1639:U:H2' | 25:BA:1640:C:H5' | 1.89 | 0.54 |
| 2:CE:92:TYR:HD2 | 2:CE:92:TYR:C | 2.10 | 0.54 |
| 35:BO:39:LYS:CB | 35:BO:45:LEU:HD22 | 2.37 | 0.54 |
| 13:CP:54:VAL:HG12 | 13:CP:58:GLU:OE1 | 2.07 | 0.54 |
| 8:AK:21:LYS:O | 8:AK:65:TYR:OH | 2.20 | 0.54 |
| 30:BG:107:LEU:HD21 | 30:BG:178:PHE:CE1 | 2.42 | 0.54 |
| 25:BA:2312:U:H6 | 25:BA:2312:U:O5' | 1.89 | 0.54 |
| 23:AC:48:U:H4' | 23:AC:49:C:C5' | 2.37 | 0.54 |
| 1:AA:1073:U:OP2 | 5:AH:57:LYS:NZ | 2.38 | 0.54 |
| 1:CA:342:C:H2' | 1:CA:343:U:H5' | 1.89 | 0.54 |
| 25:DA:389:G:H1 | 35:DO:71:VAL:HG12 | 1.72 | 0.54 |
| 20:CW:29:LYS:O | 20:CW:33:ILE:HG12 | 2.07 | 0.54 |
| 20:CW:10:LEU:O | 20:CW:10:LEU:HD22 | 2.07 | 0.54 |
| 29:DF:184:TYR:O | 29:DF:188:ARG:HB2 | 2.08 | 0.54 |
| 25:DA:2698:U:H2' | 25:DA:2699:C:C6 | 2.41 | 0.54 |
| 25:BA:445:C:O2' | 25:BA:446:G:H5' | 2.07 | 0.54 |
| 25:BA:21:A:O2' | 25:BA:22:C:H5' | 2.07 | 0.54 |
| 29:BF:129:PHE:O | 29:BF:130:ALA:HB3 | 2.07 | 0.54 |
| 30:DG:97:ASP:HA | 30:DG:100:TRP:HB2 | 1.89 | 0.54 |
| 24:C1:17:U:O2' | 24:C1:18:G:H5' | 2.07 | 0.54 |
| 1:AA:625:G:H4' | 16:AS:16:HIS:HD2 | 0.46 | 0.54 |
| 47:BZ:83:GLU:HG2 | 47:BZ:85:LEU:H | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:BD:181:GLU:CG | 27:BD:272:ALA:HB3 | 2.34 | 0.54 |
| 1:AA:1177:G:C8 | 1:AA:1178:G:C2 | 2.96 | 0.54 |
| 41:D2:81:TYR:C | 41:D2:82:ARG:CG | 2.70 | 0.54 |
| 25:BA:2415:G:H4' | 35:BO:66:GLY:CA | 2.37 | 0.54 |
| 13:AP:8:GLU:O | 13:AP:10:PRO:HD3 | 2.07 | 0.54 |
| 25:DA:2402:C:H41 | 25:DA:2416:C:H1' | 1.71 | 0.54 |
| 22:CB:17:U:H5'' | 22:CB:18:G:H8 | 1.68 | 0.54 |
| 1:AA:1004:A:O5' | 1:AA:1025:U:O4 | 2.25 | 0.54 |
| 1:AA:1059:C:O3' | 14:AQ:45:ARG:NH2 | 2.40 | 0.54 |
| 38:DQ:25:ARG:CZ | 38:DQ:40:ILE:HD12 | 2.36 | 0.54 |
| 31:BH:153:LYS:HZ2 | 31:BH:153:LYS:HA | 1.72 | 0.54 |
| 1:AA:16:A:C2' | 1:AA:17:U:H5' | 2.38 | 0.54 |
| 19:AV:65:ASN:HB3 | 50:B4:55:ARG:HH12 | 1.72 | 0.54 |
| 28:DE:14:ILE:HD11 | 28:DE:173:VAL:HG11 | 1.89 | 0.54 |
| 29:BF:63:LYS:CE | 29:BF:67:GLN:HB2 | 2.37 | 0.54 |
| 3:AF:131:ARG:NH1 | 3:AF:166:GLU:OE2 | 2.40 | 0.54 |
| 1:AA:503:C:OP2 | 12:AO:116:SER:OG | 2.16 | 0.54 |
| 45:DV:134:PRO:HG3 | 45:DV:158:PRO:HG3 | 1.89 | 0.54 |
| 23:CD:52:C:H2' | 23:CD:53:G:H8 | 1.72 | 0.54 |
| 1:CA:197:A:C6 | 1:CA:221:C:H4' | 2.42 | 0.54 |
| 25:BA:373:U:H1' | 25:BA:423:A:N3 | 2.21 | 0.54 |
| 1:CA:1386:G:N3 | 1:CA:1387:G:C8 | 2.76 | 0.54 |
| 51:B5:52:TYR:HD1 | 51:B5:53:ALA:H | 1.54 | 0.54 |
| 25:BA:265:A:H1' | 25:BA:266:G:O4' | 2.07 | 0.54 |
| 45:DV:103:ARG:HB2 | 45:DV:137:ILE:O | 2.07 | 0.54 |
| 36:BP:12:GLN:HG2 | 36:BP:73:PRO:HD2 | 1.88 | 0.54 |
| 20:CW:30:LYS:HG2 | 20:CW:80:ARG:HH22 | 1.71 | 0.54 |
| 1:AA:580:U:H2' | 1:AA:581:G:O4' | 2.08 | 0.54 |
| 1:CA:1465:C:H2' | 1:CA:1466:C:O4' | 2.07 | 0.54 |
| 25:DA:1942:C:OP2 | 25:DA:1943:U:O2' | 2.21 | 0.54 |
| 25:BA:2543:G:H2' | 25:BA:2544:G:C8 | 2.42 | 0.54 |
| 40:D1:98:LEU:O | 40:D1:99:ALA:CB | 2.55 | 0.54 |
| 28:BE:3:GLY:HA3 | 28:BE:81:ILE:CD1 | 2.37 | 0.54 |
| 1:CA:1021:G:H2' | 1:CA:1022:G:O4' | 2.07 | 0.54 |
| 44:BU:81:LYS:CG | 44:BU:96:ILE:HB | 2.37 | 0.54 |
| 26:DB:104:A:OP1 | 45:DV:72:ARG:NH2 | 2.40 | 0.54 |
| 25:DA:2415:G:H4' | 35:DO:66:GLY:CA | 2.37 | 0.54 |
| 25:DA:270(I):G:H1 | 25:DA:270(Q):C:N4 | 2.03 | 0.54 |
| 1:AA:1002:G:H2' | 1:AA:1003:G:C8 | 2.41 | 0.54 |
| 1:AA:1004:A:O5' | 1:AA:1025:U:C4 | 2.61 | 0.54 |
| 1:CA:516:U:C4 | 1:CA:517:G:C6 | 2.95 | 0.54 |
| 1:CA:631:G:H4' | 1:CA:632:A:OP1 | 2.05 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 50:D4:12:ALA:H | 50:D4:24:THR:HG21 | 1.72 | 0.54 |
| 25:DA:310:A:OP1 | 44:DU:17:SER:O | 2.24 | 0.54 |
| 44:DU:19:LYS:HE3 | 44:DU:71:LYS:NZ | 2.22 | 0.54 |
| 33:BM:96:GLU:H | 33:BM:98:VAL:HG12 | 1.73 | 0.54 |
| 35:DO:127:ALA:O | 35:DO:147:LEU:N | 2.35 | 0.54 |
| 2:CE:92:TYR:C | 2:CE:92:TYR:CD2 | 2.80 | 0.54 |
| 40:B1:79:PHE:O | 40:B1:79:PHE:CD2 | 2.56 | 0.54 |
| 1:AA:693:G:C4 | 24:A1:13:U:H1' | 2.43 | 0.54 |
| 25:BA:1164:G:H2' | 25:BA:1165:U:C6 | 2.43 | 0.54 |
| 25:BA:1203:G:H3' | 25:BA:1204:A:H5'' | 1.90 | 0.54 |
| 32:DK:77:LEU:CG | 32:DK:78:THR:N | 2.70 | 0.54 |
| 3:CF:29:TYR:HD1 | 14:CQ:36:PHE:CZ | 2.26 | 0.54 |
| 12:AO:24:VAL:HG13 | 12:AO:98:TYR:HE2 | 1.71 | 0.54 |
| 45:DV:148:ASP:CG | 45:DV:149:SER:H | 2.10 | 0.54 |
| 17:AT:82:MET:O | 17:AT:86:GLU:HB2 | 2.07 | 0.54 |
| 1:AA:375:U:O3' | 16:AS:6:LEU:HB2 | 2.07 | 0.54 |
| 6:CI:11:ASN:O | 6:CI:14:LEU:HD22 | 2.07 | 0.54 |
| 4:CG:60:GLU:OE2 | 4:CG:198:VAL:HA | 2.06 | 0.54 |
| 51:D5:52:TYR:O | 51:D5:53:ALA:HB3 | 2.07 | 0.54 |
| 25:DA:2840:C:H5'' | 37:D0:53:HIS:CD2 | 2.42 | 0.54 |
| 33:BM:26:LEU:O | 33:BM:30:ILE:HG13 | 2.07 | 0.54 |
| 1:CA:930:C:C4 | 1:CA:931:C:C5 | 2.95 | 0.54 |
| 18:AU:88:LYS:HB3 | 18:AU:88:LYS:NZ | 2.23 | 0.54 |
| 13:AP:57:ARG:HB2 | 13:AP:57:ARG:HH11 | 1.72 | 0.54 |
| 36:BP:48:GLU:HG3 | 36:BP:48:GLU:O | 2.06 | 0.54 |
| 27:DD:35:LYS:CE | 27:DD:64:ILE:C | 2.70 | 0.54 |
| 47:DZ:86:SER:N | 47:DZ:87:PRO:CD | 2.70 | 0.54 |
| 25:DA:2748:A:H62 | 25:DA:2754:U:H3 | 1.52 | 0.54 |
| 19:AV:41:VAL:CG2 | 19:AV:67:VAL:HA | 2.37 | 0.54 |
| 25:DA:2271:G:H5'' | 46:D3:20:ARG:NE | 2.21 | 0.54 |
| 13:CP:22:ILE:HD12 | 13:CP:25:ILE:HG13 | 1.87 | 0.54 |
| 1:CA:1128:C:H5'' | 9:CL:16:ARG:HH22 | 1.72 | 0.54 |
| 1:CA:1129:C:OP2 | 9:CL:62:TYR:OH | 2.22 | 0.54 |
| 25:BA:1434:A:N6 | 25:BA:1558:A:N6 | 2.47 | 0.54 |
| 25:DA:2135:A:O2' | 25:DA:2160:G:H4' | 2.08 | 0.54 |
| 20:AW:50:GLU:HA | 20:AW:100:ILE:HG22 | 1.89 | 0.54 |
| 25:DA:2689:U:H4' | 25:DA:2690:C:H5' | 1.90 | 0.54 |
| 1:AA:1287:A:H2' | 1:AA:1288:A:C8 | 2.42 | 0.54 |
| 25:DA:2262:U:P | 46:D3:19:LYS:HZ3 | 2.29 | 0.54 |
| 25:DA:1278:A:C5' | 37:D0:36:THR:HG22 | 2.37 | 0.54 |
| 50:B4:37:SER:CB | 50:B4:42:PHE:CD1 | 2.90 | 0.54 |
| 22:AB:16:U:C2 | 22:AB:70:G:N2 | 2.76 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 25:DA:2893:G:H5' | 25:DA:2894:G:OP1 | 2.06 | 0.54 |
| 23:AD:13:C:O2' | 23:AD:14:A:P | 2.65 | 0.54 |
| 23:AD:49:C:C6 | 23:AD:49:C:OP2 | 2.59 | 0.54 |
| 1:AA:166:G:O2' | 1:AA:167:G:H5' | 2.06 | 0.54 |
| 25:DA:2219:G:C2' | 25:DA:2224:G:H5' | 2.38 | 0.54 |
| 25:DA:1011:G:H1 | 25:DA:1150:C:H42 | 1.55 | 0.54 |
| 4:CG:153:ARG:HD3 | 4:CG:181:MET:SD | 2.48 | 0.54 |
| 1:AA:721:G:C6 | 1:AA:733:A:C2 | 2.95 | 0.54 |
| 1:CA:688:G:H2' | 1:CA:689:C:H6 | 1.72 | 0.54 |
| 34:DN:68:GLU:CA | 34:DN:78:ARG:HB3 | 2.38 | 0.54 |
| 25:DA:900:A:H2' | 25:DA:900:A:N3 | 2.22 | 0.54 |
| 1:AA:324:G:N1 | 1:AA:327:A:OP2 | 2.40 | 0.54 |
| 31:DH:94:TYR:N | 31:DH:94:TYR:CD1 | 2.76 | 0.54 |
| 14:CQ:12:ARG:CZ | 14:CQ:14:PRO:HG2 | 2.37 | 0.54 |
| 25:DA:94:G:H2' | 25:DA:95:G:O4' | 2.07 | 0.54 |
| 1:AA:1016:A:H2' | 1:AA:1017:G:O4' | 2.07 | 0.54 |
| 25:DA:1668:A:N3 | 25:DA:1670:C:C4 | 2.76 | 0.54 |
| 12:CO:68:ALA:CB | 12:CO:85:ILE:HD11 | 2.37 | 0.54 |
| 5:CH:100:VAL:HG12 | 5:CH:100:VAL:O | 2.06 | 0.54 |
| 1:AA:1129:C:N3 | 1:AA:1139:G:O6 | 2.40 | 0.54 |
| 25:DA:270(S):G:H5'' | 47:DZ:94:LEU:HD21 | 1.90 | 0.54 |
| 1:AA:1004:A:OP1 | 1:AA:1025:U:O4 | 2.24 | 0.54 |
| 1:CA:1129:C:N4 | 1:CA:1139:G:C2 | 2.76 | 0.54 |
| 30:BG:133:LEU:HD23 | 30:BG:157:ILE:HB | 1.89 | 0.54 |
| 1:CA:130:A:C8 | 17:CT:63:ARG:HG3 | 2.43 | 0.54 |
| 41:D2:28:GLU:HB3 | 41:D2:29:PRO:HD2 | 1.89 | 0.54 |
| 20:AW:39:LYS:HB2 | 20:AW:55:ILE:HG21 | 1.89 | 0.54 |
| 25:BA:1937:A:C2' | 25:BA:1938:A:OP1 | 2.55 | 0.54 |
| 33:DM:30:ILE:HG22 | 33:DM:34:LEU:HD22 | 1.89 | 0.54 |
| 25:DA:1138:G:H21 | 33:DM:106:MET:CE | 2.19 | 0.54 |
| 32:DK:78:THR:CB | 32:DK:104:GLN:HE22 | 2.20 | 0.54 |
| 1:CA:1014:A:H4' | 19:CV:14:HIS:CE1 | 2.43 | 0.54 |
| 29:DF:39:TRP:CH2 | 29:DF:106:ARG:HD3 | 2.42 | 0.54 |
| 4:CG:42:GLN:HG3 | 4:CG:43:HIS:CD2 | 2.42 | 0.54 |
| 1:AA:1101:A:H4' | 1:AA:1102:A:O5' | 2.08 | 0.54 |
| 25:BA:856:C:C6 | 25:BA:856:C:H3' | 2.43 | 0.54 |
| 25:DA:1101:U:H2' | 25:DA:1102:C:C6 | 2.41 | 0.54 |
| 32:DK:27:ARG:HG2 | 47:DZ:71:TYR:CZ | 2.43 | 0.54 |
| 4:AG:101:LEU:HD23 | 4:AG:121:VAL:HG11 | 1.90 | 0.54 |
| 1:CA:999:U:H2' | 1:CA:1000:A:C8 | 2.42 | 0.54 |
| 33:DM:56:ASN:H | 33:DM:125:GLY:HA3 | 1.72 | 0.54 |
| 1:CA:1194:U:H2' | 1:CA:1195:C:C6 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 47:DZ:62:VAL:HG21 | 47:DZ:70:VAL:HG21 | 1.90 | 0.54 |
| 2:AE:197:VAL:HG12 | 2:AE:200:ILE:HG13 | 1.89 | 0.54 |
| 7:AJ:6:ARG:HG2 | 7:AJ:6:ARG:O | 2.08 | 0.54 |
| 13:CP:10:PRO:HG3 | 13:CP:18:ALA:O | 2.07 | 0.54 |
| 3:AF:113:ALA:HB3 | 3:AF:114:PRO:HD3 | 1.89 | 0.54 |
| 28:BE:63:LEU:O | 28:BE:63:LEU:HD23 | 2.07 | 0.54 |
| 1:CA:1034:G:H2' | 1:CA:1035:A:C8 | 2.43 | 0.54 |
| 19:AV:41:VAL:HG13 | 19:AV:44:MET:HB2 | 1.89 | 0.54 |
| 43:DT:30:VAL:HG11 | 43:DT:39:ILE:HG12 | 1.90 | 0.54 |
| 1:AA:57:G:H2' | 1:AA:58:C:H6 | 1.70 | 0.54 |
| 25:DA:1022:G:C6 | 25:DA:1140:C:C4 | 2.95 | 0.54 |
| 29:DF:20:LEU:HD13 | 29:DF:203:GLN:OE1 | 2.07 | 0.54 |
| 54:B8:36:LYS:O | 54:B8:37:SER:C | 2.45 | 0.54 |
| 23:CD:55:U:C4 | 23:CD:56:U:H5 | 2.25 | 0.54 |
| 25:BA:1022:G:H22 | 25:BA:1142(A):A:H2 | 1.47 | 0.54 |
| 1:AA:201:C:N3 | 1:AA:216:G:N2 | 2.54 | 0.54 |
| 25:DA:903:C:O2' | 45:DV:168:GLU:HG2 | 2.08 | 0.54 |
| 45:DV:141:VAL:CG2 | 45:DV:150:LEU:HG | 2.37 | 0.54 |
| 12:CO:60:LEU:HB2 | 12:CO:64:TYR:HB2 | 1.89 | 0.54 |
| 35:BO:49:ARG:HD2 | 54:B8:58:ILE:HG21 | 1.88 | 0.54 |
| 1:CA:149:A:O2' | 1:CA:150:C:H5' | 2.08 | 0.54 |
| 1:AA:1126:U:H5 | 1:AA:1127:G:N3 | 2.06 | 0.54 |
| 1:AA:166:G:H2' | 1:AA:167:G:H8 | 1.71 | 0.54 |
| 25:BA:270(F):U:H2' | 25:BA:270(G):C:H6 | 1.71 | 0.54 |
| 25:DA:686:G:N7 | 53:D7:5:TRP:CH2 | 2.76 | 0.54 |
| 32:BK:114:LEU:O | 32:BK:115:ALA:CB | 2.55 | 0.54 |
| 28:DE:60:ASN:O | 28:DE:62:PRO:HD3 | 2.08 | 0.54 |
| 26:DB:55:U:HO2' | 30:DG:29:TRP:HD1 | 1.53 | 0.54 |
| 1:CA:1014:A:H4' | 19:CV:14:HIS:ND1 | 2.22 | 0.54 |
| 1:AA:1225:A:N3 | 1:AA:1225:A:H2' | 2.22 | 0.54 |
| 25:BA:2189:U:C3' | 25:BA:2190:G:H5'' | 2.37 | 0.54 |
| 25:BA:1436:G:H1' | 25:BA:1477:A:O2' | 2.07 | 0.54 |
| 13:CP:108:ARG:HH11 | 13:CP:108:ARG:HG3 | 1.72 | 0.54 |
| 31:DH:166:GLY:O | 31:DH:167:GLU:HG2 | 2.06 | 0.54 |
| 1:CA:457:C:H2' | 1:CA:458:C:H6 | 1.73 | 0.54 |
| 27:DD:228:PRO:HG3 | 27:DD:234:GLY:O | 2.06 | 0.54 |
| 25:DA:2511:U:O4 | 25:DA:2575:C:N3 | 2.41 | 0.54 |
| 25:BA:1942:C:OP2 | 25:BA:1943:U:O2' | 2.20 | 0.54 |
| 1:CA:664:G:H22 | 1:CA:741:G:H1 | 1.55 | 0.54 |
| 12:AO:89:ARG:HH11 | 12:AO:89:ARG:CG | 2.20 | 0.54 |
| 35:DO:75:ILE:H | 35:DO:75:ILE:HD13 | 1.71 | 0.54 |
| 49:BX:40:THR:O | 49:BX:44:ARG:HB2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 36:DP:105:GLU:HG2 | 36:DP:105:GLU:O | 2.06 | 0.54 |
| 4:AG:10:ARG:NH1 | 4:AG:10:ARG:HB2 | 2.23 | 0.54 |
| 25:DA:2059:A:H2 | 25:DA:2062:A:H61 | 1.54 | 0.54 |
| 1:CA:977:A:H2 | 1:CA:1224:G:C6 | 2.26 | 0.54 |
| 1:AA:1305:G:C5' | 21:AX:4:GLY:HA3 | 2.38 | 0.54 |
| 22:CB:70:G:H2' | 22:CB:71:U:C6 | 2.43 | 0.54 |
| 1:AA:346:G:H5' | 39:BR:41:ARG:HG2 | 1.90 | 0.54 |
| 4:AG:65:ARG:HH11 | 4:AG:65:ARG:CG | 2.20 | 0.54 |
| 25:BA:889:C:C3' | 25:BA:890:A:H4' | 2.37 | 0.54 |
| 28:BE:103:ASP:OD1 | 28:BE:201:THR:HA | 2.07 | 0.54 |
| 31:BH:83:TYR:CB | 31:BH:134:SER:HA | 2.37 | 0.54 |
| 22:AB:85:C:N4 | 25:BA:2508:G:H5' | 2.23 | 0.54 |
| 32:BK:100:ALA:O | 32:BK:101:LEU:C | 2.46 | 0.54 |
| 1:AA:397:A:N7 | 1:AA:548:G:C8 | 2.76 | 0.54 |
| 45:DV:128:VAL:HG22 | 45:DV:129:SER:N | 2.18 | 0.54 |
| 20:AW:89:ARG:HD2 | 20:AW:104:LEU:HD21 | 1.90 | 0.54 |
| 6:AI:8:ILE:HD11 | 6:AI:79:LEU:HD13 | 1.88 | 0.54 |
| 3:AF:131:ARG:HB2 | 3:AF:131:ARG:CZ | 2.38 | 0.54 |
| 9:AL:4:TYR:CG | 9:AL:88:TYR:HB2 | 2.43 | 0.54 |
| 1:AA:153:C:H42 | 1:AA:168:G:H1 | 1.56 | 0.54 |
| 36:DP:21:THR:HG22 | 36:DP:21:THR:O | 2.07 | 0.54 |
| 7:CJ:79:ARG:HG2 | 7:CJ:84:ASN:ND2 | 2.23 | 0.54 |
| 4:CG:178:VAL:C | 4:CG:180:GLY:H | 2.11 | 0.54 |
| 4:AG:29:PRO:O | 4:AG:30:LYS:HD3 | 2.08 | 0.54 |
| 25:BA:1734:C:C2' | 25:BA:1735:C:H5'' | 2.38 | 0.54 |
| 43:BT:12:VAL:HG13 | 43:BT:27:THR:O | 2.08 | 0.54 |
| 49:DX:43:ILE:O | 49:DX:47:VAL:HG23 | 2.07 | 0.54 |
| 22:AB:45:U:C2' | 22:AB:46:G:H5'' | 2.37 | 0.54 |
| 11:AN:81:ASP:HB3 | 11:AN:107:SER:OG | 2.07 | 0.54 |
| 25:BA:2121:G:H2' | 25:BA:2122:U:O4' | 2.08 | 0.54 |
| 1:AA:859:A:H2' | 1:AA:860:A:C8 | 2.42 | 0.54 |
| 25:BA:2099:U:H3 | 25:BA:2190:G:H1 | 1.56 | 0.54 |
| 48:BW:64:LEU:HD22 | 48:BW:64:LEU:O | 2.08 | 0.54 |
| 25:DA:1472:A:C2' | 25:DA:1473:G:H5' | 2.37 | 0.54 |
| 1:CA:1365:G:H2' | 1:CA:1366:C:O4' | 2.08 | 0.54 |
| 34:DN:92:GLU:OE1 | 34:DN:113:LYS:NZ | 2.38 | 0.54 |
| 1:CA:1106:G:C2 | 1:CA:1107:C:C6 | 2.95 | 0.54 |
| 1:AA:1230:C:H2' | 1:AA:1231:G:H8 | 1.72 | 0.54 |
| 25:BA:1054:A:H2' | 25:BA:1055:G:C8 | 2.43 | 0.54 |
| 19:AV:30:LEU:O | 19:AV:30:LEU:HD22 | 2.08 | 0.54 |
| 26:DB:1:U:H3 | 26:DB:119:A:H2 | 1.55 | 0.54 |
| 32:BK:144:VAL:HG22 | 32:BK:145:VAL:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 37:D0:75:LEU:HD13 | 37:D0:75:LEU:O | 2.08 | 0.54 |
| 25:BA:1062:G:OP1 | 25:BA:1070:A:H4' | 2.08 | 0.54 |
| 25:BA:1083:U:C3' | 25:BA:1084:A:H5'' | 2.38 | 0.54 |
| 25:DA:2377:A:H4' | 38:DQ:111:GLU:O | 2.08 | 0.54 |
| 38:DQ:85:VAL:HG12 | 38:DQ:86:ALA:N | 2.22 | 0.54 |
| 28:BE:46:ALA:C | 28:BE:47:VAL:HG22 | 2.27 | 0.54 |
| 1:CA:1007:C:C2 | 1:CA:1023:G:N2 | 2.75 | 0.54 |
| 25:DA:2401:U:C2' | 25:DA:2402:C:H5'' | 2.37 | 0.54 |
| 1:AA:1004:A:H8 | 1:AA:1036:G:C2 | 2.26 | 0.54 |
| 1:AA:1036:G:C8 | 1:AA:1037:C:N3 | 2.76 | 0.54 |
| 46:B3:23:VAL:HG13 | 46:B3:38:VAL:HG23 | 1.89 | 0.54 |
| 31:DH:4:ILE:HD12 | 31:DH:6:ARG:CZ | 2.38 | 0.54 |
| 36:DP:78:PRO:O | 36:DP:79:LEU:CG | 2.56 | 0.54 |
| 6:CI:60:PHE:O | 6:CI:61:LEU:HD12 | 2.07 | 0.54 |
| 1:CA:363:A:OP1 | 12:CO:33:ARG:HG3 | 2.07 | 0.54 |
| 6:CI:87:ARG:NH1 | 6:CI:87:ARG:CG | 2.63 | 0.54 |
| 2:AE:201:ILE:HG21 | 2:AE:214:ILE:HG21 | 1.89 | 0.54 |
| 29:DF:8:GLN:NE2 | 29:DF:8:GLN:O | 2.40 | 0.54 |
| 13:AP:3:ARG:HG2 | 13:AP:9:ILE:HG12 | 1.90 | 0.54 |
| 1:CA:1372:U:H2' | 1:CA:1373:G:C5' | 2.38 | 0.54 |
| 13:CP:110:ARG:HG3 | 13:CP:110:ARG:HH11 | 1.72 | 0.54 |
| 14:CQ:37:PHE:CE1 | 14:CQ:53:LEU:HD13 | 2.43 | 0.54 |
| 5:AH:84:PHE:CB | 5:AH:134:ALA:HB2 | 2.37 | 0.54 |
| 1:CA:1207:G:C6 | 1:CA:1208:C:C4 | 2.96 | 0.54 |
| 1:CA:1077:G:N2 | 1:CA:1080:A:OP2 | 2.40 | 0.54 |
| 1:AA:878:G:H5' | 8:AK:89:PRO:HG2 | 1.90 | 0.54 |
| 14:CQ:13:THR:N | 14:CQ:14:PRO:CD | 2.71 | 0.54 |
| 25:BA:389:G:H22 | 35:BO:72:PRO:HD3 | 1.72 | 0.54 |
| 25:BA:495:G:O2' | 42:BS:62:HIS:HE1 | 1.91 | 0.54 |
| 6:CI:24:GLU:O | 6:CI:28:ARG:HD2 | 2.08 | 0.54 |
| 48:BW:16:LEU:C | 48:BW:16:LEU:HD12 | 2.28 | 0.54 |
| 33:BM:90:MET:HA | 33:BM:93:THR:HG22 | 1.89 | 0.54 |
| 25:BA:2019:A:H2' | 25:BA:2020:A:O5' | 2.06 | 0.54 |
| 26:BB:116:G:H5'' | 38:BQ:55:ALA:HB2 | 1.90 | 0.54 |
| 37:D0:97:VAL:HG22 | 37:D0:114:VAL:HG22 | 1.89 | 0.54 |
| 45:DV:16:SER:O | 45:DV:20:ARG:HG3 | 2.07 | 0.54 |
| 25:DA:274:G:OP1 | 25:DA:274:G:C8 | 2.60 | 0.54 |
| 36:BP:26:TYR:HE2 | 36:BP:28:ALA:HB2 | 1.72 | 0.54 |
| 22:AB:5:A:H61 | 22:AB:79:U:H3 | 1.56 | 0.54 |
| 30:DG:110:ALA:HA | 30:DG:140:ILE:O | 2.08 | 0.54 |
| 25:BA:2320:A:H2' | 25:BA:2320:A:N3 | 2.23 | 0.54 |
| 11:AN:86:GLY:N | 11:AN:112:THR:OG1 | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 27:BD:206:LEU:HA | 27:BD:211:ARG:NH1 | 2.23 | 0.54 |
| 38:DQ:87:PHE:HD1 | 38:DQ:112:PHE:CD2 | 2.26 | 0.54 |
| 40:D1:40:PHE:HZ | 41:D2:81:TYR:CE2 | 2.26 | 0.54 |
| 25:DA:1003:G:N2 | 25:DA:1153:C:C2 | 2.76 | 0.54 |
| 25:BA:2783:G:H2' | 25:BA:2784:C:C6 | 2.42 | 0.54 |
| 23:CC:15:G:C2 | 23:CC:60:A:C2 | 2.96 | 0.54 |
| 45:DV:144:LEU:C | 45:DV:146:ILE:N | 2.61 | 0.54 |
| 13:AP:23:TYR:CE1 | 13:AP:71:ARG:HG3 | 2.43 | 0.54 |
| 19:AV:41:VAL:O | 50:B4:63:TYR:CZ | 2.61 | 0.54 |
| 25:DA:1019:U:H2' | 25:DA:1020:A:C8 | 2.43 | 0.54 |
| 25:BA:1728:G:C2 | 25:BA:1730:U:OP2 | 2.61 | 0.54 |
| 1:CA:1330:U:O4 | 1:CA:1331:G:C2 | 2.61 | 0.54 |
| 4:AG:33:MET:HE2 | 4:AG:37:PRO:HA | 1.90 | 0.54 |
| 43:BT:84:ALA:HB3 | 43:BT:87:GLN:NE2 | 2.22 | 0.54 |
| 1:AA:690:G:H2' | 1:AA:691:G:O4' | 2.08 | 0.54 |
| 25:BA:574:C:H4' | 25:BA:575:A:O5' | 2.08 | 0.54 |
| 25:DA:2689:U:C4' | 25:DA:2690:C:OP2 | 2.50 | 0.54 |
| 15:AR:87:ILE:CG2 | 15:AR:88:ARG:N | 2.67 | 0.54 |
| 28:DE:116:VAL:O | 28:DE:117:MET:CB | 2.51 | 0.54 |
| 34:BN:48:PRO:O | 34:BN:49:ARG:HB2 | 2.08 | 0.54 |
| 23:AD:22:A:C2 | 23:AD:47:G:H2' | 2.43 | 0.54 |
| 25:DA:1204:A:N1 | 25:DA:1241:A:C2 | 2.76 | 0.54 |
| 27:DD:5:LYS:HB2 | 27:DD:5:LYS:HZ2 | 1.70 | 0.54 |
| 51:B5:41:PRO:O | 51:B5:44:THR:OG1 | 2.26 | 0.54 |
| 25:BA:588:U:C2 | 29:BF:90:PHE:CE1 | 2.96 | 0.54 |
| 16:CS:48:TRP:CE3 | 16:CS:49:LEU:HB2 | 2.42 | 0.54 |
| 16:CS:49:LEU:HD12 | 16:CS:50:LYS:H | 1.73 | 0.54 |
| 22:CB:1:G:N3 | 22:CB:1:G:H2' | 2.22 | 0.54 |
| 47:BZ:53:VAL:HG21 | 47:BZ:74:VAL:HG22 | 1.90 | 0.54 |
| 33:BM:120:LEU:C | 33:BM:120:LEU:HD22 | 2.27 | 0.54 |
| 25:DA:1444:G:N2 | 25:DA:1548:C:C2 | 2.76 | 0.54 |
| 2:AE:200:ILE:H | 2:AE:200:ILE:HD12 | 1.72 | 0.54 |
| 1:AA:76:G:C6 | 1:AA:77:C:C2 | 2.96 | 0.54 |
| 1:CA:1018:C:H2' | 1:CA:1019:C:O4' | 2.08 | 0.54 |
| 1:AA:321:A:C2 | 1:AA:333:G:C2 | 2.96 | 0.54 |
| 29:DF:72:ARG:NH1 | 29:DF:72:ARG:HB3 | 2.23 | 0.54 |
| 27:BD:32:SER:O | 27:BD:33:LEU:CB | 2.56 | 0.54 |
| 28:BE:61:ARG:C | 28:BE:63:LEU:H | 2.10 | 0.54 |
| 44:BU:76:CYS:HB3 | 44:BU:96:ILE:CD1 | 2.37 | 0.54 |
| 22:CB:17:U:OP2 | 22:CB:18:G:N7 | 2.41 | 0.54 |
| 32:DK:123:LEU:HD13 | 32:DK:143:SER:HB3 | 1.89 | 0.54 |
| 48:DW:10:LEU:O | 48:DW:14:ARG:HB2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 48:DW:15:LYS:HA | 48:DW:67:LYS:HZ1 | 1.72 | 0.54 |
| 25:BA:1570:A:H2' | 25:BA:1571:A:C8 | 2.43 | 0.54 |
| 25:BA:654(M):C:C2' | 25:BA:654(N):G:H8 | 2.20 | 0.54 |
| 33:BM:63:THR:O | 33:BM:66:LYS:HG3 | 2.08 | 0.54 |
| 30:DG:44:GLY:O | 30:DG:47:LYS:HB3 | 2.08 | 0.54 |
| 1:AA:1301:U:H2' | 1:AA:1302:U:H5' | 1.90 | 0.54 |
| 50:D4:59:PHE:HD1 | 50:D4:60:GLN:NE2 | 2.06 | 0.54 |
| 2:AE:212:GLN:CD | 2:AE:235:SER:HB2 | 2.28 | 0.54 |
| 33:DM:128:HIS:HB2 | 33:DM:129:PRO:HD2 | 1.90 | 0.54 |
| 1:AA:1285:A:H4' | 1:AA:1286:A:C5' | 2.38 | 0.54 |
| 28:BE:111:ARG:CD | 28:BE:160:TYR:HE1 | 2.20 | 0.54 |
| 25:DA:2329:G:N2 | 46:D3:41:ARG:HB3 | 2.23 | 0.54 |
| 25:DA:102:G:OP1 | 48:DW:7:ARG:NH2 | 2.39 | 0.54 |
| 1:CA:170:U:O2' | 1:CA:171:A:H5' | 2.07 | 0.54 |
| 7:AJ:78:ARG:HD2 | 7:AJ:80:VAL:CG2 | 2.38 | 0.54 |
| 2:AE:178:ARG:NH2 | 2:AE:196:LEU:HA | 2.22 | 0.54 |
| 27:DD:120:GLY:HA2 | 27:DD:190:TYR:OH | 2.07 | 0.54 |
| 25:DA:2211:G:C4' | 25:DA:2212:A:OP2 | 2.56 | 0.54 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:C8 | 2.43 | 0.54 |
| 35:BO:19:VAL:HG23 | 35:BO:27:HIS:CB | 2.38 | 0.54 |
| 1:CA:1216:G:C6 | 1:CA:1217:C:N4 | 2.75 | 0.54 |
| 35:DO:57:THR:C | 35:DO:59:LEU:N | 2.61 | 0.54 |
| 1:CA:719:C:H5 | 1:CA:720:C:C4 | 2.26 | 0.54 |
| 25:BA:2282:G:H4' | 25:BA:2389:G:O2' | 2.08 | 0.54 |
| 25:BA:280:C:C2 | 25:BA:361:G:N2 | 2.76 | 0.54 |
| 25:DA:1805:U:O2 | 27:DD:50:THR:HB | 2.08 | 0.54 |
| 47:BZ:3:LYS:O | 47:BZ:12:PRO:HD3 | 2.08 | 0.54 |
| 25:BA:500:G:N2 | 25:BA:502:A:H3' | 2.23 | 0.54 |
| 27:DD:239:ARG:O | 27:DD:240:ALA:HB2 | 2.08 | 0.54 |
| 49:DX:39:ASP:OD1 | 49:DX:39:ASP:O | 2.26 | 0.54 |
| 4:CG:150:GLU:C | 4:CG:152:SER:H | 2.10 | 0.54 |
| 1:AA:1177:G:N7 | 1:AA:1178:G:N1 | 2.55 | 0.53 |
| 41:D2:75:PHE:HE2 | 41:D2:81:TYR:CE1 | 2.26 | 0.53 |
| 28:BE:81:ILE:HG22 | 28:BE:84:PHE:HB3 | 1.86 | 0.53 |
| 39:DR:45:PHE:CD1 | 39:DR:74:ARG:HD2 | 2.43 | 0.53 |
| 22:CB:85:C:H2' | 22:CB:86:C:H5' | 1.90 | 0.53 |
| 29:BF:29:ASN:N | 29:BF:112:MET:CE | 2.61 | 0.53 |
| 1:AA:974:A:P | 14:AQ:41:ARG:HH12 | 2.31 | 0.53 |
| 1:CA:992:U:O2' | 1:CA:993:G:OP2 | 2.24 | 0.53 |
| 1:CA:1149:C:O2' | 1:CA:1280:A:N1 | 2.27 | 0.53 |
| 25:DA:2303:G:O4' | 30:DG:126:ASP:HB3 | 2.08 | 0.53 |
| 1:CA:1434:A:H61 | 1:CA:1467:G:H1' | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 20:AW:100:ILE:HG13 | 20:AW:101:GLY:H | 1.71 | 0.53 |
| 31:BH:92:ILE:CD1 | 31:BH:92:ILE:H | 2.14 | 0.53 |
| 25:BA:2134:A:C5 | 25:BA:2158:A:C2 | 2.96 | 0.53 |
| 33:DM:16:ILE:HG21 | 33:DM:26:LEU:HD11 | 1.89 | 0.53 |
| 33:BM:133:GLN:O | 33:BM:134:ARG:HG2 | 2.07 | 0.53 |
| 25:BA:2292:C:O2' | 25:BA:2293:C:H5' | 2.08 | 0.53 |
| 25:BA:654(R):C:H2' | 25:BA:654(S):G:H5' | 1.89 | 0.53 |
| 1:AA:1347:G:H22 | 1:AA:1373:G:H2' | 1.69 | 0.53 |
| 45:BV:140:ASP:CG | 45:BV:156:LYS:HZ3 | 2.12 | 0.53 |
| 18:CU:22:VAL:HG22 | 18:CU:23:LYS:N | 2.23 | 0.53 |
| 25:DA:1204:A:H2 | 25:DA:1241:A:N1 | 2.05 | 0.53 |
| 29:DF:53:THR:HG22 | 29:DF:56:GLU:HG3 | 1.89 | 0.53 |
| 25:BA:1925:C:H2' | 25:BA:1926:U:H5' | 1.90 | 0.53 |
| 25:DA:963:U:H2' | 25:DA:964:C:H6 | 1.73 | 0.53 |
| 25:BA:598:G:C1' | 35:BO:12:ALA:HB2 | 2.38 | 0.53 |
| 11:CN:48:ILE:HG13 | 11:CN:63:LEU:HB2 | 1.89 | 0.53 |
| 18:CU:37:VAL:HG11 | 18:CU:78:LEU:HB3 | 1.89 | 0.53 |
| 7:CJ:99:LEU:HD22 | 7:CJ:103:TRP:CZ2 | 2.42 | 0.53 |
| 25:DA:2780:G:OP1 | 33:DM:118:LYS:HE2 | 2.07 | 0.53 |
| 1:AA:851:G:O2' | 1:AA:852:G:H5' | 2.08 | 0.53 |
| 53:B7:5:TRP:NE1 | 53:B7:7:PRO:HG3 | 2.23 | 0.53 |
| 25:BA:1292:U:H2' | 25:BA:1293:C:C6 | 2.43 | 0.53 |
| 25:DA:2836:U:C4 | 25:DA:2883:A:N6 | 2.76 | 0.53 |
| 8:CK:29:SER:HB3 | 8:CK:32:LYS:HB2 | 1.90 | 0.53 |
| 25:DA:1445:C:H2' | 25:DA:1446:C:H6 | 1.72 | 0.53 |
| 42:BS:96:ILE:HD13 | 42:BS:96:ILE:O | 2.09 | 0.53 |
| 33:DM:130:HIS:CD2 | 33:DM:130:HIS:O | 2.60 | 0.53 |
| 32:BK:133:HIS:O | 32:BK:134:PRO:C | 2.45 | 0.53 |
| 23:CC:73:A:N6 | 23:CC:74:A:N6 | 2.56 | 0.53 |
| 25:DA:593:G:C1' | 54:D8:4:MET:HE1 | 2.39 | 0.53 |
| 54:D8:33:ASN:C | 54:D8:34:TRP:CD1 | 2.81 | 0.53 |
| 25:DA:9:U:O4 | 25:DA:2629:A:N1 | 2.41 | 0.53 |
| 27:DD:35:LYS:HB3 | 27:DD:63:ARG:CA | 2.27 | 0.53 |
| 25:DA:779:U:OP1 | 27:DD:49:ILE:CG2 | 2.57 | 0.53 |
| 41:D2:81:TYR:CD1 | 41:D2:81:TYR:N | 2.76 | 0.53 |
| 1:CA:1004:A:C5' | 1:CA:1025:U:H3 | 2.22 | 0.53 |
| 52:B6:30:THR:HA | 52:B6:32:ASN:N | 2.22 | 0.53 |
| 36:DP:30:GLY:HA2 | 36:DP:107:ALA:CB | 2.38 | 0.53 |
| 19:AV:41:VAL:CG2 | 19:AV:67:VAL:HG22 | 2.37 | 0.53 |
| 39:BR:36:GLU:CG | 39:BR:41:ARG:HD2 | 2.28 | 0.53 |
| 1:AA:1349:A:OP2 | 9:AL:118:LYS:NZ | 2.39 | 0.53 |
| 1:CA:1132:C:H2' | 1:CA:1133:G:C8 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|---------------------|-------------|----------|
| 30:BG:37:VAL:HG23 | 30:BG:99:MET:CE | 2.38 | 0.53 |
| 7:CJ:115:ARG:HB2 | 7:CJ:118:VAL:CG1 | 2.38 | 0.53 |
| 25:DA:1464:C:O2' | 25:DA:1528:A:C8 | 2.42 | 0.53 |
| 45:DV:141:VAL:HG21 | 45:DV:150:LEU:HG | 1.90 | 0.53 |
| 25:DA:2320:A:H4' | 25:DA:2321:G:C8 | 2.43 | 0.53 |
| 2:AE:42:ILE:HD11 | 2:AE:202:PRO:HB2 | 1.90 | 0.53 |
| 34:BN:85:VAL:HG11 | 34:BN:114:ILE:CD1 | 2.35 | 0.53 |
| 19:CV:31:ILE:HG13 | 19:CV:32:LYS:N | 2.22 | 0.53 |
| 25:BA:2702:U:OP1 | 25:BA:2702:U:C6 | 2.61 | 0.53 |
| 1:AA:475:G:O2' | 1:AA:476:G:H5' | 2.08 | 0.53 |
| 1:AA:381:C:H2' | 1:AA:382:A:O4' | 2.08 | 0.53 |
| 45:BV:166:SER:N | 45:BV:167:PRO:HD3 | 2.23 | 0.53 |
| 54:D8:16:ILE:HD11 | 54:D8:60:LEU:HD12 | 1.91 | 0.53 |
| 12:CO:86:ARG:HB2 | 12:CO:101:VAL:HG23 | 1.90 | 0.53 |
| 25:DA:963:U:H2' | 25:DA:964:C:C6 | 2.43 | 0.53 |
| 1:CA:1032:A:H3' | 1:CA:1032(A):G:H5'' | 1.90 | 0.53 |
| 27:DD:236:GLY:O | 27:DD:237:GLU:O | 2.26 | 0.53 |
| 9:CL:122:ALA:HB1 | 9:CL:123:PRO:HD2 | 1.90 | 0.53 |
| 25:BA:1651:G:N7 | 37:B0:11:ASN:ND2 | 2.55 | 0.53 |
| 25:DA:881:G:O6 | 25:DA:895:U:O2 | 2.25 | 0.53 |
| 6:CI:23:LYS:O | 6:CI:27:GLN:HB2 | 2.08 | 0.53 |
| 25:BA:2766:G:N3 | 25:BA:2766:G:H2' | 2.23 | 0.53 |
| 25:BA:667:U:O2 | 54:B8:2:PRO:HD2 | 2.08 | 0.53 |
| 15:CR:55:GLY:O | 15:CR:59:MET:HE2 | 2.08 | 0.53 |
| 25:DA:2208:U:O2' | 25:DA:2209:C:H5' | 2.08 | 0.53 |
| 8:CK:138:TRP:OXT | 8:CK:138:TRP:HE3 | 1.90 | 0.53 |
| 1:AA:1075:C:O2' | 1:AA:1076:C:H5' | 2.09 | 0.53 |
| 25:DA:496:G:H2' | 25:DA:497:A:H5' | 1.90 | 0.53 |
| 13:AP:50:GLU:O | 13:AP:54:VAL:HG23 | 2.08 | 0.53 |
| 29:BF:107:LYS:HE3 | 29:BF:207:GLY:H | 1.73 | 0.53 |
| 25:DA:2371:G:C1' | 52:D6:45:LYS:HE2 | 2.35 | 0.53 |
| 35:BO:75:ILE:N | 35:BO:75:ILE:HD13 | 2.14 | 0.53 |
| 25:BA:1026:U:H1' | 25:BA:1027:A:P | 2.48 | 0.53 |
| 1:AA:1025:U:HO2' | 1:AA:1026:G:C5' | 2.19 | 0.53 |
| 22:CB:38:G:C2' | 22:CB:39:U:H5' | 2.39 | 0.53 |
| 19:AV:42:PRO:O | 19:AV:45:VAL:HG22 | 2.08 | 0.53 |
| 25:DA:2470:G:OP2 | 36:DP:56:ARG:NH1 | 2.41 | 0.53 |
| 25:DA:2712(A):A:C5' | 25:DA:2713:A:OP2 | 2.48 | 0.53 |
| 1:CA:1276:G:H2' | 1:CA:1277:C:H6 | 1.73 | 0.53 |
| 25:DA:2872:G:N7 | 25:DA:2873:A:H2 | 2.07 | 0.53 |
| 2:AE:211:ILE:O | 2:AE:215:LEU:HB2 | 2.08 | 0.53 |
| 40:D1:108:GLU:OE1 | 41:D2:45:THR:HA | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:674:G:H1' | 29:BF:74:ARG:CD | 2.34 | 0.53 |
| 43:DT:36:LYS:HG2 | 43:DT:54:VAL:HB | 1.90 | 0.53 |
| 1:AA:607:A:C2' | 1:AA:608:A:H5' | 2.38 | 0.53 |
| 36:DP:10:ARG:HA | 36:DP:10:ARG:NE | 2.23 | 0.53 |
| 1:CA:1327:C:H2' | 1:CA:1328:C:C6 | 2.42 | 0.53 |
| 43:DT:63:LYS:HE3 | 43:DT:63:LYS:N | 2.21 | 0.53 |
| 4:AG:133:VAL:HG11 | 4:AG:138:TYR:HD1 | 1.73 | 0.53 |
| 12:CO:84:LEU:HD12 | 12:CO:104:VAL:HG11 | 1.91 | 0.53 |
| 18:CU:22:VAL:C | 18:CU:24:ALA:H | 2.11 | 0.53 |
| 25:DA:1309:G:H4' | 53:D7:7:PRO:HB2 | 1.90 | 0.53 |
| 25:BA:1465:G:H5' | 25:BA:1528:A:H1' | 1.90 | 0.53 |
| 1:AA:736:C:H2' | 1:AA:737:A:H8 | 1.72 | 0.53 |
| 2:AE:103:THR:HG22 | 2:AE:180:LEU:HD21 | 1.90 | 0.53 |
| 25:BA:1494:A:C2' | 25:BA:1495:A:H5' | 2.38 | 0.53 |
| 30:DG:146:TYR:CD2 | 30:DG:146:TYR:C | 2.81 | 0.53 |
| 27:DD:108:PRO:HB3 | 27:DD:143:HIS:CE1 | 2.43 | 0.53 |
| 36:BP:51:ARG:NH2 | 36:BP:52:VAL:HG23 | 2.23 | 0.53 |
| 42:DS:78:GLU:OE1 | 42:DS:99:ARG:HD3 | 2.08 | 0.53 |
| 46:D3:51:VAL:N | 46:D3:62:LEU:HD12 | 2.22 | 0.53 |
| 2:AE:28:PHE:CD1 | 2:AE:190:THR:HA | 2.43 | 0.53 |
| 26:BB:1(M):A:H2' | 26:BB:0:A:H5' | 1.89 | 0.53 |
| 25:DA:1488:G:H5' | 25:DA:1489:U:OP2 | 2.08 | 0.53 |
| 29:DF:79:GLY:HA2 | 29:DF:86:GLY:HA2 | 1.88 | 0.53 |
| 41:B2:60:GLU:O | 41:B2:62:LEU:HD13 | 2.08 | 0.53 |
| 39:DR:29:ARG:CB | 39:DR:29:ARG:HH11 | 2.21 | 0.53 |
| 3:CF:173:VAL:HG12 | 3:CF:175:LEU:HD23 | 1.90 | 0.53 |
| 6:CI:82:ARG:HB2 | 6:CI:85:VAL:HG23 | 1.89 | 0.53 |
| 12:AO:47:LYS:HA | 12:AO:49:ASN:H | 1.72 | 0.53 |
| 25:BA:1062:G:H1' | 25:BA:1088:A:C5 | 2.44 | 0.53 |
| 25:DA:2062:A:H62 | 25:DA:2503:A:H62 | 1.54 | 0.53 |
| 54:D8:24:ALA:O | 54:D8:48:PHE:CD1 | 2.62 | 0.53 |
| 25:DA:1088:A:H5' | 25:DA:1089:G:H5' | 1.89 | 0.53 |
| 1:AA:972:C:O2' | 10:AM:55:LYS:HG3 | 2.08 | 0.53 |
| 30:BG:121:ASN:HD22 | 30:BG:123:ASN:N | 1.91 | 0.53 |
| 25:BA:2749:A:H4' | 31:BH:62:LYS:HB3 | 1.90 | 0.53 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:N6 | 2.07 | 0.53 |
| 25:BA:2062:A:C2' | 25:BA:2062:A:N3 | 2.69 | 0.53 |
| 33:BM:59:LYS:CE | 33:BM:61:ARG:HH22 | 2.22 | 0.53 |
| 25:BA:2134:A:C5 | 25:BA:2158:A:H2 | 2.26 | 0.53 |
| 2:AE:80:ILE:O | 2:AE:80:ILE:HG22 | 2.09 | 0.53 |
| 13:CP:68:GLY:HA3 | 30:DG:116:ASP:OD1 | 2.08 | 0.53 |
| 43:DT:54:VAL:C | 43:DT:55:ASN:HD22 | 2.11 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 22:AB:18:G:C4' | 22:AB:19:G:OP2 | 2.54 | 0.53 |
| 45:DV:69:THR:HB | 45:DV:88:PHE:HB3 | 1.91 | 0.53 |
| 5:AH:51:VAL:HB | 5:AH:52:PRO:HD3 | 1.89 | 0.53 |
| 1:CA:192:U:O4' | 20:CW:103:GLY:HA3 | 2.08 | 0.53 |
| 47:DZ:11:ARG:HB2 | 47:DZ:12:PRO:HD2 | 1.90 | 0.53 |
| 10:CM:22:LYS:HE2 | 10:CM:90:LEU:HD11 | 1.90 | 0.53 |
| 1:CA:197:A:H1' | 1:CA:198:G:OP2 | 2.08 | 0.53 |
| 1:CA:244:U:H5' | 1:CA:244:U:H6 | 1.73 | 0.53 |
| 12:CO:82:VAL:HB | 12:CO:105:TYR:HB3 | 1.91 | 0.53 |
| 1:CA:923:A:OP1 | 5:CH:21:ALA:HB2 | 2.08 | 0.53 |
| 31:BH:116:GLU:HG3 | 31:BH:117:PRO:HD2 | 1.90 | 0.53 |
| 25:BA:495:G:H21 | 42:BS:61:ASN:HD21 | 1.57 | 0.53 |
| 46:B3:66:VAL:HG22 | 46:B3:82:ARG:HG2 | 1.91 | 0.53 |
| 5:AH:69:VAL:O | 5:AH:71:LEU:N | 2.41 | 0.53 |
| 25:BA:2025:C:H2' | 25:BA:2026:C:C6 | 2.44 | 0.53 |
| 25:DA:2461:C:H2' | 25:DA:2462:U:C6 | 2.42 | 0.53 |
| 1:CA:373:A:N3 | 1:CA:374:A:C8 | 2.77 | 0.53 |
| 25:DA:2103:C:H2' | 25:DA:2104:G:C8 | 2.43 | 0.53 |
| 25:BA:1816:G:H8 | 27:BD:62:TYR:HH | 1.54 | 0.53 |
| 3:CF:155:GLY:O | 3:CF:196:LEU:HD22 | 2.07 | 0.53 |
| 44:DU:9:LYS:O | 44:DU:27:VAL:HG22 | 2.07 | 0.53 |
| 25:DA:654:A:N3 | 25:DA:654:A:H2' | 2.23 | 0.53 |
| 3:AF:42:LEU:O | 3:AF:46:GLU:HG2 | 2.08 | 0.53 |
| 1:AA:615:C:C2 | 1:AA:616:G:C8 | 2.96 | 0.53 |
| 25:DA:51:G:N3 | 25:DA:119:A:C2 | 2.76 | 0.53 |
| 9:AL:16:ARG:HB2 | 9:AL:64:THR:HG22 | 1.90 | 0.53 |
| 23:CC:56:U:O2 | 23:CC:58:A:N7 | 2.41 | 0.53 |
| 25:DA:2748:A:N7 | 25:DA:2754:U:C4 | 2.73 | 0.53 |
| 2:CE:204:ASN:HB2 | 2:CE:210:SER:HB3 | 1.89 | 0.53 |
| 35:BO:64:LYS:HD2 | 54:B8:25:MET:HE1 | 1.84 | 0.53 |
| 25:DA:531:C:OP1 | 25:DA:561:G:N1 | 2.41 | 0.53 |
| 1:CA:1132:C:O2' | 1:CA:1133:G:H5' | 2.08 | 0.53 |
| 22:AB:85:C:H2' | 22:AB:86:C:H5' | 1.91 | 0.53 |
| 12:CO:46:LYS:NZ | 12:CO:47:LYS:HD3 | 2.20 | 0.53 |
| 25:BA:2789:C:H3' | 25:BA:2790:A:H5'' | 1.89 | 0.53 |
| 28:BE:119:ARG:NH1 | 28:BE:119:ARG:HG3 | 2.22 | 0.53 |
| 35:DO:101:VAL:CG2 | 35:DO:108:LYS:H | 2.22 | 0.53 |
| 31:DH:136:ILE:H | 31:DH:136:ILE:HD12 | 1.72 | 0.53 |
| 41:B2:44:LYS:HG2 | 41:B2:45:THR:H | 1.72 | 0.53 |
| 25:BA:534:U:H5' | 40:B1:42:ALA:CB | 2.36 | 0.53 |
| 25:DA:1006:C:C2 | 25:DA:1138:G:N2 | 2.77 | 0.53 |
| 36:BP:20:ALA:O | 36:BP:21:THR:HG23 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 14:CQ:45:ARG:NH1 | 14:CQ:45:ARG:HG3 | 2.21 | 0.53 |
| 1:CA:1400:C:H42 | 23:CC:35:C:H1' | 1.74 | 0.53 |
| 1:AA:353:A:C2' | 1:AA:354:G:OP2 | 2.56 | 0.53 |
| 2:AE:111:ARG:HH11 | 2:AE:111:ARG:CG | 2.22 | 0.53 |
| 1:AA:411:A:C2 | 1:AA:431:A:N6 | 2.77 | 0.53 |
| 26:DB:29:A:C2 | 26:DB:56:G:C2 | 2.97 | 0.53 |
| 39:BR:108:ARG:HA | 39:BR:111:ARG:NE | 2.23 | 0.53 |
| 19:CV:41:VAL:HG22 | 50:D4:63:TYR:CZ | 2.44 | 0.53 |
| 13:AP:60:VAL:CG1 | 13:AP:66:LEU:HD11 | 2.38 | 0.53 |
| 25:DA:128:C:H4' | 25:DA:129:C:OP1 | 2.09 | 0.53 |
| 1:AA:881:G:OP2 | 12:AO:12:ARG:NH2 | 2.41 | 0.53 |
| 25:BA:614:U:C4 | 29:BF:168:ARG:HG2 | 2.44 | 0.53 |
| 25:BA:1710:C:O2' | 25:BA:1711:C:H5' | 2.09 | 0.53 |
| 46:D3:70:GLN:HE21 | 46:D3:80:HIS:HE2 | 1.54 | 0.53 |
| 35:BO:94:GLU:O | 35:BO:124:LYS:O | 2.26 | 0.53 |
| 26:BB:94:C:C4 | 26:BB:95:U:C5 | 2.97 | 0.53 |
| 5:AH:64:ARG:HH11 | 5:AH:64:ARG:HG3 | 1.73 | 0.53 |
| 25:DA:880:G:H2' | 25:DA:880:G:N3 | 2.22 | 0.53 |
| 30:BG:128:ARG:NH2 | 30:BG:128:ARG:HB2 | 2.23 | 0.53 |
| 38:DQ:39:ILE:HG22 | 38:DQ:39:ILE:O | 2.08 | 0.53 |
| 25:BA:1247:A:OP1 | 29:BF:95:ARG:NH2 | 2.41 | 0.53 |
| 25:DA:1686:C:C2' | 25:DA:1687:G:H5' | 2.39 | 0.53 |
| 30:BG:70:VAL:CG2 | 30:BG:87:PRO:HB3 | 2.39 | 0.53 |
| 25:DA:2287:A:N1 | 25:DA:2346:A:N1 | 2.56 | 0.53 |
| 54:B8:23:VAL:CG1 | 54:B8:46:ARG:HD3 | 2.39 | 0.53 |
| 28:BE:78:LEU:CD1 | 28:BE:79:ARG:CG | 2.86 | 0.53 |
| 41:D2:89:GLN:HE21 | 41:D2:90:PRO:HD2 | 1.72 | 0.53 |
| 1:CA:449:C:O4' | 1:CA:449:C:O2 | 2.26 | 0.53 |
| 36:BP:88:GLY:C | 36:BP:90:VAL:H | 2.12 | 0.53 |
| 22:CB:40:G:C2 | 22:CB:41:G:C5 | 2.97 | 0.53 |
| 19:AV:40:ILE:HG22 | 19:AV:69:HIS:O | 2.08 | 0.53 |
| 35:BO:64:LYS:HD2 | 54:B8:25:MET:HE2 | 1.83 | 0.53 |
| 25:BA:2056:G:C2 | 25:BA:2057:A:C8 | 2.96 | 0.53 |
| 25:BA:1141:U:OP2 | 33:BM:63:THR:CG2 | 2.56 | 0.53 |
| 30:DG:91:ARG:HD2 | 30:DG:92:VAL:N | 2.23 | 0.53 |
| 25:DA:887:A:N3 | 25:DA:887:A:H2' | 2.22 | 0.53 |
| 1:AA:397:A:H5' | 1:AA:398:C:OP1 | 2.09 | 0.53 |
| 35:DO:21:ARG:NE | 35:DO:21:ARG:HA | 2.17 | 0.53 |
| 33:BM:133:GLN:HB2 | 33:BM:135:PRO:HD3 | 1.90 | 0.53 |
| 41:D2:44:LYS:C | 41:D2:46:VAL:N | 2.57 | 0.53 |
| 35:DO:78:PRO:HA | 35:DO:110:TYR:CD2 | 2.43 | 0.53 |
| 41:B2:34:GLU:O | 41:B2:34:GLU:HG3 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:101:G:H2' | 25:DA:102:G:OP1 | 2.09 | 0.53 |
| 1:CA:1286:A:H8 | 1:CA:1287:A:H4' | 1.69 | 0.53 |
| 13:AP:3:ARG:CD | 13:AP:7:VAL:HG13 | 2.39 | 0.53 |
| 22:CB:45:U:O2' | 22:CB:46:G:H5'' | 2.08 | 0.53 |
| 1:CA:465:A:N6 | 1:CA:467:G:C2 | 2.77 | 0.53 |
| 39:BR:108:ARG:HA | 39:BR:111:ARG:HE | 1.74 | 0.53 |
| 25:BA:1309:G:P | 53:B7:9:ARG:HD3 | 2.47 | 0.53 |
| 25:BA:1311:G:O6 | 53:B7:9:ARG:NH2 | 2.41 | 0.53 |
| 25:BA:1735:C:C5' | 25:BA:1735:C:H6 | 2.21 | 0.53 |
| 22:CB:1:G:H5'' | 22:CB:2:C:OP1 | 2.09 | 0.53 |
| 1:AA:66:G:N2 | 1:AA:172:A:C2 | 2.77 | 0.53 |
| 46:D3:29:GLN:O | 46:D3:67:VAL:HG23 | 2.08 | 0.53 |
| 25:BA:1657:C:H2' | 25:BA:1658:C:H6 | 1.72 | 0.53 |
| 22:AB:45:U:H3' | 22:AB:45:U:C6 | 2.44 | 0.53 |
| 25:BA:821:A:H5'' | 25:BA:822:U:H6 | 1.73 | 0.53 |
| 1:AA:640:A:O2' | 8:AK:115:SER:HB2 | 2.08 | 0.53 |
| 25:BA:705:A:C2 | 25:BA:727:A:H1' | 2.44 | 0.53 |
| 25:BA:1820:U:H4' | 25:BA:1821:A:OP2 | 2.08 | 0.53 |
| 1:CA:1263:C:H42 | 1:CA:1272:G:H1 | 1.56 | 0.53 |
| 4:CG:117:ALA:O | 4:CG:121:VAL:HG23 | 2.09 | 0.53 |
| 1:CA:194:C:C3' | 1:CA:195:A:H5'' | 2.38 | 0.53 |
| 29:DF:129:PHE:HA | 29:DF:142:TRP:CD1 | 2.44 | 0.53 |
| 27:DD:35:LYS:NZ | 27:DD:104:TYR:HB2 | 2.24 | 0.53 |
| 25:DA:690:G:O2' | 27:DD:43:ARG:NH2 | 2.36 | 0.53 |
| 22:CB:40:G:H2' | 22:CB:41:G:H8 | 1.74 | 0.53 |
| 1:AA:818:G:O2' | 1:AA:819:A:H5' | 2.09 | 0.53 |
| 26:DB:3:C:H2' | 26:DB:3:C:O2 | 2.07 | 0.53 |
| 25:DA:527:C:N4 | 25:DA:2779:U:OP2 | 2.42 | 0.53 |
| 1:CA:1128:C:C2 | 1:CA:1139:G:C6 | 2.97 | 0.53 |
| 22:AB:85:C:H42 | 25:BA:2508:G:H5' | 1.74 | 0.53 |
| 1:CA:1443:G:N2 | 39:DR:119:LYS:HB2 | 2.22 | 0.53 |
| 31:BH:54:ARG:NH1 | 31:BH:65:HIS:ND1 | 2.56 | 0.53 |
| 25:DA:2129:C:C4 | 25:DA:2130:U:N3 | 2.77 | 0.53 |
| 45:DV:108:PRO:CB | 45:DV:143:GLY:N | 2.72 | 0.53 |
| 27:BD:25:THR:CG2 | 27:BD:26:LYS:N | 2.71 | 0.53 |
| 13:CP:3:ARG:HB2 | 50:D4:34:GLU:OE2 | 2.09 | 0.53 |
| 25:BA:2712:U:O2' | 25:BA:2712(A):A:P | 2.67 | 0.53 |
| 8:AK:87:SER:HB2 | 8:AK:93:VAL:CA | 2.38 | 0.53 |
| 37:B0:104:ARG:NH1 | 37:B0:107:ASP:CG | 2.62 | 0.53 |
| 25:DA:654(Q):C:H2' | 25:DA:654(R):C:C6 | 2.44 | 0.53 |
| 7:CJ:23:VAL:CG1 | 7:CJ:43:PHE:HE2 | 2.21 | 0.53 |
| 25:BA:1771:C:HO2' | 25:BA:1786:A:C1' | 2.22 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 39:DR:47:GLY:CA | 39:DR:63:VAL:HG12 | 2.37 | 0.53 |
| 2:AE:68:ILE:O | 2:AE:91:PRO:HD2 | 2.09 | 0.53 |
| 39:BR:39:ARG:CG | 39:BR:40:THR:H | 2.21 | 0.53 |
| 1:AA:250:A:H4' | 1:AA:251:G:O5' | 2.07 | 0.53 |
| 25:BA:372:G:O2' | 25:BA:373:U:OP2 | 2.27 | 0.53 |
| 25:DA:2765:A:C2 | 25:DA:2766:G:O4' | 2.61 | 0.53 |
| 1:CA:1122:U:C4 | 1:CA:1123:A:N7 | 2.75 | 0.53 |
| 25:DA:854:G:O2' | 25:DA:855:G:H5' | 2.09 | 0.53 |
| 8:CK:111:ILE:HG22 | 8:CK:112:LEU:N | 2.24 | 0.53 |
| 25:DA:1412:A:H2' | 25:DA:1413:G:C8 | 2.42 | 0.53 |
| 31:BH:84:SER:O | 31:BH:133:VAL:O | 2.26 | 0.53 |
| 3:AF:36:ASP:OD2 | 3:AF:57:ILE:HG21 | 2.08 | 0.53 |
| 25:DA:2031:A:C6 | 25:DA:2498:C:H1' | 2.43 | 0.53 |
| 44:BU:90:LEU:N | 44:BU:90:LEU:HD13 | 2.23 | 0.53 |
| 37:D0:91:GLN:HG2 | 37:D0:91:GLN:O | 2.08 | 0.53 |
| 1:CA:1056:U:H5' | 3:CF:163:ALA:CB | 2.38 | 0.53 |
| 6:CI:50:TYR:HE1 | 18:CU:74:ARG:O | 1.91 | 0.53 |
| 12:AO:75:HIS:HD2 | 12:AO:77:LEU:H | 1.55 | 0.53 |
| 25:BA:1069:A:H4' | 25:BA:1070:A:H5'' | 1.91 | 0.53 |
| 27:DD:35:LYS:HG2 | 27:DD:64:ILE:N | 2.21 | 0.53 |
| 33:DM:4:TYR:CD2 | 40:D1:100:VAL:HG11 | 2.44 | 0.53 |
| 28:BE:27:LEU:CD1 | 39:BR:1:MET:CE | 2.76 | 0.53 |
| 23:CC:19:G:O2' | 23:CC:20:G:O5' | 2.26 | 0.53 |
| 25:BA:535:C:O3' | 40:B1:53:ARG:NH1 | 2.42 | 0.53 |
| 10:AM:55:LYS:O | 10:AM:56:HIS:CG | 2.62 | 0.53 |
| 54:B8:33:ASN:HA | 54:B8:36:LYS:HE3 | 1.91 | 0.53 |
| 25:BA:2115:G:O6 | 25:BA:2117:A:H3' | 2.08 | 0.53 |
| 45:DV:108:PRO:CA | 45:DV:143:GLY:HA2 | 2.37 | 0.53 |
| 25:DA:2320:A:C6 | 25:DA:2333:A:C8 | 2.97 | 0.53 |
| 39:BR:90:GLN:HG3 | 39:BR:91:ARG:N | 2.24 | 0.53 |
| 29:DF:5:ALA:HB1 | 29:DF:125:LEU:HD21 | 1.91 | 0.53 |
| 1:AA:1226:C:N4 | 13:AP:104:ARG:HG3 | 2.24 | 0.53 |
| 6:CI:33:TYR:OH | 6:CI:78:GLU:HG3 | 2.09 | 0.53 |
| 30:BG:114:ILE:CD1 | 30:BG:140:ILE:HG21 | 2.39 | 0.53 |
| 25:BA:2646:C:H6 | 25:BA:2646:C:O5' | 1.92 | 0.53 |
| 5:CH:147:ASP:HA | 5:CH:150:ARG:HB2 | 1.91 | 0.53 |
| 25:DA:1416:G:O2' | 25:DA:1417:C:H6 | 1.91 | 0.53 |
| 25:DA:322:A:OP2 | 29:DF:169:ASN:HB2 | 2.09 | 0.53 |
| 36:DP:68:ILE:HG21 | 36:DP:103:MET:HB3 | 1.91 | 0.53 |
| 39:BR:107:ASP:O | 39:BR:110:ILE:HG23 | 2.08 | 0.53 |
| 25:BA:1079:C:H3' | 25:BA:1080:A:C8 | 2.43 | 0.53 |
| 26:BB:90:C:P | 36:BP:16:ARG:HH21 | 2.31 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:148:G:C2 | 1:AA:149:A:N7 | 2.76 | 0.53 |
| 25:BA:988:A:P | 49:BX:11:SER:HB3 | 2.49 | 0.53 |
| 2:AE:236:TYR:HA | 2:AE:239:VAL:CG2 | 2.38 | 0.53 |
| 20:AW:13:LEU:HD12 | 20:AW:13:LEU:O | 2.09 | 0.53 |
| 27:DD:79:VAL:HG21 | 27:DD:111:LEU:HD11 | 1.91 | 0.53 |
| 1:AA:339:C:OP2 | 34:BN:97:ARG:NH1 | 2.42 | 0.53 |
| 14:CQ:38:GLY:O | 14:CQ:39:LEU:HD23 | 2.09 | 0.53 |
| 1:AA:614:A:OP1 | 4:AG:86:LYS:NZ | 2.42 | 0.53 |
| 1:AA:295:C:H2' | 1:AA:296:U:O4' | 2.08 | 0.53 |
| 8:CK:10:LEU:HD22 | 8:CK:83:ILE:HD11 | 1.90 | 0.53 |
| 25:DA:2593:U:H2' | 25:DA:2594:C:C6 | 2.43 | 0.53 |
| 2:CE:172:ILE:O | 2:CE:176:GLU:HG3 | 2.09 | 0.53 |
| 52:B6:36:LEU:H | 52:B6:36:LEU:CD2 | 2.20 | 0.53 |
| 1:AA:433:C:O2' | 1:AA:434:U:H5' | 2.09 | 0.53 |
| 36:BP:43:THR:OG1 | 36:BP:46:GLN:HB2 | 2.08 | 0.53 |
| 25:DA:994:C:H1' | 41:D2:10:LYS:HE2 | 1.90 | 0.53 |
| 25:DA:1061:U:H4' | 25:DA:1070:A:H1' | 1.91 | 0.53 |
| 2:AE:21:ARG:CB | 2:AE:39:ILE:HA | 2.39 | 0.53 |
| 1:AA:976:G:H5' | 1:AA:1358:U:O2' | 2.09 | 0.53 |
| 25:DA:528:A:C3' | 25:DA:528:A:C8 | 2.91 | 0.53 |
| 25:DA:90:U:H2' | 25:DA:90:U:O2 | 2.08 | 0.53 |
| 38:BQ:42:ASP:O | 38:BQ:43:GLU:HG2 | 2.09 | 0.53 |
| 25:DA:607:U:OP1 | 29:DF:102:PRO:HA | 2.08 | 0.53 |
| 2:CE:153:ARG:CG | 2:CE:154:LEU:H | 2.13 | 0.53 |
| 25:DA:2112:G:N3 | 25:DA:2169:A:N6 | 2.56 | 0.53 |
| 1:CA:1238:A:N7 | 1:CA:1301:U:O4 | 2.41 | 0.53 |
| 25:DA:2872:G:N7 | 25:DA:2873:A:C2 | 2.77 | 0.53 |
| 25:DA:321:G:H5' | 29:DF:134:GLY:O | 2.08 | 0.53 |
| 25:DA:2410:G:C2 | 25:DA:2411:A:H1' | 2.44 | 0.53 |
| 25:DA:2335:A:C8 | 25:DA:2337:G:C5 | 2.97 | 0.53 |
| 29:DF:110:LEU:HD22 | 29:DF:202:PHE:CE1 | 2.41 | 0.53 |
| 19:CV:42:PRO:O | 19:CV:43:GLU:HG2 | 2.08 | 0.53 |
| 25:BA:1079:C:H3' | 25:BA:1080:A:H8 | 1.73 | 0.53 |
| 10:AM:32:ALA:CB | 10:AM:76:ASN:HB2 | 2.38 | 0.53 |
| 26:DB:31:C:C2' | 26:DB:32:C:H5' | 2.39 | 0.53 |
| 1:CA:57:G:H2' | 1:CA:58:C:C6 | 2.44 | 0.53 |
| 45:BV:107:THR:C | 45:BV:109:ALA:N | 2.62 | 0.53 |
| 25:DA:2143:C:H2' | 25:DA:2144:U:O4' | 2.09 | 0.53 |
| 18:CU:29:PHE:N | 18:CU:29:PHE:CD2 | 2.77 | 0.53 |
| 25:DA:1412:A:H2' | 25:DA:1413:G:H8 | 1.74 | 0.53 |
| 4:AG:88:VAL:HG13 | 5:AH:97:GLY:HA2 | 1.91 | 0.53 |
| 42:DS:88:ARG:NH1 | 42:DS:94:ASP:OD1 | 2.30 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:CO:37:CYS:SG | 12:CO:81:SER:OG | 2.66 | 0.53 |
| 25:DA:273:G:H1 | 25:DA:364:C:H42 | 1.56 | 0.53 |
| 1:CA:568:G:O6 | 12:CO:5:PRO:HD3 | 2.09 | 0.53 |
| 1:CA:587:G:N1 | 1:CA:754:C:OP2 | 2.42 | 0.53 |
| 20:CW:12:ALA:O | 20:CW:15:ARG:HB2 | 2.08 | 0.53 |
| 21:AX:3:LYS:HB3 | 21:AX:14:TRP:CD1 | 2.43 | 0.53 |
| 14:CQ:15:LYS:NZ | 14:CQ:15:LYS:HB3 | 2.23 | 0.53 |
| 1:AA:445:G:H1 | 1:AA:489:C:H42 | 1.56 | 0.53 |
| 25:DA:1769:G:O2' | 25:DA:1958:C:OP1 | 2.22 | 0.53 |
| 25:DA:2638:G:OP2 | 28:DE:82:ARG:NH2 | 2.42 | 0.53 |
| 25:BA:1063:G:H1 | 25:BA:1075:C:N4 | 2.06 | 0.53 |
| 38:DQ:106:ARG:HA | 38:DQ:110:LEU:HG | 1.90 | 0.53 |
| 39:DR:56:GLY:C | 39:DR:58:ASN:H | 2.12 | 0.53 |
| 1:CA:1061:G:H2' | 1:CA:1062:U:C5' | 2.38 | 0.53 |
| 29:DF:25:PRO:HB2 | 29:DF:27:GLU:H | 1.74 | 0.53 |
| 25:DA:528:A:C2' | 25:DA:529:A:H5' | 2.39 | 0.53 |
| 9:CL:5:TYR:CD2 | 9:CL:18:PHE:CE2 | 2.97 | 0.53 |
| 2:CE:115:LEU:O | 2:CE:118:LEU:HB2 | 2.08 | 0.53 |
| 25:DA:1496:A:C8 | 25:DA:1577:C:O2' | 2.51 | 0.53 |
| 9:CL:49:PRO:HD3 | 9:CL:78:LYS:HE3 | 1.90 | 0.53 |
| 45:DV:141:VAL:O | 45:DV:142:SER:C | 2.47 | 0.53 |
| 28:BE:16:ARG:O | 28:BE:16:ARG:CG | 2.51 | 0.53 |
| 29:DF:9:ILE:HA | 29:DF:13:SER:O | 2.08 | 0.53 |
| 41:B2:38:LEU:C | 41:B2:38:LEU:HD23 | 2.29 | 0.53 |
| 33:DM:30:ILE:O | 33:DM:34:LEU:HD22 | 2.08 | 0.53 |
| 3:AF:166:GLU:CG | 3:AF:167:TRP:N | 2.72 | 0.53 |
| 1:CA:411:A:N7 | 1:CA:413:G:N3 | 2.57 | 0.53 |
| 1:AA:382:A:H2' | 1:AA:383:A:H8 | 1.68 | 0.53 |
| 25:BA:2681:C:H1' | 25:BA:2682:U:OP2 | 2.09 | 0.53 |
| 44:BU:41:GLY:O | 44:BU:42:VAL:C | 2.48 | 0.53 |
| 32:DK:77:LEU:CD1 | 32:DK:78:THR:H | 2.22 | 0.53 |
| 41:D2:48:GLY:C | 41:D2:49:THR:O | 2.45 | 0.53 |
| 3:AF:78:GLY:HA3 | 3:AF:83:ARG:CB | 2.38 | 0.53 |
| 1:AA:312:C:C2' | 1:AA:313:A:H5' | 2.39 | 0.53 |
| 22:CB:3:C:H2' | 22:CB:4:G:C8 | 2.44 | 0.53 |
| 1:AA:170:U:O2' | 1:AA:171:A:H5' | 2.07 | 0.53 |
| 8:AK:41:ARG:O | 8:AK:41:ARG:HD2 | 2.09 | 0.53 |
| 22:AB:27:G:H3' | 22:AB:28:C:H6 | 1.72 | 0.53 |
| 26:BB:61:G:C6 | 26:BB:62:C:C4 | 2.97 | 0.53 |
| 25:BA:1694:C:H5' | 25:BA:1694:C:C6 | 2.44 | 0.53 |
| 25:DA:274:G:C5 | 25:DA:275:G:C6 | 2.97 | 0.53 |
| 25:BA:2839:G:H5'' | 37:B0:46:GLY:HA2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 12:CO:111:LYS:O | 12:CO:112:ASP:HB2 | 2.09 | 0.53 |
| 25:DA:284:U:C2' | 25:DA:285:C:H5' | 2.39 | 0.53 |
| 1:CA:114:U:O2' | 1:CA:115:G:H5' | 2.09 | 0.53 |
| 1:CA:1267:C:H2' | 1:CA:1267:C:O2 | 2.09 | 0.53 |
| 10:AM:23:ILE:HD12 | 10:AM:85:LEU:HD22 | 1.90 | 0.53 |
| 1:CA:1137:C:H5'' | 1:CA:1138:G:OP1 | 2.09 | 0.53 |
| 41:D2:5:VAL:HB | 41:D2:37:VAL:HG11 | 1.90 | 0.52 |
| 41:D2:87:HIS:CE1 | 41:D2:89:GLN:HB2 | 2.44 | 0.52 |
| 31:DH:152:ARG:C | 31:DH:154:PRO:HD3 | 2.29 | 0.52 |
| 29:BF:178:PRO:HB3 | 29:BF:198:ALA:CB | 2.38 | 0.52 |
| 1:AA:1004:A:C4 | 1:AA:1025:U:O2 | 2.63 | 0.52 |
| 1:CA:1160:G:N3 | 1:CA:1160:G:H2' | 2.24 | 0.52 |
| 1:CA:126:G:H4' | 1:CA:634:C:H1' | 1.90 | 0.52 |
| 25:BA:1021:A:C8 | 25:BA:1022:G:H5'' | 2.42 | 0.52 |
| 1:CA:1256:A:N6 | 1:CA:1277:C:H3' | 2.24 | 0.52 |
| 32:BK:104:GLN:O | 32:BK:105:HIS:CD2 | 2.62 | 0.52 |
| 35:DO:47:ASP:O | 35:DO:50:ARG:N | 2.42 | 0.52 |
| 50:D4:33:VAL:HG23 | 50:D4:33:VAL:O | 2.09 | 0.52 |
| 1:AA:1369:C:H2' | 1:AA:1370:G:O4' | 2.09 | 0.52 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.44 | 0.52 |
| 25:BA:2702:U:H6 | 25:BA:2702:U:OP1 | 1.92 | 0.52 |
| 1:AA:922:G:C6 | 1:AA:923:A:C6 | 2.97 | 0.52 |
| 25:BA:2682:U:H6 | 25:BA:2682:U:H5' | 1.74 | 0.52 |
| 3:AF:58:GLU:N | 3:AF:65:ALA:HB3 | 2.24 | 0.52 |
| 8:AK:104:ARG:O | 8:AK:107:LEU:HB2 | 2.09 | 0.52 |
| 1:CA:280:C:H3' | 1:CA:281:G:H5' | 1.90 | 0.52 |
| 1:AA:412:A:H4' | 1:AA:413:G:O5' | 2.09 | 0.52 |
| 27:BD:228:PRO:HD3 | 27:BD:234:GLY:C | 2.29 | 0.52 |
| 26:DB:28:C:H2' | 26:DB:29:A:O4' | 2.09 | 0.52 |
| 31:DH:86:GLU:CD | 31:DH:86:GLU:H | 2.13 | 0.52 |
| 4:CG:9:CYS:O | 4:CG:12:CYS:HB2 | 2.09 | 0.52 |
| 8:AK:29:SER:OG | 8:AK:32:LYS:HB2 | 2.09 | 0.52 |
| 25:BA:2820:A:O2' | 25:BA:2821:A:OP1 | 2.25 | 0.52 |
| 6:CI:2:ARG:HH21 | 6:CI:69:GLU:HG3 | 1.74 | 0.52 |
| 25:BA:989:G:N7 | 49:BX:13:ILE:CD1 | 2.72 | 0.52 |
| 40:D1:110:VAL:O | 40:D1:114:LYS:HG2 | 2.09 | 0.52 |
| 15:CR:8:LYS:O | 15:CR:12:ILE:HG13 | 2.08 | 0.52 |
| 27:DD:93:ALA:HB3 | 27:DD:105:ILE:HG22 | 1.92 | 0.52 |
| 25:BA:1575:C:H2' | 25:BA:1576:U:C6 | 2.44 | 0.52 |
| 25:DA:2859:G:C8 | 25:DA:2859:G:H3' | 2.45 | 0.52 |
| 35:DO:90:ARG:HG3 | 35:DO:91:PHE:CD1 | 2.44 | 0.52 |
| 8:CK:51:VAL:HG11 | 8:CK:60:ARG:HH11 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 36:BP:58:PHE:O | 36:BP:58:PHE:HD1 | 1.90 | 0.52 |
| 25:BA:1057:A:H2' | 25:BA:1058:U:C6 | 2.45 | 0.52 |
| 25:BA:1057:A:O2' | 25:BA:1058:U:H5' | 2.09 | 0.52 |
| 40:D1:50:ARG:HB2 | 40:D1:50:ARG:NH2 | 2.25 | 0.52 |
| 41:D2:6:LYS:HG3 | 41:D2:11:GLN:HG2 | 1.91 | 0.52 |
| 9:AL:29:ASN:OD1 | 9:AL:64:THR:HA | 2.09 | 0.52 |
| 1:CA:977:A:C2 | 1:CA:1224:G:C5 | 2.97 | 0.52 |
| 1:CA:973:G:H1' | 10:CM:55:LYS:HG3 | 1.92 | 0.52 |
| 36:BP:75:THR:HA | 36:BP:88:GLY:C | 2.30 | 0.52 |
| 43:DT:40:LYS:HA | 43:DT:51:VAL:HG11 | 1.91 | 0.52 |
| 31:DH:4:ILE:HG13 | 31:DH:6:ARG:H | 1.75 | 0.52 |
| 25:BA:1797:C:C2' | 25:BA:1798:U:H5' | 2.39 | 0.52 |
| 25:BA:2210:G:H5' | 25:BA:2211:G:C5 | 2.44 | 0.52 |
| 40:B1:90:VAL:HG12 | 40:B1:91:ASP:CA | 2.39 | 0.52 |
| 25:DA:886:C:C2 | 25:DA:890:A:N1 | 2.77 | 0.52 |
| 25:DA:1025:G:C5 | 25:DA:1135:C:H1' | 2.45 | 0.52 |
| 27:BD:270:ILE:CG2 | 27:BD:271:ILE:N | 2.72 | 0.52 |
| 19:CV:67:VAL:O | 19:CV:69:HIS:N | 2.42 | 0.52 |
| 1:CA:362:G:H4' | 12:CO:33:ARG:HH21 | 1.74 | 0.52 |
| 25:BA:1385:G:H4' | 25:BA:1386:C:OP1 | 2.09 | 0.52 |
| 43:DT:55:ASN:HB2 | 43:DT:80:ILE:HG12 | 1.91 | 0.52 |
| 40:B1:79:PHE:CE1 | 40:B1:106:PHE:CZ | 2.94 | 0.52 |
| 22:AB:15:A:C2 | 22:AB:70:G:C6 | 2.96 | 0.52 |
| 40:B1:76:TYR:C | 40:B1:76:TYR:CD2 | 2.82 | 0.52 |
| 30:BG:114:ILE:HD13 | 30:BG:140:ILE:HG21 | 1.90 | 0.52 |
| 13:CP:110:ARG:NH1 | 13:CP:110:ARG:CG | 2.68 | 0.52 |
| 5:CH:47:LYS:O | 5:CH:57:LYS:HD3 | 2.10 | 0.52 |
| 1:AA:1333:A:H2' | 1:AA:1334:G:O5' | 2.09 | 0.52 |
| 26:DB:29:A:OP2 | 38:DQ:31:SER:HB2 | 2.09 | 0.52 |
| 12:AO:24:VAL:HG12 | 12:AO:27:LEU:HG | 1.90 | 0.52 |
| 1:AA:1255:G:O2' | 1:AA:1258:G:H1' | 2.09 | 0.52 |
| 1:CA:1014:A:H2' | 1:CA:1015:A:N9 | 2.24 | 0.52 |
| 1:AA:51:A:OP2 | 1:AA:52:G:C8 | 2.62 | 0.52 |
| 4:CG:127:THR:HB | 4:CG:131:ARG:O | 2.10 | 0.52 |
| 22:CB:76:U:C4 | 22:CB:77:C:C4 | 2.98 | 0.52 |
| 1:CA:20:U:H2' | 1:CA:21:G:H5' | 1.92 | 0.52 |
| 26:DB:1:U:O4 | 26:DB:119:A:N1 | 2.42 | 0.52 |
| 4:CG:101:LEU:HD23 | 4:CG:121:VAL:CG1 | 2.40 | 0.52 |
| 8:CK:95:VAL:HB | 8:CK:99:GLU:HB2 | 1.91 | 0.52 |
| 1:CA:1449:C:O3' | 1:CA:1450:U:H4' | 2.08 | 0.52 |
| 42:BS:21:VAL:HG23 | 42:BS:47:VAL:HG21 | 1.91 | 0.52 |
| 30:DG:75:LYS:O | 30:DG:76:SER:HB2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:BA:1590:U:H2' | 25:BA:1591:G:C8 | 2.43 | 0.52 |
| 22:AB:71:U:OP2 | 22:AB:71:U:H6 | 1.92 | 0.52 |
| 1:AA:1164:G:H2' | 1:AA:1165:C:C6 | 2.45 | 0.52 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:H6 | 1.74 | 0.52 |
| 45:DV:40:ASP:OD1 | 45:DV:42:VAL:HB | 2.09 | 0.52 |
| 25:DA:2638:G:O2' | 25:DA:2639:A:H8 | 1.91 | 0.52 |
| 25:BA:1069:A:O2' | 25:BA:1072:C:OP1 | 2.27 | 0.52 |
| 40:D1:90:VAL:O | 40:D1:92:ARG:HB3 | 2.10 | 0.52 |
| 1:CA:1004:A:C5' | 1:CA:1025:U:C4 | 2.92 | 0.52 |
| 52:B6:15:GLU:HG3 | 52:B6:47:THR:HG21 | 1.91 | 0.52 |
| 22:CB:21:A:H1' | 22:CB:22:G:P | 2.49 | 0.52 |
| 25:DA:1012:U:O2 | 25:DA:1143:A:C2 | 2.61 | 0.52 |
| 51:D5:45:VAL:CG1 | 51:D5:56:LYS:HG2 | 2.40 | 0.52 |
| 25:BA:880:G:N2 | 25:BA:898:C:C2 | 2.77 | 0.52 |
| 1:CA:1175:G:N1 | 1:CA:1176:A:C6 | 2.77 | 0.52 |
| 23:CD:59:A:H8 | 23:CD:59:A:OP2 | 1.92 | 0.52 |
| 25:BA:2210:G:H5' | 25:BA:2211:G:N7 | 2.24 | 0.52 |
| 25:DA:307:G:N2 | 25:DA:309:G:H3' | 2.24 | 0.52 |
| 25:BA:443:A:H3' | 29:BF:45:ARG:NH1 | 2.24 | 0.52 |
| 32:BK:9:LEU:CB | 32:BK:11:ASN:O | 2.55 | 0.52 |
| 25:DA:863:A:O2' | 25:DA:864:G:H5' | 2.10 | 0.52 |
| 19:CV:30:LEU:HD12 | 19:CV:31:ILE:H | 1.74 | 0.52 |
| 25:BA:2700:C:O2' | 25:BA:2701:C:H5' | 2.09 | 0.52 |
| 25:DA:1277:G:H4' | 37:D0:20:LEU:HD11 | 1.91 | 0.52 |
| 25:BA:2733:A:H3' | 25:BA:2734:A:H5'' | 1.91 | 0.52 |
| 1:AA:530:G:C4' | 1:AA:531:U:OP2 | 2.56 | 0.52 |
| 25:BA:2068:U:N3 | 25:BA:2430:A:H2 | 2.04 | 0.52 |
| 25:BA:1678:G:N2 | 25:BA:1989:G:N2 | 2.58 | 0.52 |
| 25:DA:443:A:H5'' | 25:DA:444:C:OP1 | 2.09 | 0.52 |
| 25:BA:2065:C:H2' | 25:BA:2066:C:H6 | 1.73 | 0.52 |
| 25:DA:634:C:H2' | 25:DA:635:C:C6 | 2.45 | 0.52 |
| 25:DA:908:C:O2' | 25:DA:909:A:H5' | 2.09 | 0.52 |
| 4:CG:110:PHE:HZ | 4:CG:182:LYS:HA | 1.73 | 0.52 |
| 15:AR:21:ASP:OD1 | 15:AR:24:SER:HB3 | 2.09 | 0.52 |
| 7:CJ:71:PRO:HD3 | 7:CJ:103:TRP:HZ3 | 1.75 | 0.52 |
| 1:CA:999:U:H3 | 1:CA:1041:A:H61 | 1.57 | 0.52 |
| 37:D0:84:ALA:HB3 | 37:D0:85:PRO:HD3 | 1.92 | 0.52 |
| 7:AJ:111:ARG:HB3 | 7:AJ:112:PRO:HD2 | 1.92 | 0.52 |
| 8:AK:103:VAL:CG2 | 8:AK:110:ALA:HB2 | 2.39 | 0.52 |
| 36:DP:110:THR:O | 36:DP:113:GLN:HB2 | 2.09 | 0.52 |
| 25:DA:1385:G:HO2' | 25:DA:1396:U:H6 | 1.56 | 0.52 |
| 19:AV:7:LYS:O | 19:AV:7:LYS:HD2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 2:AE:106:LYS:O | 2:AE:110:GLN:HG3 | 2.10 | 0.52 |
| 25:BA:2815:C:H2' | 25:BA:2816:C:H6 | 1.75 | 0.52 |
| 52:D6:25:LYS:HE2 | 52:D6:27:LYS:HZ2 | 1.75 | 0.52 |
| 28:BE:79:ARG:CZ | 28:BE:197:ILE:CG2 | 2.87 | 0.52 |
| 1:AA:1157:A:H62 | 1:AA:1178:G:N2 | 2.07 | 0.52 |
| 25:DA:9:U:O4 | 25:DA:2629:A:C2 | 2.63 | 0.52 |
| 40:D1:50:ARG:HG2 | 40:D1:53:ARG:NH2 | 2.24 | 0.52 |
| 25:BA:1794:U:H2' | 25:BA:1795:C:C6 | 2.43 | 0.52 |
| 28:DE:5:LEU:HD12 | 28:DE:50:GLY:O | 2.10 | 0.52 |
| 23:CC:58:A:H2' | 23:CC:59:A:H5' | 1.91 | 0.52 |
| 52:B6:46:HIS:O | 52:B6:47:THR:OG1 | 2.26 | 0.52 |
| 1:CA:972:C:O3' | 10:CM:57:LYS:CG | 2.57 | 0.52 |
| 47:DZ:91:LYS:HE3 | 47:DZ:92:LYS:H | 1.73 | 0.52 |
| 36:BP:104:PHE:CE1 | 36:BP:125:LEU:HD11 | 2.41 | 0.52 |
| 25:DA:2469:A:O2' | 36:DP:56:ARG:HG2 | 2.10 | 0.52 |
| 25:DA:2713:A:H3' | 25:DA:2714:G:C5' | 2.40 | 0.52 |
| 23:CD:56:U:C4 | 23:CD:59:A:N6 | 2.78 | 0.52 |
| 1:CA:1131:G:H2' | 1:CA:1132:C:C6 | 2.36 | 0.52 |
| 25:BA:1478:G:O2' | 25:BA:1558:A:H2 | 1.93 | 0.52 |
| 2:CE:153:ARG:HG3 | 2:CE:154:LEU:N | 2.15 | 0.52 |
| 25:BA:1538:G:O5' | 25:BA:1538:G:H8 | 1.92 | 0.52 |
| 50:D4:16:CYS:HB3 | 50:D4:20:ASN:H | 1.74 | 0.52 |
| 31:BH:152:ARG:HE | 31:BH:153:LYS:HZ3 | 1.57 | 0.52 |
| 25:DA:2327:A:H2' | 25:DA:2328:A:H8 | 1.73 | 0.52 |
| 25:BA:1937:A:O2' | 25:BA:1938:A:P | 2.67 | 0.52 |
| 25:BA:1177:A:H5' | 25:BA:1178:C:H6 | 1.74 | 0.52 |
| 19:CV:49:ILE:H | 19:CV:49:ILE:HD12 | 1.74 | 0.52 |
| 1:AA:5:U:O2' | 1:AA:6:G:N3 | 2.42 | 0.52 |
| 36:BP:36:ALA:O | 36:BP:99:PRO:HA | 2.09 | 0.52 |
| 25:BA:1264:G:H3' | 25:BA:1265:A:H5'' | 1.91 | 0.52 |
| 29:DF:82:ILE:CD1 | 29:DF:82:ILE:C | 2.75 | 0.52 |
| 33:BM:60:ILE:H | 33:BM:60:ILE:HD13 | 1.74 | 0.52 |
| 25:DA:1839:G:N3 | 25:DA:1839:G:H2' | 2.24 | 0.52 |
| 1:CA:142:G:H1 | 1:CA:221:C:H42 | 1.58 | 0.52 |
| 25:BA:2688:U:H3' | 25:BA:2688:U:O2 | 2.10 | 0.52 |
| 30:BG:101:ILE:HG13 | 50:B4:25:TYR:O | 2.09 | 0.52 |
| 7:AJ:109:ASN:OD1 | 7:AJ:119:ARG:NH2 | 2.37 | 0.52 |
| 41:B2:25:LEU:H | 41:B2:92:THR:HG21 | 1.75 | 0.52 |
| 25:BA:796:C:H2' | 25:BA:797:C:C6 | 2.43 | 0.52 |
| 20:CW:50:GLU:CD | 20:CW:100:ILE:HG12 | 2.29 | 0.52 |
| 2:CE:5:ILE:HD12 | 2:CE:59:GLU:CD | 2.30 | 0.52 |
| 25:DA:979:G:H3' | 25:DA:980:A:H5'' | 1.89 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:986:A:N3 | 19:CV:52:TYR:OH | 2.29 | 0.52 |
| 25:BA:1364:G:OP2 | 47:BZ:2:SER:OG | 2.26 | 0.52 |
| 6:CI:53:ALA:O | 6:CI:54:LYS:HB2 | 2.10 | 0.52 |
| 17:AT:66:SER:OG | 17:AT:69:LYS:HB2 | 2.09 | 0.52 |
| 34:BN:25:LEU:O | 34:BN:26:LYS:HG2 | 2.09 | 0.52 |
| 2:CE:24:TRP:C | 2:CE:24:TRP:CD1 | 2.80 | 0.52 |
| 25:DA:534:U:O2' | 40:D1:49:HIS:HD2 | 1.93 | 0.52 |
| 25:DA:1568:G:H21 | 27:DD:58:HIS:CE1 | 2.27 | 0.52 |
| 36:DP:134:ARG:NH2 | 45:DV:122:ARG:HD2 | 2.24 | 0.52 |
| 27:BD:44:ASN:N | 27:BD:44:ASN:ND2 | 2.57 | 0.52 |
| 1:AA:1131:G:OP2 | 1:AA:1131:G:H8 | 1.92 | 0.52 |
| 28:DE:37:ARG:HD3 | 28:DE:44:TYR:CZ | 2.44 | 0.52 |
| 28:DE:8:LYS:HG2 | 28:DE:192:ASN:HD22 | 1.73 | 0.52 |
| 31:DH:152:ARG:C | 31:DH:154:PRO:HD2 | 2.28 | 0.52 |
| 35:DO:64:LYS:HB2 | 54:D8:25:MET:CG | 2.21 | 0.52 |
| 4:CG:13:ARG:HB3 | 4:CG:33:MET:SD | 2.49 | 0.52 |
| 25:DA:2752:C:O4' | 25:DA:2752:C:OP2 | 2.27 | 0.52 |
| 23:AC:76:C:OP2 | 23:AC:77:A:O3' | 2.26 | 0.52 |
| 1:CA:1160:G:N1 | 1:CA:1177:G:N2 | 2.33 | 0.52 |
| 1:CA:1235:U:O2' | 1:CA:1305:G:O5' | 2.26 | 0.52 |
| 1:CA:1330:U:H5' | 1:CA:1331:G:O5' | 2.09 | 0.52 |
| 25:DA:2776:A:H4' | 25:DA:2777:G:O5' | 2.09 | 0.52 |
| 36:DP:78:PRO:O | 36:DP:79:LEU:HG | 2.09 | 0.52 |
| 25:DA:1300:U:H5'' | 25:DA:1301:A:H5'' | 1.91 | 0.52 |
| 25:DA:1677:A:H2' | 25:DA:1678:G:O4' | 2.09 | 0.52 |
| 40:B1:98:LEU:C | 40:B1:98:LEU:HD23 | 2.30 | 0.52 |
| 20:AW:24:LEU:HD12 | 20:AW:24:LEU:C | 2.26 | 0.52 |
| 25:BA:2119:A:H61 | 25:BA:2170:A:H62 | 1.55 | 0.52 |
| 25:BA:2168:G:C2' | 25:BA:2168:G:N3 | 2.73 | 0.52 |
| 25:DA:2329:G:H2' | 25:DA:2330:G:C8 | 2.45 | 0.52 |
| 25:DA:910:A:C5 | 36:DP:13:GLN:HG3 | 2.44 | 0.52 |
| 25:BA:141:A:H8 | 25:BA:1595:G:H21 | 1.56 | 0.52 |
| 47:BZ:92:LYS:HA | 47:BZ:95:LEU:CB | 2.39 | 0.52 |
| 27:BD:166:GLN:HA | 27:BD:166:GLN:NE2 | 2.21 | 0.52 |
| 51:B5:51:TYR:H | 51:B5:56:LYS:CB | 2.23 | 0.52 |
| 25:DA:84:A:O5' | 44:DU:8:LYS:HD3 | 2.09 | 0.52 |
| 1:AA:1226:C:O2 | 19:AV:83:HIS:HE1 | 1.92 | 0.52 |
| 12:CO:40:VAL:HG11 | 12:CO:77:LEU:O | 2.09 | 0.52 |
| 5:CH:57:LYS:O | 5:CH:61:TYR:CD2 | 2.63 | 0.52 |
| 25:BA:2250:G:C6 | 36:BP:82:ARG:HD3 | 2.44 | 0.52 |
| 52:B6:33:LYS:O | 52:B6:35:GLU:HG3 | 2.09 | 0.52 |
| 1:AA:96:G:C6 | 1:AA:97:U:C2 | 2.98 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:2875:C:C4' | 39:BR:5:ALA:HB2 | 2.40 | 0.52 |
| 25:DA:154:G:H3' | 25:DA:155:C:H6 | 1.73 | 0.52 |
| 10:CM:8:LEU:HD22 | 10:CM:20:ALA:CB | 2.40 | 0.52 |
| 28:BE:170:LEU:HD11 | 28:BE:187:ALA:HB3 | 1.90 | 0.52 |
| 38:BQ:48:LEU:HD23 | 38:BQ:82:ILE:HD11 | 1.90 | 0.52 |
| 35:DO:113:LYS:HG2 | 35:DO:115:LEU:HD21 | 1.91 | 0.52 |
| 2:CE:55:PHE:CD1 | 2:CE:58:ILE:HD12 | 2.44 | 0.52 |
| 25:BA:1045:A:N3 | 25:BA:1111:A:N6 | 2.57 | 0.52 |
| 25:BA:2019:A:C2' | 25:BA:2020:A:O5' | 2.57 | 0.52 |
| 25:BA:2505:G:O6 | 25:BA:2576:G:H2' | 2.09 | 0.52 |
| 52:D6:12:GLU:HG3 | 52:D6:21:TYR:HB3 | 1.92 | 0.52 |
| 1:AA:757:U:H2' | 1:AA:758:G:O4' | 2.09 | 0.52 |
| 35:BO:96:THR:C | 35:BO:98:GLU:H | 2.11 | 0.52 |
| 37:B0:42:LYS:O | 37:B0:45:ARG:HD2 | 2.10 | 0.52 |
| 25:BA:6:A:H2' | 25:BA:7:G:O4' | 2.09 | 0.52 |
| 25:DA:2010:G:H5'' | 42:DS:42:ARG:HB2 | 1.91 | 0.52 |
| 25:BA:2352:A:C4 | 25:BA:2366:A:C2 | 2.97 | 0.52 |
| 25:BA:1085:A:C4' | 25:BA:1086:A:OP1 | 2.57 | 0.52 |
| 38:DQ:106:ARG:O | 38:DQ:107:GLU:HB2 | 2.10 | 0.52 |
| 33:BM:35:ARG:HG3 | 33:BM:37:LYS:HG3 | 1.89 | 0.52 |
| 27:DD:27:THR:CG2 | 27:DD:28:GLU:N | 2.72 | 0.52 |
| 1:CA:1356:G:N2 | 1:CA:1367:C:O2 | 2.43 | 0.52 |
| 2:AE:21:ARG:HG2 | 2:AE:21:ARG:O | 2.05 | 0.52 |
| 29:BF:46:ARG:NH1 | 29:BF:46:ARG:CG | 2.67 | 0.52 |
| 25:DA:1022:G:C2' | 25:DA:1023:U:OP2 | 2.58 | 0.52 |
| 1:AA:973:G:OP1 | 10:AM:57:LYS:HD3 | 2.09 | 0.52 |
| 1:CA:1309:G:C6 | 1:CA:1329:A:C2 | 2.98 | 0.52 |
| 13:CP:37:THR:HG23 | 13:CP:59:TYR:CD2 | 2.45 | 0.52 |
| 1:CA:634:C:H2' | 1:CA:635:G:H8 | 1.75 | 0.52 |
| 1:CA:1149:C:OP2 | 9:CL:9:ARG:NH1 | 2.43 | 0.52 |
| 26:DB:40:U:O2 | 26:DB:46:A:C6 | 2.62 | 0.52 |
| 38:BQ:15:ARG:HD3 | 38:BQ:88:ASP:OD2 | 2.10 | 0.52 |
| 17:CT:63:ARG:HG2 | 17:CT:64:PRO:HD2 | 1.90 | 0.52 |
| 25:DA:1495:A:O2' | 25:DA:1496:A:H5' | 2.09 | 0.52 |
| 25:BA:1358:G:N2 | 25:BA:1372:U:C5 | 2.78 | 0.52 |
| 25:BA:811:U:C4 | 35:BO:21:ARG:NH2 | 2.78 | 0.52 |
| 30:DG:143:GLU:N | 30:DG:143:GLU:OE2 | 2.41 | 0.52 |
| 17:CT:59:ILE:CG2 | 17:CT:71:PHE:HB3 | 2.39 | 0.52 |
| 41:B2:44:LYS:C | 41:B2:46:VAL:N | 2.63 | 0.52 |
| 25:BA:1153:C:OP1 | 40:B1:76:TYR:OH | 2.26 | 0.52 |
| 1:CA:927:G:N2 | 1:CA:1391:U:H1' | 2.25 | 0.52 |
| 23:AD:60:A:C2' | 23:AD:61:U:H5' | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:AD:9:G:N2 | 23:AD:46:G:C8 | 2.77 | 0.52 |
| 9:CL:125:TYR:CD2 | 9:CL:125:TYR:C | 2.83 | 0.52 |
| 23:CC:2:G:N3 | 23:CC:2:G:H2' | 2.24 | 0.52 |
| 39:BR:107:ASP:H | 39:BR:110:ILE:HG23 | 1.74 | 0.52 |
| 53:D7:43:THR:HG22 | 53:D7:44:PRO:O | 2.09 | 0.52 |
| 20:CW:104:LEU:O | 20:CW:105:SER:HB3 | 2.10 | 0.52 |
| 25:DA:372:G:O2' | 25:DA:373:U:OP2 | 2.28 | 0.52 |
| 28:DE:66:HIS:HE1 | 28:DE:73:GLU:HG3 | 1.74 | 0.52 |
| 1:AA:1258:G:C6 | 1:AA:1259:C:N4 | 2.77 | 0.52 |
| 25:BA:1931:U:O4' | 25:BA:1931:U:O2 | 2.24 | 0.52 |
| 3:AF:83:ARG:O | 3:AF:86:VAL:HG22 | 2.10 | 0.52 |
| 1:CA:920:U:O4' | 1:CA:1080:A:C2 | 2.62 | 0.52 |
| 46:D3:72:ARG:CB | 46:D3:75:LEU:HB2 | 2.39 | 0.52 |
| 1:AA:149:A:C2 | 1:AA:150:C:C2 | 2.98 | 0.52 |
| 1:AA:73:G:N3 | 1:AA:74:C:C5 | 2.78 | 0.52 |
| 29:BF:117:ARG:NH2 | 35:BO:1:MET:O | 2.43 | 0.52 |
| 1:CA:35:G:N2 | 1:CA:550:G:H1' | 2.24 | 0.52 |
| 1:AA:368:U:P | 32:DK:91:SER:OG | 2.68 | 0.52 |
| 25:DA:1638:C:H4' | 25:DA:2710:C:O2 | 2.09 | 0.52 |
| 42:DS:88:ARG:HD3 | 42:DS:94:ASP:OD1 | 2.09 | 0.52 |
| 1:CA:567:G:H2' | 1:CA:568:G:O4' | 2.09 | 0.52 |
| 28:DE:7:VAL:HG21 | 39:DR:1:MET:HE3 | 1.91 | 0.52 |
| 37:D0:45:ARG:HA | 37:D0:95:THR:HG21 | 1.91 | 0.52 |
| 23:AD:51:U:H2' | 23:AD:52:C:C6 | 2.45 | 0.52 |
| 25:BA:84:A:N1 | 25:BA:98:G:O2' | 2.33 | 0.52 |
| 1:AA:1428:A:H2' | 1:AA:1429:C:C6 | 2.45 | 0.52 |
| 32:DK:51:ILE:HG22 | 32:DK:52:ARG:N | 2.24 | 0.52 |
| 34:BN:8:LEU:HD13 | 34:BN:82:ASN:HB2 | 1.91 | 0.52 |
| 46:B3:50:ASN:HB3 | 46:B3:63:VAL:HG22 | 1.91 | 0.52 |
| 52:D6:31:PRO:HB2 | 52:D6:33:LYS:H | 1.74 | 0.52 |
| 25:DA:2393:A:O3' | 35:DO:62:LEU:HA | 2.10 | 0.52 |
| 25:DA:2801:A:H5' | 25:DA:2895:U:O2' | 2.10 | 0.52 |
| 38:DQ:24:LEU:HD12 | 38:DQ:41:ASP:HB2 | 1.91 | 0.52 |
| 28:BE:59:VAL:CG1 | 28:BE:63:LEU:HB3 | 2.39 | 0.52 |
| 25:BA:1793:C:O2 | 25:BA:1900:A:H2 | 1.93 | 0.52 |
| 1:CA:1319:A:C5' | 1:CA:1320:C:OP1 | 2.57 | 0.52 |
| 45:DV:145:GLU:O | 45:DV:145:GLU:CG | 2.57 | 0.52 |
| 35:BO:50:ARG:HD3 | 54:B8:7:HIS:CD2 | 2.45 | 0.52 |
| 2:CE:115:LEU:HD21 | 2:CE:153:ARG:NH1 | 2.25 | 0.52 |
| 53:B7:11:LYS:HE3 | 53:B7:15:THR:OG1 | 2.10 | 0.52 |
| 4:CG:3:ARG:NH1 | 4:CG:115:ARG:HB3 | 2.23 | 0.52 |
| 30:DG:109:VAL:HG22 | 50:D4:33:VAL:HG11 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 6:CI:63:TYR:CD2 | 6:CI:63:TYR:N | 2.78 | 0.52 |
| 2:AE:69:LEU:HD13 | 2:AE:91:PRO:HB2 | 1.92 | 0.52 |
| 29:DF:123:LEU:HD11 | 29:DF:125:LEU:HD22 | 1.91 | 0.52 |
| 25:BA:1188:U:H2' | 25:BA:1189:A:H5' | 1.92 | 0.52 |
| 36:DP:7:MET:CB | 36:DP:10:ARG:NH2 | 2.71 | 0.52 |
| 22:CB:55:G:C4 | 22:CB:56:G:N7 | 2.78 | 0.52 |
| 1:CA:353:A:H2' | 1:CA:354:G:OP2 | 2.10 | 0.52 |
| 23:AD:9:G:C6 | 23:AD:47:G:N1 | 2.77 | 0.52 |
| 25:DA:239:U:H2' | 25:DA:240:G:O4' | 2.10 | 0.52 |
| 37:B0:74:LYS:O | 37:B0:75:LEU:HB3 | 2.09 | 0.52 |
| 27:BD:239:ARG:O | 27:BD:240:ALA:HB2 | 2.08 | 0.52 |
| 50:B4:12:ALA:HB3 | 50:B4:24:THR:HB | 1.90 | 0.52 |
| 28:BE:25:VAL:CG1 | 28:BE:183:LEU:HG | 2.39 | 0.52 |
| 16:CS:48:TRP:CH2 | 16:CS:76:GLN:NE2 | 2.78 | 0.52 |
| 25:DA:1858:G:H1' | 25:DA:1884:A:H61 | 1.73 | 0.52 |
| 9:AL:9:ARG:HA | 9:AL:76:ALA:HB1 | 1.91 | 0.52 |
| 45:BV:141:VAL:HG12 | 45:BV:142:SER:H | 1.75 | 0.52 |
| 1:AA:256:U:OP1 | 17:AT:17:LYS:NZ | 2.43 | 0.52 |
| 25:DA:78:A:H2' | 25:DA:79:G:H8 | 1.74 | 0.52 |
| 4:CG:139:ARG:NH1 | 4:CG:139:ARG:HG3 | 2.25 | 0.52 |
| 25:DA:2646:C:OP2 | 25:DA:2732:G:O2' | 2.23 | 0.52 |
| 20:CW:10:LEU:C | 20:CW:10:LEU:HD22 | 2.30 | 0.52 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:N7 | 2.78 | 0.52 |
| 1:CA:1106:G:N3 | 1:CA:1107:C:C6 | 2.78 | 0.52 |
| 23:CC:73:A:N6 | 23:CC:74:A:C6 | 2.78 | 0.52 |
| 31:DH:54:ARG:HB3 | 31:DH:65:HIS:CD2 | 2.45 | 0.52 |
| 25:DA:1449(A):G:H2' | 25:DA:1450:C:H6 | 1.73 | 0.52 |
| 1:CA:10:A:H2' | 1:CA:11:G:H8 | 1.75 | 0.52 |
| 39:BR:129:ARG:O | 39:BR:133:GLU:HG3 | 2.09 | 0.52 |
| 32:DK:142:VAL:HG22 | 32:DK:142:VAL:O | 2.09 | 0.52 |
| 25:BA:2818:G:O2' | 25:BA:2819:G:H5' | 2.09 | 0.52 |
| 25:BA:1339:G:N2 | 25:BA:1603:A:H1' | 2.24 | 0.52 |
| 43:DT:67:GLY:C | 43:DT:69:TYR:H | 2.13 | 0.52 |
| 25:BA:1103:A:H2' | 25:BA:1104:C:H5' | 1.92 | 0.52 |
| 27:BD:273:ARG:HG2 | 27:BD:273:ARG:O | 2.08 | 0.52 |
| 30:BG:67:LYS:NZ | 50:B4:6:HIS:NE2 | 2.57 | 0.52 |
| 54:D8:25:MET:O | 54:D8:48:PHE:CE1 | 2.62 | 0.52 |
| 54:B8:36:LYS:O | 54:B8:38:GLY:N | 2.43 | 0.52 |
| 25:BA:2211:G:C4' | 25:BA:2212:A:OP2 | 2.56 | 0.52 |
| 30:DG:41:GLN:NE2 | 30:DG:60:LEU:HD12 | 2.25 | 0.52 |
| 26:DB:42:C:O2 | 30:DG:92:VAL:HA | 2.10 | 0.52 |
| 25:DA:309:G:N3 | 25:DA:329:G:O2' | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 43:DT:24:GLY:O | 43:DT:83:VAL:HG12 | 2.10 | 0.52 |
| 39:BR:90:GLN:NE2 | 39:BR:116:ALA:HA | 2.25 | 0.52 |
| 25:BA:1593:G:H2' | 25:BA:1594:G:H8 | 1.72 | 0.52 |
| 29:DF:7:TYR:HA | 29:DF:125:LEU:O | 2.10 | 0.52 |
| 25:BA:527:C:H4' | 25:BA:528:A:O5' | 2.10 | 0.52 |
| 1:AA:129(A):G:N2 | 1:AA:191(A):G:N7 | 2.57 | 0.52 |
| 1:CA:1219:U:OP1 | 14:CQ:19:ARG:NH1 | 2.35 | 0.52 |
| 1:CA:245:C:O2 | 1:CA:283:C:N3 | 2.43 | 0.52 |
| 4:CG:162:LEU:HD12 | 4:CG:181:MET:HE3 | 1.91 | 0.52 |
| 25:DA:443:A:N7 | 29:DF:45:ARG:HD2 | 2.25 | 0.52 |
| 30:DG:124:SER:HB2 | 30:DG:131:TYR:CE1 | 2.44 | 0.52 |
| 4:CG:139:ARG:CG | 4:CG:139:ARG:HH11 | 2.22 | 0.52 |
| 25:BA:2751:G:HO2' | 25:BA:2752:C:P | 2.32 | 0.52 |
| 31:DH:41:MET:CE | 31:DH:64:LEU:HB2 | 2.39 | 0.52 |
| 25:DA:751:A:H5' | 42:DS:90:ARG:HA | 1.92 | 0.52 |
| 11:AN:54:ARG:NH2 | 23:AD:40:C:O3' | 2.42 | 0.52 |
| 1:AA:1250:A:H4' | 9:AL:68:GLY:N | 2.25 | 0.52 |
| 1:CA:369:C:O2 | 1:CA:369:C:H2' | 2.09 | 0.52 |
| 25:BA:2901:C:C4 | 25:BA:2902:C:N4 | 2.74 | 0.52 |
| 25:DA:56:A:C2 | 25:DA:115:C:O2 | 2.63 | 0.52 |
| 25:BA:26:G:H1' | 25:BA:515:A:H61 | 1.75 | 0.52 |
| 3:CF:186:PHE:CE2 | 3:CF:188:LEU:HD21 | 2.45 | 0.52 |
| 40:D1:52:ARG:HB3 | 40:D1:52:ARG:NH1 | 2.25 | 0.52 |
| 28:BE:1:MET:HB3 | 28:BE:200:GLU:OE1 | 2.09 | 0.52 |
| 54:D8:51:ALA:O | 54:D8:52:LYS:C | 2.49 | 0.52 |
| 27:DD:32:SER:HA | 27:DD:35:LYS:O | 2.09 | 0.52 |
| 39:DR:55:ASN:CG | 39:DR:55:ASN:O | 2.47 | 0.52 |
| 13:CP:87:TYR:O | 13:CP:91:ARG:HG2 | 2.09 | 0.52 |
| 1:CA:1061:G:C2' | 1:CA:1062:U:H5' | 2.38 | 0.52 |
| 25:DA:2469:A:C2 | 25:DA:2470:G:C5 | 2.98 | 0.52 |
| 38:BQ:11:LYS:HD2 | 38:BQ:15:ARG:NH2 | 2.23 | 0.52 |
| 2:CE:67:THR:HG21 | 2:CE:155:LEU:HG | 1.92 | 0.52 |
| 31:BH:6:ARG:HA | 31:BH:66:GLY:HA2 | 1.91 | 0.52 |
| 26:DB:8:U:H3 | 26:DB:112:G:H1 | 1.58 | 0.52 |
| 25:BA:784:A:C5 | 27:BD:229:VAL:HG21 | 2.45 | 0.52 |
| 19:CV:12:ASP:O | 19:CV:16:LEU:HD13 | 2.09 | 0.52 |
| 39:DR:6:LEU:O | 39:DR:10:VAL:HG23 | 2.10 | 0.52 |
| 31:DH:78:GLY:O | 31:DH:136:ILE:HG22 | 2.09 | 0.52 |
| 1:AA:606:G:N2 | 1:AA:631:G:C8 | 2.78 | 0.52 |
| 5:AH:31:LEU:HD23 | 5:AH:45:PHE:CD1 | 2.38 | 0.52 |
| 1:AA:1399:C:C2 | 1:AA:1401:G:C5 | 2.98 | 0.52 |
| 23:AD:21:U:C3' | 23:AD:22:A:C5' | 2.88 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:197:A:N6 | 25:BA:2430:A:H2' | 2.24 | 0.52 |
| 26:BB:13:A:H2' | 26:BB:70:C:O2' | 2.10 | 0.52 |
| 15:CR:24:SER:O | 15:CR:28:GLN:HG3 | 2.09 | 0.52 |
| 16:CS:43:LYS:HB3 | 16:CS:48:TRP:CD1 | 2.45 | 0.52 |
| 25:BA:1192:G:O2' | 25:BA:1193:G:H5' | 2.10 | 0.52 |
| 22:AB:42:U:H3' | 22:AB:43:A:H8 | 1.75 | 0.52 |
| 25:DA:838:C:O2' | 25:DA:839:U:H5' | 2.10 | 0.52 |
| 1:CA:838:G:H1 | 1:CA:848:C:H42 | 1.58 | 0.52 |
| 25:DA:855:G:O2' | 46:D3:27:GLU:OE2 | 2.27 | 0.52 |
| 38:BQ:4:LEU:O | 38:BQ:5:THR:HG23 | 2.10 | 0.52 |
| 45:BV:48:PHE:HE2 | 45:BV:71:VAL:HG21 | 1.74 | 0.52 |
| 1:AA:321:A:N7 | 1:AA:328:C:O2' | 2.36 | 0.52 |
| 25:DA:2249:U:N3 | 25:DA:2253:G:OP2 | 2.35 | 0.52 |
| 25:BA:270(J):G:H2' | 25:BA:270(K):C:O4' | 2.10 | 0.52 |
| 25:BA:943:U:OP2 | 35:BO:36:LYS:CE | 2.58 | 0.52 |
| 1:AA:945:G:C2 | 1:AA:946:A:C8 | 2.98 | 0.52 |
| 2:AE:73:THR:OG1 | 2:AE:170:GLU:OE2 | 2.22 | 0.52 |
| 25:BA:1939:U:OP1 | 25:BA:2604:U:O2' | 2.23 | 0.52 |
| 1:AA:151:A:H2' | 1:AA:151:A:N3 | 2.23 | 0.52 |
| 6:CI:15:ASP:C | 6:CI:15:ASP:OD1 | 2.49 | 0.52 |
| 5:AH:41:VAL:CG1 | 5:AH:113:ALA:HB2 | 2.39 | 0.52 |
| 25:DA:1217:C:P | 40:D1:15:LYS:HE3 | 2.50 | 0.52 |
| 27:DD:35:LYS:CE | 27:DD:104:TYR:HD1 | 2.23 | 0.52 |
| 33:BM:35:ARG:O | 33:BM:37:LYS:HG3 | 2.10 | 0.52 |
| 1:CA:976:G:C8 | 1:CA:1358:U:C2 | 2.98 | 0.52 |
| 28:DE:52:LEU:O | 28:DE:75:VAL:N | 2.43 | 0.52 |
| 27:DD:25:THR:C | 27:DD:27:THR:N | 2.63 | 0.52 |
| 52:B6:41:PRO:HD2 | 52:B6:46:HIS:CA | 2.39 | 0.52 |
| 1:AA:1005:A:C2 | 1:AA:1006:C:C2 | 2.98 | 0.52 |
| 25:DA:2271:G:OP1 | 46:D3:18:ALA:HB1 | 2.10 | 0.52 |
| 1:CA:1306:A:H61 | 1:CA:1331:G:H1' | 1.75 | 0.52 |
| 25:DA:747:U:H5 | 51:D5:3:LYS:HB2 | 1.67 | 0.52 |
| 25:DA:2713:A:H3' | 25:DA:2714:G:H5' | 1.91 | 0.52 |
| 25:BA:1798:U:H5'' | 27:BD:259:THR:CG2 | 2.31 | 0.52 |
| 1:CA:1281:U:H3' | 1:CA:1282:C:C5 | 2.45 | 0.52 |
| 40:B1:98:LEU:HD23 | 40:B1:99:ALA:N | 2.25 | 0.52 |
| 26:DB:15:A:C3' | 26:DB:16:G:H5' | 2.36 | 0.52 |
| 23:CD:57:C:N4 | 25:DA:2112:G:H22 | 1.98 | 0.52 |
| 25:DA:2173:A:C2 | 25:DA:2174:C:H4' | 2.45 | 0.52 |
| 41:D2:27:ALA:HB3 | 41:D2:61:VAL:HG21 | 1.92 | 0.52 |
| 25:BA:1332:G:H21 | 25:BA:1610:A:H8 | 1.57 | 0.52 |
| 31:BH:153:LYS:HZ3 | 31:BH:153:LYS:H | 1.56 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:1210:A:H5'' | 25:BA:1212:G:O4' | 2.10 | 0.52 |
| 6:AI:8:ILE:HG22 | 6:AI:10:LEU:HD12 | 1.90 | 0.52 |
| 1:CA:1187:G:P | 9:CL:113:LYS:HZ1 | 2.33 | 0.52 |
| 1:CA:407:G:H1 | 1:CA:435:C:N4 | 2.04 | 0.52 |
| 5:CH:67:VAL:HG21 | 5:CH:140:ARG:HG3 | 1.91 | 0.52 |
| 1:AA:351:G:H4' | 1:AA:352:C:OP1 | 2.09 | 0.52 |
| 36:DP:20:ALA:O | 36:DP:21:THR:HG22 | 2.10 | 0.52 |
| 32:DK:76:THR:HG23 | 32:DK:77:LEU:H | 1.75 | 0.52 |
| 1:AA:883:C:H2' | 1:AA:884:U:H5' | 1.90 | 0.52 |
| 25:DA:1287:A:H5'' | 25:DA:1288:U:OP2 | 2.09 | 0.52 |
| 25:BA:602:G:N2 | 25:BA:655:A:C8 | 2.74 | 0.52 |
| 26:BB:73:A:C4 | 26:BB:104:A:C2 | 2.98 | 0.52 |
| 23:AD:31:G:H2' | 23:AD:32:G:C8 | 2.45 | 0.52 |
| 25:BA:2281:C:O2' | 25:BA:2282:G:H5' | 2.09 | 0.52 |
| 1:AA:627:G:O2' | 1:AA:628:G:H5' | 2.10 | 0.52 |
| 25:DA:2483:C:O2 | 25:DA:2483:C:H2' | 2.10 | 0.52 |
| 1:AA:835:U:OP2 | 18:AU:60:ALA:HB3 | 2.10 | 0.52 |
| 25:DA:200:U:O4 | 25:DA:250:G:N2 | 2.43 | 0.52 |
| 25:BA:744:G:OP1 | 28:BE:132:HIS:ND1 | 2.35 | 0.52 |
| 25:DA:734:A:O2' | 25:DA:1635:G:H5' | 2.10 | 0.52 |
| 3:CF:190:ARG:HD2 | 3:CF:190:ARG:H | 1.75 | 0.52 |
| 3:AF:104:GLN:HA | 3:AF:104:GLN:HE21 | 1.75 | 0.52 |
| 38:BQ:106:ARG:HA | 38:BQ:110:LEU:HD21 | 1.91 | 0.51 |
| 27:BD:35:LYS:CE | 27:BD:64:ILE:C | 2.78 | 0.51 |
| 28:BE:59:VAL:HG13 | 28:BE:63:LEU:CB | 2.40 | 0.51 |
| 28:BE:34:VAL:HG21 | 28:BE:64:LYS:HZ1 | 1.76 | 0.51 |
| 1:AA:1054:C:O2' | 1:AA:1055:A:H5'' | 2.10 | 0.51 |
| 25:DA:2061:G:H5'' | 25:DA:2503:A:C2 | 2.44 | 0.51 |
| 29:DF:63:LYS:CE | 29:DF:67:GLN:HB3 | 2.40 | 0.51 |
| 1:CA:952:U:H4' | 1:CA:964:A:N1 | 2.26 | 0.51 |
| 36:DP:63:LYS:O | 36:DP:63:LYS:HD3 | 1.93 | 0.51 |
| 25:DA:1085:A:C4' | 25:DA:1086:A:OP1 | 2.58 | 0.51 |
| 51:D5:49:CYS:O | 51:D5:56:LYS:HB3 | 2.10 | 0.51 |
| 25:BA:1380:G:N2 | 25:BA:1570:A:C2 | 2.77 | 0.51 |
| 1:CA:1142:G:H2' | 1:CA:1143:G:C8 | 2.45 | 0.51 |
| 26:DB:43:C:H1' | 30:DG:93:THR:O | 2.10 | 0.51 |
| 26:DB:44:G:H1' | 26:DB:47:C:N4 | 2.25 | 0.51 |
| 1:AA:39:G:N7 | 1:AA:547:A:C8 | 2.75 | 0.51 |
| 25:BA:229:A:O2' | 25:BA:230:U:OP1 | 2.26 | 0.51 |
| 33:BM:130:HIS:CD2 | 33:BM:134:ARG:HH12 | 2.29 | 0.51 |
| 7:CJ:24:THR:HA | 7:CJ:27:ILE:HD12 | 1.91 | 0.51 |
| 2:CE:178:ARG:HH22 | 2:CE:196:LEU:C | 2.14 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 31:BH:86:GLU:HG2 | 31:BH:87:LEU:H | 1.76 | 0.51 |
| 25:BA:2689:U:H4' | 25:BA:2690:C:OP2 | 2.10 | 0.51 |
| 1:AA:129(A):G:C2 | 1:AA:191(A):G:C8 | 2.98 | 0.51 |
| 23:AD:8:U:H5'' | 23:AD:9:G:OP2 | 2.10 | 0.51 |
| 25:BA:1047:G:HO2' | 25:BA:1048:A:H8 | 1.55 | 0.51 |
| 8:AK:63:LEU:HB3 | 8:AK:65:TYR:CE1 | 2.45 | 0.51 |
| 1:AA:620:C:C6 | 4:AG:135:LEU:HD23 | 2.45 | 0.51 |
| 1:CA:652:U:C4 | 1:CA:752:G:N3 | 2.77 | 0.51 |
| 32:DK:25:TYR:CE2 | 32:DK:29:TYR:HD2 | 2.27 | 0.51 |
| 45:DV:114:GLY:C | 45:DV:116:VAL:H | 2.13 | 0.51 |
| 1:AA:389:A:H2' | 1:AA:390:C:C5' | 2.40 | 0.51 |
| 25:BA:2209:C:O2 | 25:BA:2216:G:C2 | 2.62 | 0.51 |
| 45:BV:142:SER:N | 45:BV:143:GLY:HA2 | 2.24 | 0.51 |
| 45:BV:128:VAL:HG23 | 45:BV:160:GLY:HA3 | 1.92 | 0.51 |
| 22:CB:76:U:O4 | 22:CB:77:C:N4 | 2.43 | 0.51 |
| 30:BG:26:GLN:NE2 | 30:BG:27:ASN:HB2 | 2.25 | 0.51 |
| 1:CA:375:U:OP1 | 16:CS:69:THR:OG1 | 2.16 | 0.51 |
| 20:AW:96:GLY:O | 20:AW:97:ALA:HB3 | 2.09 | 0.51 |
| 30:DG:171:ALA:O | 30:DG:174:GLU:N | 2.43 | 0.51 |
| 25:DA:1504:C:O2' | 25:DA:1505:C:H5' | 2.09 | 0.51 |
| 13:AP:82:MET:O | 13:AP:83:ASP:HB2 | 2.11 | 0.51 |
| 1:AA:130:A:O2' | 1:AA:131:C:O5' | 2.25 | 0.51 |
| 37:B0:57:ARG:HB3 | 37:B0:59:ASP:OD1 | 2.10 | 0.51 |
| 25:BA:2884:U:H2' | 25:BA:2885:C:H5' | 1.91 | 0.51 |
| 1:CA:1291:G:C6 | 1:CA:1292:U:C4 | 2.97 | 0.51 |
| 25:DA:657:U:H2' | 25:DA:658:C:C6 | 2.45 | 0.51 |
| 40:D1:74:LEU:HD12 | 40:D1:74:LEU:N | 2.25 | 0.51 |
| 25:BA:654(I):C:O2 | 25:BA:654(I):C:H3' | 2.10 | 0.51 |
| 1:AA:812:C:H4' | 1:AA:813:U:O5' | 2.09 | 0.51 |
| 25:BA:1063:G:H2' | 25:BA:1064:C:C6 | 2.44 | 0.51 |
| 40:D1:76:TYR:OH | 40:D1:93:LYS:HE2 | 2.10 | 0.51 |
| 41:D2:35:LEU:O | 41:D2:37:VAL:HG13 | 2.09 | 0.51 |
| 33:DM:39:ARG:HH11 | 33:DM:48:MET:HE2 | 1.75 | 0.51 |
| 27:BD:35:LYS:H | 27:BD:64:ILE:CG2 | 2.23 | 0.51 |
| 28:BE:47:VAL:O | 28:BE:48:GLN:C | 2.49 | 0.51 |
| 28:BE:50:GLY:HA2 | 28:BE:76:ARG:O | 2.10 | 0.51 |
| 23:CC:14:A:C2 | 23:CC:15:G:H1' | 2.45 | 0.51 |
| 1:CA:1355:G:O2' | 1:CA:1356:G:H5' | 2.10 | 0.51 |
| 22:AB:7:G:C3' | 22:AB:8:U:C5' | 2.82 | 0.51 |
| 1:AA:789:U:C5 | 1:AA:792:A:OP2 | 2.60 | 0.51 |
| 54:B8:36:LYS:HB2 | 54:B8:40:GLU:HB3 | 1.91 | 0.51 |
| 25:DA:528:A:C2 | 25:DA:2043:C:H4' | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 44:DU:19:LYS:HE3 | 44:DU:71:LYS:HZ2 | 1.75 | 0.51 |
| 25:BA:479:A:O2' | 25:BA:481:G:H2' | 2.10 | 0.51 |
| 44:BU:50:ARG:O | 44:BU:53:PRO:HD2 | 2.10 | 0.51 |
| 19:CV:66:MET:HA | 19:CV:67:VAL:HB | 1.92 | 0.51 |
| 25:DA:2353:G:H2' | 25:DA:2354:G:O4' | 2.09 | 0.51 |
| 25:DA:654(S):G:C4' | 25:DA:654(T):A:OP1 | 2.57 | 0.51 |
| 25:BA:1168:G:C2 | 25:BA:1182:A:C2 | 2.98 | 0.51 |
| 41:B2:39:LEU:HD13 | 41:B2:51:VAL:HG22 | 1.91 | 0.51 |
| 12:CO:41:ARG:CB | 12:CO:41:ARG:HH11 | 2.21 | 0.51 |
| 25:DA:2531:A:C5' | 31:DH:157:TYR:CE2 | 2.91 | 0.51 |
| 36:DP:3:MET:HG3 | 36:DP:4:PRO:O | 2.10 | 0.51 |
| 50:B4:15:ILE:O | 50:B4:33:VAL:HG12 | 2.10 | 0.51 |
| 1:AA:1008:C:N4 | 1:AA:1021:G:H1 | 2.06 | 0.51 |
| 1:CA:464:G:C5 | 1:CA:466:C:OP2 | 2.63 | 0.51 |
| 47:BZ:49:VAL:CG1 | 47:BZ:70:VAL:HG11 | 2.39 | 0.51 |
| 44:DU:63:LYS:HA | 44:DU:63:LYS:HZ3 | 1.72 | 0.51 |
| 32:BK:95:LYS:O | 32:BK:98:ALA:HB3 | 2.11 | 0.51 |
| 23:AD:11:A:N1 | 23:AD:26:C:O2 | 2.43 | 0.51 |
| 1:CA:57:G:C6 | 1:CA:58:C:C4 | 2.98 | 0.51 |
| 34:BN:3:GLN:HG3 | 34:BN:4:PRO:HD2 | 1.91 | 0.51 |
| 27:BD:72:LYS:HE3 | 27:BD:75:ILE:HD12 | 1.91 | 0.51 |
| 1:AA:1363:A:H1' | 1:AA:1365:G:N7 | 2.25 | 0.51 |
| 25:DA:1570:A:H2' | 25:DA:1571:A:C8 | 2.45 | 0.51 |
| 25:BA:2628:C:O2' | 25:BA:2781:A:H2' | 2.10 | 0.51 |
| 44:BU:5:MET:CE | 44:BU:32:PRO:HA | 2.40 | 0.51 |
| 25:BA:963:U:H2' | 25:BA:964:C:C6 | 2.46 | 0.51 |
| 25:BA:125:G:H4' | 25:BA:126:A:OP2 | 2.10 | 0.51 |
| 49:BX:43:ILE:O | 49:BX:47:VAL:HG23 | 2.11 | 0.51 |
| 47:BZ:56:GLN:HG3 | 47:BZ:83:GLU:C | 2.29 | 0.51 |
| 35:BO:62:LEU:CD2 | 54:B8:30:ARG:HH22 | 2.08 | 0.51 |
| 25:DA:1226:G:P | 41:D2:85:LYS:HA | 2.50 | 0.51 |
| 27:BD:34:VAL:O | 27:BD:34:VAL:CG1 | 2.57 | 0.51 |
| 29:DF:84:VAL:HG22 | 29:DF:84:VAL:O | 2.11 | 0.51 |
| 33:BM:42:TRP:O | 40:B1:64:ARG:NH2 | 2.43 | 0.51 |
| 23:CC:21:U:O2 | 23:CC:21:U:C2' | 2.50 | 0.51 |
| 31:DH:151:ILE:O | 31:DH:152:ARG:NE | 2.42 | 0.51 |
| 1:CA:978:A:C5' | 1:CA:979:C:OP2 | 2.58 | 0.51 |
| 1:CA:1061:G:H1' | 10:CM:56:HIS:CE1 | 2.45 | 0.51 |
| 36:DP:31:ASP:H | 36:DP:107:ALA:CB | 2.23 | 0.51 |
| 1:CA:1157:A:C2 | 1:CA:1181:G:H1' | 2.46 | 0.51 |
| 25:DA:1609:A:O2' | 25:DA:1610:A:H5' | 2.11 | 0.51 |
| 13:CP:29:ARG:HD3 | 13:CP:64:TRP:CD2 | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:CD:61:U:O2' | 23:CD:62:C:H5' | 2.10 | 0.51 |
| 32:BK:101:LEU:HD22 | 32:BK:109:ILE:HG23 | 1.92 | 0.51 |
| 1:CA:560:U:H4' | 1:CA:561:U:O5' | 2.09 | 0.51 |
| 25:BA:1359:A:N3 | 25:BA:1359:A:O4' | 2.43 | 0.51 |
| 9:CL:99:LEU:HB3 | 9:CL:101:PHE:CE1 | 2.45 | 0.51 |
| 23:AD:19:G:C1' | 23:AD:59:A:H2 | 2.21 | 0.51 |
| 2:CE:233:SER:HB3 | 2:CE:234:PRO:CD | 2.36 | 0.51 |
| 27:BD:25:THR:O | 27:BD:26:LYS:C | 2.47 | 0.51 |
| 37:B0:2:ARG:HG3 | 37:B0:5:LYS:NZ | 2.25 | 0.51 |
| 1:CA:1065:U:C5 | 1:CA:1190:G:H1' | 2.46 | 0.51 |
| 1:AA:961:U:OP2 | 1:AA:1223:C:H1' | 2.10 | 0.51 |
| 29:DF:125:LEU:HD12 | 29:DF:196:LEU:HD21 | 1.92 | 0.51 |
| 1:AA:965:A:C2 | 1:AA:969:A:C2 | 2.98 | 0.51 |
| 2:AE:22:LYS:HA | 2:AE:22:LYS:HZ2 | 1.75 | 0.51 |
| 29:DF:155:LEU:HD23 | 29:DF:186:ILE:HD13 | 1.92 | 0.51 |
| 27:DD:73:VAL:HG13 | 27:DD:120:GLY:HA3 | 1.92 | 0.51 |
| 25:DA:2056:G:H2' | 25:DA:2056:G:N3 | 2.25 | 0.51 |
| 1:CA:827:U:H5'' | 1:CA:828:A:OP2 | 2.11 | 0.51 |
| 48:DW:17:SER:HB2 | 48:DW:18:PRO:CA | 2.40 | 0.51 |
| 48:DW:17:SER:CB | 48:DW:18:PRO:CA | 2.88 | 0.51 |
| 25:BA:2565:A:H62 | 34:BN:28:SER:HB2 | 1.76 | 0.51 |
| 25:BA:1983:C:H2' | 25:BA:1984:G:H5' | 1.93 | 0.51 |
| 13:AP:115:LYS:O | 13:AP:117:VAL:CG1 | 2.58 | 0.51 |
| 1:AA:374:A:C6 | 1:AA:375:U:C4 | 2.98 | 0.51 |
| 1:AA:942:G:C2 | 1:AA:943:U:C6 | 2.99 | 0.51 |
| 1:CA:332:G:OP2 | 20:CW:10:LEU:HD13 | 2.10 | 0.51 |
| 28:DE:27:LEU:HG | 28:DE:27:LEU:O | 2.11 | 0.51 |
| 25:BA:447:A:N1 | 25:BA:454:A:O2' | 2.39 | 0.51 |
| 25:DA:1796:U:H2' | 25:DA:1797:C:C6 | 2.45 | 0.51 |
| 25:BA:827:U:H5' | 25:BA:828:U:O5' | 2.11 | 0.51 |
| 25:DA:19:C:H2' | 25:DA:20:C:C6 | 2.45 | 0.51 |
| 2:AE:17:PHE:HD1 | 2:AE:17:PHE:O | 1.93 | 0.51 |
| 1:AA:147:G:C2 | 1:AA:176:C:O2 | 2.64 | 0.51 |
| 25:DA:2065:C:H2' | 25:DA:2066:C:H6 | 1.74 | 0.51 |
| 25:BA:1085:A:N3 | 25:BA:1086:A:N7 | 2.58 | 0.51 |
| 52:D6:9:LEU:HD13 | 52:D6:11:LEU:HD21 | 1.92 | 0.51 |
| 27:DD:43:ARG:CB | 27:DD:54:ARG:HB2 | 2.40 | 0.51 |
| 28:BE:31:CYS:N | 28:BE:91:VAL:O | 2.39 | 0.51 |
| 25:DA:588:U:H2' | 25:DA:589:C:C6 | 2.45 | 0.51 |
| 25:DA:1063:G:C6 | 25:DA:1064:C:C2 | 2.99 | 0.51 |
| 1:CA:1305:G:H5' | 21:CX:4:GLY:HA3 | 1.91 | 0.51 |
| 23:CD:6:G:C2 | 23:CD:7:G:N7 | 2.78 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:180:U:H2' | 1:CA:181:G:H5' | 1.92 | 0.51 |
| 30:DG:41:GLN:HE21 | 30:DG:60:LEU:HD12 | 1.76 | 0.51 |
| 2:AE:8:LYS:CE | 2:AE:8:LYS:H | 2.23 | 0.51 |
| 25:DA:2117:A:N1 | 25:DA:2162:G:OP1 | 2.43 | 0.51 |
| 5:CH:90:VAL:O | 5:CH:120:THR:HA | 2.10 | 0.51 |
| 25:DA:1421:G:C2 | 25:DA:1422:G:C8 | 2.99 | 0.51 |
| 25:BA:1786:A:H1' | 25:BA:1938:A:N6 | 2.25 | 0.51 |
| 2:CE:231:GLU:HB3 | 2:CE:232:PRO:HD3 | 1.92 | 0.51 |
| 23:AC:2:G:H2' | 23:AC:3:C:C6 | 2.45 | 0.51 |
| 9:AL:81:ILE:O | 9:AL:85:LEU:HG | 2.10 | 0.51 |
| 23:CC:76:C:H2' | 23:CC:77:A:C8 | 2.46 | 0.51 |
| 25:DA:1027:A:N6 | 25:DA:1126:A:C4 | 2.79 | 0.51 |
| 44:BU:42:VAL:HG12 | 44:BU:65:ALA:HB3 | 1.91 | 0.51 |
| 28:DE:60:ASN:O | 28:DE:62:PRO:CD | 2.59 | 0.51 |
| 28:DE:64:LYS:HB3 | 28:DE:66:HIS:HD2 | 1.73 | 0.51 |
| 10:CM:48:THR:HA | 10:CM:62:HIS:CB | 2.40 | 0.51 |
| 25:DA:2389:G:H5'' | 25:DA:2390:U:O4' | 2.11 | 0.51 |
| 29:BF:64:ILE:HG23 | 29:BF:65:TRP:CD1 | 2.46 | 0.51 |
| 33:BM:34:LEU:HD21 | 33:BM:120:LEU:HB2 | 1.91 | 0.51 |
| 1:CA:668:G:C2' | 1:CA:669:U:H5' | 2.41 | 0.51 |
| 50:B4:36:CYS:O | 50:B4:39:CYS:SG | 2.69 | 0.51 |
| 25:BA:18:C:O3' | 40:B1:23:GLY:HA2 | 2.10 | 0.51 |
| 2:AE:189:ASP:OD1 | 2:AE:191:ASP:HB2 | 2.11 | 0.51 |
| 25:DA:646:A:H2' | 25:DA:647:G:O4' | 2.10 | 0.51 |
| 25:DA:17:G:H4' | 40:D1:25:TRP:CH2 | 2.45 | 0.51 |
| 25:DA:2121:G:H1 | 25:DA:2177:C:H42 | 1.58 | 0.51 |
| 25:BA:325:G:O2' | 25:BA:326:G:H5' | 2.09 | 0.51 |
| 25:DA:64:A:C4 | 43:DT:66:LEU:HD12 | 2.45 | 0.51 |
| 54:D8:32:LEU:HB2 | 54:D8:36:LYS:CE | 2.39 | 0.51 |
| 27:DD:44:ASN:OD1 | 27:DD:44:ASN:N | 2.43 | 0.51 |
| 41:D2:5:VAL:HB | 41:D2:37:VAL:CG1 | 2.41 | 0.51 |
| 23:AC:19:G:H4' | 23:AC:20:G:OP1 | 2.10 | 0.51 |
| 39:DR:74:ARG:NH1 | 39:DR:74:ARG:CG | 2.65 | 0.51 |
| 1:AA:1053:G:O6 | 1:AA:1199:U:H2' | 2.10 | 0.51 |
| 25:DA:973:A:O4' | 25:DA:1188:U:C6 | 2.64 | 0.51 |
| 27:DD:27:THR:O | 27:DD:28:GLU:HB2 | 2.11 | 0.51 |
| 47:DZ:91:LYS:O | 47:DZ:92:LYS:C | 2.48 | 0.51 |
| 25:DA:1060:U:C2 | 25:DA:1088:A:H8 | 2.29 | 0.51 |
| 25:DA:1060:U:N3 | 25:DA:1088:A:H8 | 2.08 | 0.51 |
| 25:DA:2274:A:N1 | 25:DA:2276:G:H1' | 2.26 | 0.51 |
| 1:CA:1128:C:H2' | 1:CA:1129:C:O5' | 2.09 | 0.51 |
| 30:BG:131:TYR:O | 30:BG:159:VAL:HG13 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:AE:16:HIS:N | 2:AE:16:HIS:ND1 | 2.56 | 0.51 |
| 25:BA:2119:A:N1 | 25:BA:2170:A:C5 | 2.78 | 0.51 |
| 2:CE:239:VAL:O | 2:CE:240:GLN:HB2 | 2.09 | 0.51 |
| 26:DB:87:G:N2 | 26:DB:89(A):A:OP2 | 2.44 | 0.51 |
| 19:CV:18:LYS:HA | 19:CV:21:GLU:HG2 | 1.93 | 0.51 |
| 29:BF:32:LEU:C | 29:BF:32:LEU:HD12 | 2.30 | 0.51 |
| 25:BA:2261:C:O2' | 25:BA:2262:U:H5' | 2.10 | 0.51 |
| 45:DV:59:LEU:HG | 45:DV:69:THR:OG1 | 2.10 | 0.51 |
| 22:CB:27:G:O6 | 22:CB:45:U:O2 | 2.28 | 0.51 |
| 1:CA:1269:A:C2 | 1:CA:1313:U:H1' | 2.45 | 0.51 |
| 3:AF:58:GLU:HB2 | 3:AF:65:ALA:HB3 | 1.91 | 0.51 |
| 25:BA:613:U:O2 | 25:BA:613:U:O4' | 2.23 | 0.51 |
| 25:DA:1011:G:OP1 | 40:D1:75:ASN:HB3 | 2.09 | 0.51 |
| 25:BA:1388:G:C2' | 25:BA:1389:G:H5' | 2.39 | 0.51 |
| 30:BG:2:PRO:HB3 | 50:B4:25:TYR:CE1 | 2.45 | 0.51 |
| 1:AA:724:G:C2 | 1:AA:725:G:C8 | 2.98 | 0.51 |
| 23:CD:71:G:C2' | 23:CD:72:C:H5' | 2.40 | 0.51 |
| 45:BV:48:PHE:CE2 | 45:BV:71:VAL:HG21 | 2.46 | 0.51 |
| 1:CA:116:A:OP2 | 1:CA:116:A:C8 | 2.64 | 0.51 |
| 27:DD:96:HIS:CE1 | 27:DD:102:LYS:HD3 | 2.45 | 0.51 |
| 9:AL:34:ASN:O | 9:AL:38:GLN:HB2 | 2.10 | 0.51 |
| 1:CA:1213:A:N1 | 1:CA:1215:G:H1' | 2.26 | 0.51 |
| 25:DA:1763:G:OP1 | 25:DA:1763:G:C4' | 2.59 | 0.51 |
| 23:CC:40:C:O5' | 23:CC:40:C:H6 | 1.93 | 0.51 |
| 25:DA:767:U:O2' | 25:DA:768:G:H5' | 2.11 | 0.51 |
| 54:D8:52:LYS:HD3 | 54:D8:52:LYS:H | 1.75 | 0.51 |
| 40:D1:95:LEU:HD21 | 41:D2:13:ARG:HB2 | 1.91 | 0.51 |
| 28:BE:59:VAL:CG2 | 28:BE:73:GLU:HB3 | 2.38 | 0.51 |
| 23:AC:77:A:C8 | 23:AC:77:A:H5' | 2.46 | 0.51 |
| 25:DA:954:G:O2' | 25:DA:2274:A:N1 | 2.41 | 0.51 |
| 44:DU:84:ARG:O | 44:DU:84:ARG:HG3 | 2.11 | 0.51 |
| 3:AF:20:SER:CB | 3:AF:40:ARG:HH22 | 2.23 | 0.51 |
| 37:D0:117:VAL:O | 37:D0:118:GLU:HB2 | 2.11 | 0.51 |
| 41:D2:61:VAL:O | 41:D2:61:VAL:HG13 | 2.10 | 0.51 |
| 25:BA:2392:A:H2 | 25:BA:2424:C:N4 | 2.07 | 0.51 |
| 3:CF:6:HIS:NE2 | 3:CF:184:TYR:CE2 | 2.79 | 0.51 |
| 25:BA:1177:A:H5'' | 25:BA:1178:C:O5' | 2.09 | 0.51 |
| 1:AA:926:G:C5' | 1:AA:927:G:O5' | 2.58 | 0.51 |
| 35:DO:122:PRO:CB | 35:DO:141:ALA:HB1 | 2.39 | 0.51 |
| 25:DA:2057:A:HO2' | 25:DA:2058:A:H5' | 1.76 | 0.51 |
| 1:CA:1268:A:O2' | 1:CA:1269:A:O5' | 2.26 | 0.51 |
| 25:DA:2446:G:C3' | 25:DA:2447:G:H5'' | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 36:DP:20:ALA:O | 36:DP:21:THR:CB | 2.58 | 0.51 |
| 8:AK:64:LYS:O | 8:AK:65:TYR:HD1 | 1.93 | 0.51 |
| 31:DH:169:VAL:HG22 | 31:DH:170:ARG:H | 1.76 | 0.51 |
| 48:BW:65:ASN:ND2 | 48:BW:69:ARG:HE | 2.08 | 0.51 |
| 25:BA:2199:A:H5' | 47:BZ:50:ARG:HH21 | 1.74 | 0.51 |
| 25:BA:1760:A:O2' | 25:BA:1761:C:H5' | 2.10 | 0.51 |
| 1:AA:941:G:N2 | 1:AA:942:G:H1' | 2.25 | 0.51 |
| 25:BA:2148:G:H2' | 25:BA:2149:G:H8 | 1.75 | 0.51 |
| 25:DA:4:C:H2' | 25:DA:5:A:O4' | 2.11 | 0.51 |
| 5:AH:142:LEU:O | 5:AH:143:ARG:NH1 | 2.43 | 0.51 |
| 45:DV:23:LYS:HD3 | 45:DV:39:VAL:O | 2.11 | 0.51 |
| 25:BA:125:G:C6 | 53:B7:10:ARG:HG3 | 2.45 | 0.51 |
| 1:AA:644:G:H2' | 1:AA:645:C:O4' | 2.11 | 0.51 |
| 4:AG:126:ILE:CG2 | 4:AG:127:THR:N | 2.73 | 0.51 |
| 34:DN:8:LEU:HD13 | 34:DN:82:ASN:HB3 | 1.92 | 0.51 |
| 25:DA:83:G:N2 | 25:DA:103:A:OP2 | 2.43 | 0.51 |
| 22:CB:66:U:O2 | 22:CB:68:A:N7 | 2.44 | 0.51 |
| 4:AG:141:ARG:HB3 | 4:AG:142:PRO:HD2 | 1.91 | 0.51 |
| 1:AA:81:G:H2' | 1:AA:82:U:O4' | 2.10 | 0.51 |
| 15:CR:76:GLU:HA | 15:CR:79:ARG:HD2 | 1.91 | 0.51 |
| 1:CA:67:C:H2' | 1:CA:68:G:C8 | 2.45 | 0.51 |
| 25:DA:743:G:C2' | 25:DA:744:G:H5' | 2.41 | 0.51 |
| 25:BA:910:A:N1 | 25:BA:2277:G:H1' | 2.25 | 0.51 |
| 2:CE:56:ARG:HH11 | 2:CE:56:ARG:HA | 1.75 | 0.51 |
| 25:BA:930:U:O4' | 25:BA:930:U:O2 | 2.26 | 0.51 |
| 44:BU:43:ASN:HA | 44:BU:64:GLU:HA | 1.93 | 0.51 |
| 25:DA:305:U:H2' | 25:DA:306:U:C6 | 2.46 | 0.51 |
| 2:CE:48:MET:HA | 2:CE:51:LEU:HB2 | 1.92 | 0.51 |
| 27:BD:272:ALA:HB1 | 27:BD:273:ARG:HA | 0.68 | 0.51 |
| 25:DA:2377:A:H2' | 25:DA:2378:A:C8 | 2.46 | 0.51 |
| 29:DF:51:THR:HG21 | 29:DF:92:PRO:HD2 | 1.93 | 0.51 |
| 30:BG:67:LYS:HG2 | 50:B4:5:ILE:HG23 | 1.93 | 0.51 |
| 52:B6:40:CYS:HA | 52:B6:46:HIS:CA | 2.34 | 0.51 |
| 25:DA:2750:A:C8 | 25:DA:2752:C:N4 | 2.76 | 0.51 |
| 25:BA:883:G:N2 | 25:BA:893:C:N3 | 2.52 | 0.51 |
| 1:CA:1162:C:N4 | 1:CA:1174:G:H1 | 2.06 | 0.51 |
| 25:DA:2779:U:O4' | 25:DA:2779:U:O2 | 2.29 | 0.51 |
| 30:BG:7:LEU:HD23 | 30:BG:100:TRP:HZ3 | 1.74 | 0.51 |
| 25:DA:330:A:H2 | 25:DA:1210:A:H2' | 1.76 | 0.51 |
| 25:DA:607:U:N3 | 25:DA:621:A:C2 | 2.71 | 0.51 |
| 25:DA:260:G:O4' | 25:DA:621:A:H1' | 2.11 | 0.51 |
| 32:BK:99:GLU:O | 32:BK:102:SER:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:1526:G:H2' | 25:BA:1527:G:O4' | 2.11 | 0.51 |
| 25:BA:1266:G:O2' | 25:BA:2012:G:O6 | 2.20 | 0.51 |
| 5:CH:102:ALA:HB2 | 5:CH:120:THR:OG1 | 2.11 | 0.51 |
| 25:DA:2571:C:C5' | 25:DA:2572:A:H5'' | 2.35 | 0.51 |
| 36:DP:58:PHE:C | 36:DP:60:ARG:H | 2.13 | 0.51 |
| 11:AN:121:PRO:HG2 | 11:AN:126:ARG:CG | 2.34 | 0.51 |
| 28:BE:119:ARG:HD3 | 28:BE:160:TYR:CD2 | 2.46 | 0.51 |
| 31:DH:136:ILE:O | 31:DH:137:ASP:HB2 | 2.11 | 0.51 |
| 2:AE:31:TYR:O | 2:AE:42:ILE:HG13 | 2.10 | 0.51 |
| 25:BA:330:A:C2 | 25:BA:1210:A:H2' | 2.44 | 0.51 |
| 3:AF:50:ALA:O | 3:AF:70:VAL:HG13 | 2.10 | 0.51 |
| 2:AE:91:PRO:HG3 | 2:AE:155:LEU:HB2 | 1.92 | 0.51 |
| 45:DV:156:LYS:O | 45:DV:157:LEU:HB2 | 2.09 | 0.51 |
| 25:DA:2447:G:H1' | 25:DA:2448:A:OP2 | 2.10 | 0.51 |
| 25:BA:1800:C:H5'' | 27:BD:147:LEU:HD21 | 1.91 | 0.51 |
| 53:D7:12:ARG:NH2 | 53:D7:44:PRO:HB3 | 2.26 | 0.51 |
| 1:AA:1256:A:H4' | 1:AA:1258:G:C4 | 2.45 | 0.51 |
| 38:BQ:93:LYS:HG2 | 38:BQ:95:HIS:HB2 | 1.92 | 0.51 |
| 3:AF:11:ARG:HH21 | 3:AF:180:ALA:HB3 | 1.74 | 0.51 |
| 43:BT:55:ASN:HB2 | 43:BT:80:ILE:HG13 | 1.93 | 0.51 |
| 1:CA:1112:C:C2 | 3:CF:178:LEU:HB2 | 2.46 | 0.51 |
| 4:AG:117:ALA:O | 4:AG:121:VAL:HG23 | 2.10 | 0.51 |
| 7:CJ:65:ALA:O | 7:CJ:69:VAL:HG23 | 2.10 | 0.51 |
| 26:DB:1:U:H2' | 26:DB:2:C:O4' | 2.10 | 0.51 |
| 25:DA:2209:C:O2 | 25:DA:2216:G:C2 | 2.63 | 0.51 |
| 26:BB:0:A:H2' | 26:BB:1:U:C6 | 2.46 | 0.51 |
| 1:CA:374:A:C6 | 1:CA:375:U:C4 | 2.99 | 0.51 |
| 1:CA:1267:C:O2 | 1:CA:1267:C:C2' | 2.59 | 0.51 |
| 25:DA:705:A:H1' | 27:DD:9:TYR:CE1 | 2.46 | 0.51 |
| 25:DA:971:C:H2' | 25:DA:972:G:C5' | 2.41 | 0.51 |
| 38:DQ:38:GLN:OE1 | 38:DQ:47:THR:OG1 | 2.22 | 0.51 |
| 1:CA:1486:G:H2' | 1:CA:1487:G:O4' | 2.11 | 0.51 |
| 2:AE:130:ARG:HH21 | 2:AE:138:LEU:HD11 | 1.75 | 0.51 |
| 25:DA:2346:A:H5' | 25:DA:2383:G:H1' | 1.93 | 0.51 |
| 27:DD:35:LYS:CE | 27:DD:104:TYR:CD1 | 2.93 | 0.51 |
| 27:DD:36:PRO:HA | 27:DD:62:TYR:O | 2.11 | 0.51 |
| 1:AA:1128:C:O2' | 1:AA:1130:A:C8 | 2.50 | 0.51 |
| 1:CA:977:A:C2 | 1:CA:1224:G:C6 | 2.98 | 0.51 |
| 1:CA:952:U:C5 | 13:CP:104:ARG:NH2 | 2.74 | 0.51 |
| 1:AA:1305:G:H5'' | 21:AX:4:GLY:C | 2.31 | 0.51 |
| 52:B6:28:ARG:NH1 | 52:B6:28:ARG:HB3 | 2.26 | 0.51 |
| 52:B6:48:VAL:O | 52:B6:49:HIS:HB2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 36:BP:88:GLY:O | 36:BP:90:VAL:O | 2.29 | 0.51 |
| 25:DA:1341:U:H2' | 25:DA:1397:U:O2 | 2.11 | 0.51 |
| 28:DE:134:ILE:HA | 28:DE:137:HIS:CD2 | 2.46 | 0.51 |
| 1:CA:1279:A:O2' | 1:CA:1281:U:OP2 | 2.24 | 0.51 |
| 31:DH:102:ALA:HA | 31:DH:117:PRO:HD3 | 1.92 | 0.51 |
| 19:CV:65:ASN:HB2 | 19:CV:66:MET:CE | 2.39 | 0.51 |
| 25:BA:1331:A:O2' | 25:BA:1332:G:H8 | 1.93 | 0.51 |
| 48:DW:41:ILE:CD1 | 48:DW:44:LEU:HG | 2.37 | 0.51 |
| 1:CA:960:U:O2 | 1:CA:960:U:C2' | 2.59 | 0.51 |
| 25:BA:1937:A:H1' | 25:BA:1938:A:OP1 | 2.11 | 0.51 |
| 25:BA:1403:C:C5' | 25:BA:1471:A:H1' | 2.38 | 0.51 |
| 43:DT:36:LYS:HD2 | 43:DT:56:THR:OG1 | 2.11 | 0.51 |
| 1:AA:191:G:C4 | 20:AW:105:SER:HB2 | 2.45 | 0.51 |
| 20:AW:89:ARG:NH2 | 20:AW:104:LEU:HD11 | 2.23 | 0.51 |
| 2:CE:136:VAL:O | 2:CE:139:LYS:HB3 | 2.11 | 0.51 |
| 23:CC:35:C:O2 | 23:CC:36:A:C8 | 2.64 | 0.51 |
| 23:AD:10:G:C6 | 23:AD:27:G:N2 | 2.79 | 0.51 |
| 49:BX:8:LEU:HD13 | 49:BX:31:LEU:CD2 | 2.41 | 0.51 |
| 1:CA:243:A:C2 | 1:CA:245:C:C2 | 2.99 | 0.51 |
| 25:DA:833:U:O2 | 35:DO:55:ARG:NH1 | 2.40 | 0.51 |
| 25:BA:1449(A):G:H2' | 25:BA:1450:C:H6 | 1.76 | 0.51 |
| 27:BD:134:ARG:HG3 | 27:BD:135:PHE:CE2 | 2.46 | 0.51 |
| 25:DA:1170:G:O6 | 25:DA:1179:C:N3 | 2.44 | 0.51 |
| 1:CA:575:G:H4' | 1:CA:576:G:OP1 | 2.10 | 0.51 |
| 6:CI:69:GLU:N | 6:CI:69:GLU:OE1 | 2.26 | 0.51 |
| 25:BA:1952:A:C4 | 34:BN:22:ILE:HG13 | 2.46 | 0.51 |
| 25:BA:511:U:C5 | 25:BA:512:G:C5 | 2.99 | 0.51 |
| 25:DA:748:G:C8 | 42:DS:89:ALA:HB1 | 2.46 | 0.51 |
| 16:AS:51:VAL:HG12 | 16:AS:52:ASP:N | 2.26 | 0.51 |
| 5:CH:43:LEU:HD22 | 5:CH:136:MET:HG3 | 1.93 | 0.51 |
| 25:BA:57:C:H2' | 25:BA:58:G:O4' | 2.11 | 0.51 |
| 5:CH:63:ARG:HA | 5:CH:66:MET:CE | 2.41 | 0.51 |
| 22:AB:64:G:O2' | 22:AB:65:U:H5' | 2.11 | 0.51 |
| 25:DA:729:G:C6 | 27:DD:208:LYS:HB2 | 2.46 | 0.51 |
| 1:CA:757:U:H2' | 1:CA:758:G:O4' | 2.11 | 0.51 |
| 33:DM:137:LYS:HA | 33:DM:137:LYS:NZ | 2.25 | 0.51 |
| 27:DD:58:HIS:HD2 | 27:DD:59:LYS:O | 1.93 | 0.51 |
| 25:DA:2784:C:O2 | 28:DE:37:ARG:NH2 | 2.43 | 0.51 |
| 28:DE:13:ARG:O | 39:DR:57:PHE:HE1 | 1.93 | 0.51 |
| 25:BA:2287:A:N1 | 25:BA:2346:A:H2 | 2.09 | 0.51 |
| 1:CA:485:G:H1' | 1:CA:486:U:H5 | 1.75 | 0.51 |
| 36:BP:105:GLU:O | 36:BP:105:GLU:HG2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 40:B1:50:ARG:HG2 | 40:B1:53:ARG:NH2 | 2.25 | 0.51 |
| 39:BR:61:PHE:CD2 | 39:BR:61:PHE:N | 2.79 | 0.51 |
| 23:CD:15:G:H22 | 23:CD:60:A:H1' | 1.76 | 0.51 |
| 30:BG:133:LEU:HD21 | 30:BG:157:ILE:HB | 1.93 | 0.51 |
| 30:BG:172:LEU:O | 30:BG:176:LEU:HD12 | 2.11 | 0.51 |
| 36:DP:59:ARG:NH2 | 36:DP:59:ARG:CG | 2.71 | 0.51 |
| 25:DA:1444(A):A:H4' | 25:DA:1460:A:H2' | 1.93 | 0.51 |
| 25:BA:2135:A:N6 | 25:BA:2156:G:O2' | 2.43 | 0.51 |
| 25:BA:1535:U:H3' | 25:BA:1536:A:C5' | 2.38 | 0.51 |
| 35:DO:98:GLU:O | 35:DO:102:ARG:HB2 | 2.11 | 0.51 |
| 25:DA:2439:A:C5' | 25:DA:2439:A:H8 | 2.22 | 0.51 |
| 30:BG:115:ARG:O | 30:BG:116:ASP:HB2 | 2.10 | 0.51 |
| 49:DX:23:LEU:HD11 | 49:DX:53:LEU:CD1 | 2.41 | 0.51 |
| 49:DX:23:LEU:HD11 | 49:DX:53:LEU:HD11 | 1.92 | 0.51 |
| 9:CL:8:GLY:HA2 | 9:CL:79:LEU:HD12 | 1.93 | 0.51 |
| 23:CD:52:C:C2 | 23:CD:53:G:C8 | 2.99 | 0.51 |
| 7:CJ:86:GLN:HE22 | 23:CD:32:G:H21 | 1.58 | 0.51 |
| 25:BA:2264:C:H2' | 25:BA:2264:C:O2 | 2.11 | 0.51 |
| 30:BG:107:LEU:HD11 | 30:BG:178:PHE:CE1 | 2.46 | 0.51 |
| 1:CA:555:C:H2' | 1:CA:556:C:C6 | 2.46 | 0.51 |
| 1:AA:673:G:H5'' | 6:AI:87:ARG:NH1 | 2.26 | 0.51 |
| 14:CQ:29:ARG:O | 14:CQ:30:ALA:CB | 2.59 | 0.51 |
| 1:AA:533:A:C2 | 1:AA:536:C:C5 | 2.98 | 0.51 |
| 52:B6:11:LEU:HD11 | 52:B6:51:GLU:OE2 | 2.11 | 0.51 |
| 2:CE:32:ILE:HG13 | 2:CE:32:ILE:O | 2.06 | 0.51 |
| 32:BK:110:ASP:HB3 | 32:BK:111:PRO:C | 2.30 | 0.51 |
| 1:AA:1436:U:H2' | 1:AA:1437:C:O4' | 2.10 | 0.51 |
| 25:DA:912:C:C2 | 25:DA:913:U:C5 | 2.98 | 0.51 |
| 5:CH:36:ASP:OD2 | 5:CH:38:GLN:HB2 | 2.10 | 0.51 |
| 1:CA:677:U:H3 | 1:CA:713:G:H22 | 1.59 | 0.51 |
| 35:BO:94:GLU:HA | 35:BO:94:GLU:OE2 | 2.11 | 0.51 |
| 3:CF:199:LYS:HG2 | 3:CF:201:TYR:HE1 | 1.76 | 0.51 |
| 2:AE:19:HIS:HD2 | 2:AE:20:GLU:OE1 | 1.93 | 0.51 |
| 11:AN:18:ARG:HB3 | 11:AN:33:THR:OG1 | 2.11 | 0.51 |
| 25:BA:2031:A:C6 | 25:BA:2498:C:H1' | 2.45 | 0.51 |
| 44:BU:19:LYS:HG2 | 44:BU:20:TYR:CD1 | 2.46 | 0.51 |
| 13:CP:66:LEU:HA | 13:CP:70:LEU:HD12 | 1.93 | 0.51 |
| 25:DA:21:A:O2' | 25:DA:22:C:H5' | 2.11 | 0.51 |
| 20:CW:75:ASN:N | 20:CW:75:ASN:OD1 | 2.44 | 0.51 |
| 10:CM:6:ILE:HG22 | 10:CM:98:ILE:HG23 | 1.91 | 0.51 |
| 25:BA:2291:U:O2' | 25:BA:2374:C:O2 | 2.28 | 0.51 |
| 54:D8:52:LYS:C | 54:D8:54:GLU:H | 2.15 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 28:BE:23:VAL:CG1 | 28:BE:185:LYS:CB | 2.57 | 0.51 |
| 1:CA:1027:C:O2' | 1:CA:1028:C:O5' | 2.28 | 0.51 |
| 1:CA:1002:G:H1 | 1:CA:1038:C:H42 | 1.58 | 0.51 |
| 35:DO:65:ARG:CG | 35:DO:65:ARG:NH1 | 2.58 | 0.51 |
| 47:DZ:87:PRO:CA | 47:DZ:90:ILE:HG23 | 2.30 | 0.51 |
| 39:BR:74:ARG:HD3 | 39:BR:76:PHE:HZ | 1.75 | 0.51 |
| 50:B4:59:PHE:HA | 50:B4:62:ARG:HG2 | 1.93 | 0.51 |
| 2:AE:39:ILE:HG22 | 2:AE:40:HIS:O | 2.11 | 0.51 |
| 25:BA:444:C:C4' | 29:BF:49:ALA:HB2 | 2.41 | 0.51 |
| 9:CL:97:LYS:HG3 | 9:CL:98:PRO:N | 2.26 | 0.51 |
| 13:AP:61:GLU:O | 50:B4:49:PHE:HE2 | 1.93 | 0.51 |
| 33:DM:90:MET:SD | 33:DM:97:ARG:HB3 | 2.50 | 0.51 |
| 23:CD:54:G:H2' | 23:CD:55:U:H6 | 1.76 | 0.51 |
| 40:B1:58:ARG:HA | 40:B1:61:TRP:CE3 | 2.46 | 0.51 |
| 45:DV:108:PRO:O | 45:DV:143:GLY:HA3 | 2.11 | 0.51 |
| 2:CE:215:LEU:O | 2:CE:219:VAL:HG12 | 2.11 | 0.51 |
| 19:CV:66:MET:CE | 50:D4:55:ARG:HB2 | 2.41 | 0.51 |
| 17:CT:45:HIS:CD2 | 17:CT:47:PRO:HD3 | 2.46 | 0.51 |
| 51:B5:51:TYR:H | 51:B5:56:LYS:HB3 | 1.76 | 0.51 |
| 2:CE:6:THR:HG23 | 2:CE:7:VAL:N | 2.25 | 0.51 |
| 37:B0:103:ARG:NH1 | 42:BS:40:ASN:HD22 | 2.06 | 0.51 |
| 25:BA:2862:G:C5 | 25:BA:2863:C:C5 | 2.99 | 0.51 |
| 25:DA:1599:C:C5' | 43:DT:35:THR:HG22 | 2.39 | 0.51 |
| 13:AP:25:ILE:HD11 | 13:AP:60:VAL:CG1 | 2.41 | 0.51 |
| 4:CG:91:SER:OG | 4:CG:191:ARG:HG3 | 2.11 | 0.51 |
| 1:CA:57:G:C5 | 1:CA:58:C:C4 | 2.99 | 0.51 |
| 35:DO:134:ALA:O | 35:DO:138:LEU:HD12 | 2.11 | 0.51 |
| 25:BA:751:A:H5' | 42:BS:90:ARG:HA | 1.93 | 0.51 |
| 1:AA:989:C:N4 | 1:AA:1216:G:H1 | 2.09 | 0.51 |
| 25:DA:2816:C:O3' | 37:D0:99:LYS:NZ | 2.44 | 0.51 |
| 36:BP:57:HIS:ND1 | 36:BP:117:ALA:HB2 | 2.26 | 0.51 |
| 33:BM:7:LYS:HD2 | 33:BM:7:LYS:H | 1.75 | 0.51 |
| 25:DA:1973:G:H2' | 25:DA:1974:C:C6 | 2.46 | 0.51 |
| 38:BQ:51:ALA:HB3 | 38:BQ:73:LEU:HG | 1.92 | 0.51 |
| 25:DA:43:G:H2' | 25:DA:44:A:O4' | 2.11 | 0.51 |
| 12:AO:39:VAL:HG12 | 12:AO:41:ARG:HG2 | 1.92 | 0.51 |
| 16:AS:58:TYR:C | 16:AS:58:TYR:HD1 | 2.15 | 0.51 |
| 25:DA:2138:C:H42 | 25:DA:2153:G:H1 | 1.59 | 0.51 |
| 1:CA:877:C:H5'' | 8:CK:88:LYS:HE3 | 1.93 | 0.51 |
| 25:DA:226:G:N2 | 25:DA:228:A:H62 | 1.82 | 0.50 |
| 54:D8:33:ASN:O | 54:D8:34:TRP:HD1 | 1.87 | 0.50 |
| 54:D8:52:LYS:CB | 54:D8:53:PRO:CD | 2.90 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:2811:G:H2' | 25:BA:2812:G:H5' | 1.92 | 0.50 |
| 23:AC:59:A:C5 | 23:AC:62:C:N3 | 2.79 | 0.50 |
| 33:BM:32:THR:HG22 | 33:BM:37:LYS:HB2 | 1.93 | 0.50 |
| 25:DA:1144:G:C2 | 25:DA:1145:C:C2 | 2.99 | 0.50 |
| 39:DR:93:ARG:CG | 39:DR:117:ASP:HB2 | 2.40 | 0.50 |
| 39:DR:26:ASP:HB2 | 39:DR:90:GLN:O | 2.11 | 0.50 |
| 54:B8:36:LYS:CG | 54:B8:40:GLU:HG2 | 2.40 | 0.50 |
| 25:DA:2777:G:C5' | 25:DA:2778:A:H5' | 2.30 | 0.50 |
| 1:CA:1128:C:C2' | 1:CA:1129:C:O5' | 2.59 | 0.50 |
| 25:DA:2129:C:C2' | 25:DA:2130:U:H5' | 2.41 | 0.50 |
| 27:BD:25:THR:HG22 | 27:BD:26:LYS:N | 2.25 | 0.50 |
| 25:BA:1386:C:OP2 | 25:BA:1396:U:H5 | 1.94 | 0.50 |
| 41:B2:34:GLU:HA | 41:B2:57:VAL:O | 2.10 | 0.50 |
| 25:BA:242:G:C5' | 54:B8:62:LEU:HD13 | 2.40 | 0.50 |
| 1:AA:953:G:C5' | 1:AA:965:A:H61 | 2.23 | 0.50 |
| 25:BA:2689:U:C4' | 25:BA:2690:C:OP2 | 2.58 | 0.50 |
| 25:DA:2682:U:C5 | 28:DE:11:MET:HE1 | 2.46 | 0.50 |
| 1:AA:428:G:O4' | 1:AA:430:A:C8 | 2.64 | 0.50 |
| 46:D3:53:MET:HA | 46:D3:58:THR:O | 2.12 | 0.50 |
| 1:CA:1122:U:N3 | 1:CA:1123:A:N7 | 2.59 | 0.50 |
| 25:BA:2496:C:P | 36:BP:81:VAL:HG13 | 2.51 | 0.50 |
| 11:CN:63:LEU:N | 11:CN:63:LEU:HD23 | 2.25 | 0.50 |
| 25:BA:287:C:H2' | 25:BA:288:C:C6 | 2.46 | 0.50 |
| 18:CU:29:PHE:HD2 | 18:CU:29:PHE:N | 2.09 | 0.50 |
| 23:AD:67:C:N4 | 23:AD:68:C:H41 | 2.07 | 0.50 |
| 23:AD:71:G:C2' | 23:AD:72:C:H5' | 2.40 | 0.50 |
| 25:DA:2513:G:N2 | 28:DE:143:ASN:HD21 | 2.09 | 0.50 |
| 4:AG:86:LYS:HD2 | 4:AG:86:LYS:H | 1.75 | 0.50 |
| 25:BA:26:G:C6 | 25:BA:27:G:N1 | 2.79 | 0.50 |
| 1:AA:185:A:H2' | 1:AA:186:C:H6 | 1.75 | 0.50 |
| 25:DA:270(L):U:H3 | 32:DK:50:ARG:NH1 | 2.09 | 0.50 |
| 47:DZ:19:GLN:HB2 | 47:DZ:35:THR:O | 2.11 | 0.50 |
| 23:AC:24:C:H2' | 23:AC:25:U:C6 | 2.46 | 0.50 |
| 1:CA:439:A:H2' | 1:CA:440:A:O5' | 2.11 | 0.50 |
| 25:BA:2774:C:H2' | 25:BA:2775:A:O4' | 2.11 | 0.50 |
| 25:DA:1531:C:H42 | 25:DA:1540:G:H1 | 1.59 | 0.50 |
| 1:CA:1009:G:C2 | 1:CA:1010:G:C8 | 2.99 | 0.50 |
| 35:DO:124:LYS:HA | 35:DO:143:GLY:O | 2.11 | 0.50 |
| 29:BF:7:TYR:CD1 | 29:BF:7:TYR:N | 2.78 | 0.50 |
| 8:CK:136:GLU:HG3 | 8:CK:136:GLU:O | 2.10 | 0.50 |
| 9:AL:97:LYS:HB3 | 9:AL:98:PRO:HD3 | 1.93 | 0.50 |
| 25:BA:2564:A:C2 | 25:BA:2647:U:H4' | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:BA:1065:U:H1' | 25:BA:1074:G:N2 | 2.26 | 0.50 |
| 52:D6:11:LEU:HD23 | 52:D6:26:ASN:CB | 2.35 | 0.50 |
| 38:BQ:85:VAL:CG2 | 38:BQ:112:PHE:HE1 | 2.15 | 0.50 |
| 27:DD:33:LEU:HD23 | 27:DD:34:VAL:N | 2.26 | 0.50 |
| 27:BD:35:LYS:CB | 27:BD:64:ILE:H | 2.24 | 0.50 |
| 4:AG:7:PRO:HB2 | 4:AG:10:ARG:HD2 | 1.92 | 0.50 |
| 28:DE:12:THR:HG22 | 39:DR:58:ASN:ND2 | 2.27 | 0.50 |
| 23:AD:6:G:H2' | 23:AD:7:G:H8 | 1.77 | 0.50 |
| 44:BU:84:ARG:HH12 | 44:BU:97:ARG:HB2 | 1.76 | 0.50 |
| 1:CA:961:U:OP2 | 1:CA:1223:C:O2' | 2.17 | 0.50 |
| 1:CA:972:C:OP2 | 10:CM:57:LYS:CD | 2.59 | 0.50 |
| 47:DZ:91:LYS:O | 47:DZ:93:GLU:HB2 | 2.10 | 0.50 |
| 1:AA:1002:G:C4 | 1:AA:1003:G:C8 | 2.99 | 0.50 |
| 25:DA:1061:U:H4' | 25:DA:1070:A:O2' | 2.12 | 0.50 |
| 25:DA:1089:G:H5'' | 25:DA:1090:U:OP1 | 2.10 | 0.50 |
| 25:DA:1313:U:H2' | 25:DA:1610:A:C2 | 2.46 | 0.50 |
| 29:DF:116:ASP:O | 29:DF:120:GLU:HG2 | 2.11 | 0.50 |
| 23:CD:55:U:N3 | 23:CD:56:U:H5 | 2.07 | 0.50 |
| 25:DA:2751:G:N2 | 31:DH:2:SER:N | 2.58 | 0.50 |
| 25:DA:528:A:O2' | 25:DA:529:A:H5' | 2.11 | 0.50 |
| 1:CA:1141:C:H2' | 1:CA:1142:G:C8 | 2.44 | 0.50 |
| 1:CA:1128:C:C5' | 9:CL:16:ARG:HH22 | 2.24 | 0.50 |
| 30:BG:124:SER:HB2 | 30:BG:131:TYR:CE1 | 2.46 | 0.50 |
| 25:BA:1510:A:OP1 | 25:BA:1510:A:H4' | 2.10 | 0.50 |
| 25:DA:1653:G:C6 | 37:D0:9:LYS:HB2 | 2.46 | 0.50 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:N9 | 2.24 | 0.50 |
| 25:DA:2795:G:C3' | 25:DA:2797:U:H5'' | 2.36 | 0.50 |
| 25:DA:2468:G:C4 | 25:DA:2481:G:N2 | 2.79 | 0.50 |
| 25:BA:2133:G:N3 | 25:BA:2158:A:N6 | 2.58 | 0.50 |
| 30:DG:111:LEU:O | 30:DG:117:PHE:HD2 | 1.93 | 0.50 |
| 31:BH:11:VAL:CB | 31:BH:12:PRO:HD2 | 2.37 | 0.50 |
| 25:BA:2701:C:C3' | 25:BA:2702:U:H5'' | 2.39 | 0.50 |
| 28:DE:173:VAL:N | 28:DE:183:LEU:O | 2.37 | 0.50 |
| 23:AC:2:G:H2' | 23:AC:3:C:H6 | 1.77 | 0.50 |
| 35:BO:38:GLN:HG2 | 35:BO:45:LEU:CD1 | 2.41 | 0.50 |
| 1:CA:1392:G:N2 | 1:CA:1502:A:C8 | 2.76 | 0.50 |
| 18:CU:22:VAL:CG2 | 18:CU:23:LYS:N | 2.75 | 0.50 |
| 8:AK:51:VAL:HG11 | 8:AK:60:ARG:HG3 | 1.93 | 0.50 |
| 25:DA:1283:G:N2 | 25:DA:1285:G:H3' | 2.26 | 0.50 |
| 25:BA:1528:A:C2 | 25:BA:1543:A:N1 | 2.79 | 0.50 |
| 31:DH:26:VAL:HG13 | 31:DH:27:LYS:H | 1.75 | 0.50 |
| 25:DA:627:A:H4' | 25:DA:628:G:OP1 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:660:G:N2 | 35:BO:12:ALA:HA | 2.26 | 0.50 |
| 25:DA:1784:A:H4' | 25:DA:1785:A:H5'' | 1.91 | 0.50 |
| 1:AA:389:A:H2' | 1:AA:390:C:H5' | 1.94 | 0.50 |
| 25:DA:1169:G:N2 | 25:DA:1181:C:C2 | 2.79 | 0.50 |
| 25:DA:2847:U:C2' | 25:DA:2848:G:H5' | 2.42 | 0.50 |
| 18:AU:22:VAL:HA | 18:AU:25:THR:OG1 | 2.11 | 0.50 |
| 2:AE:237:ALA:H | 2:AE:239:VAL:HG23 | 1.76 | 0.50 |
| 30:DG:43:LEU:HD12 | 30:DG:45:GLU:HG3 | 1.92 | 0.50 |
| 11:CN:34:ASP:HB2 | 11:CN:35:PRO:HD2 | 1.93 | 0.50 |
| 25:DA:2575:C:H5' | 28:DE:143:ASN:O | 2.10 | 0.50 |
| 1:CA:358:U:H2' | 1:CA:359:U:H6 | 1.76 | 0.50 |
| 50:D4:50:VAL:O | 50:D4:51:ASP:CG | 2.50 | 0.50 |
| 9:AL:22:GLY:HA3 | 9:AL:60:ASP:CG | 2.32 | 0.50 |
| 25:BA:88:G:O2' | 25:BA:89:G:H5' | 2.11 | 0.50 |
| 25:BA:236:C:H2' | 25:BA:237:C:C6 | 2.47 | 0.50 |
| 52:D6:17:LYS:NZ | 52:D6:17:LYS:HA | 2.27 | 0.50 |
| 25:DA:1791:A:OP2 | 25:DA:1791:A:H8 | 1.94 | 0.50 |
| 25:BA:1060:U:C4' | 25:BA:1061:U:O5' | 2.59 | 0.50 |
| 25:DA:2393:A:H5'' | 54:D8:30:ARG:HG2 | 1.93 | 0.50 |
| 28:BE:38:THR:C | 28:BE:40:GLU:N | 2.64 | 0.50 |
| 1:AA:972:C:OP2 | 10:AM:57:LYS:HE2 | 2.11 | 0.50 |
| 13:CP:15:VAL:HG13 | 13:CP:43:THR:O | 2.11 | 0.50 |
| 25:DA:2013:A:N6 | 25:DA:2014:A:C6 | 2.79 | 0.50 |
| 25:DA:2712:U:O2' | 25:DA:2712(A):A:P | 2.69 | 0.50 |
| 1:CA:1139:G:N2 | 1:CA:1143:G:N1 | 2.50 | 0.50 |
| 26:DB:46:A:H2' | 26:DB:47:C:C6 | 2.46 | 0.50 |
| 25:DA:90:U:O2 | 25:DA:90:U:C2' | 2.59 | 0.50 |
| 25:DA:2128:C:H42 | 25:DA:2160:G:H1 | 1.57 | 0.50 |
| 25:BA:2168:G:N2 | 25:BA:2170:A:P | 2.84 | 0.50 |
| 1:CA:624:C:H2' | 1:CA:625:G:H8 | 1.76 | 0.50 |
| 25:BA:2790:A:H2 | 25:BA:2894:G:C5' | 2.25 | 0.50 |
| 27:BD:28:GLU:O | 27:BD:29:PRO:C | 2.49 | 0.50 |
| 2:CE:69:LEU:HD21 | 2:CE:93:VAL:HG23 | 1.92 | 0.50 |
| 1:AA:1392:G:C2' | 1:AA:1393:U:H5' | 2.42 | 0.50 |
| 2:AE:178:ARG:HH22 | 2:AE:196:LEU:CA | 2.23 | 0.50 |
| 13:AP:7:VAL:HB | 30:BG:115:ARG:HH22 | 1.76 | 0.50 |
| 1:CA:878:G:H5' | 8:CK:89:PRO:HG2 | 1.93 | 0.50 |
| 18:CU:22:VAL:O | 18:CU:23:LYS:HB3 | 2.10 | 0.50 |
| 1:AA:991:U:H2' | 1:AA:1212:U:O2 | 2.11 | 0.50 |
| 28:DE:62:PRO:C | 28:DE:64:LYS:N | 2.63 | 0.50 |
| 1:CA:1015:A:N6 | 1:CA:1016:A:C6 | 2.79 | 0.50 |
| 2:AE:220:ASP:O | 2:AE:223:ILE:HG13 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:2329:G:H2' | 25:BA:2330:G:C8 | 2.47 | 0.50 |
| 4:CG:190:ASP:OD1 | 4:CG:191:ARG:N | 2.45 | 0.50 |
| 25:BA:2875:C:H4' | 39:BR:5:ALA:HB2 | 1.93 | 0.50 |
| 1:AA:1118:C:H1' | 1:AA:1179:A:C4 | 2.46 | 0.50 |
| 45:BV:142:SER:HB3 | 45:BV:143:GLY:HA2 | 1.94 | 0.50 |
| 25:DA:394:A:H5'' | 25:DA:395:U:OP2 | 2.11 | 0.50 |
| 25:DA:93:C:H5' | 25:DA:94:G:OP2 | 2.11 | 0.50 |
| 1:CA:1040:U:H2' | 1:CA:1041:A:C8 | 2.46 | 0.50 |
| 4:CG:150:GLU:O | 4:CG:152:SER:N | 2.43 | 0.50 |
| 26:BB:1(M):A:C2' | 26:BB:0:A:H5' | 2.41 | 0.50 |
| 25:DA:2139:C:H2' | 25:DA:2140:C:H5' | 1.93 | 0.50 |
| 49:DX:31:LEU:O | 49:DX:32:GLN:HB2 | 2.12 | 0.50 |
| 35:BO:86:LYS:HB3 | 35:BO:118:GLY:HA3 | 1.94 | 0.50 |
| 8:CK:11:THR:HG22 | 8:CK:15:ASN:ND2 | 2.27 | 0.50 |
| 32:BK:35:LEU:O | 32:BK:36:ALA:HB2 | 2.10 | 0.50 |
| 26:DB:10:C:C4 | 26:DB:11:C:C5 | 2.98 | 0.50 |
| 25:BA:1502:C:C2' | 25:BA:1503:U:H5' | 2.41 | 0.50 |
| 25:DA:631:A:H2' | 25:DA:632:A:O4' | 2.10 | 0.50 |
| 26:BB:7:G:H2' | 26:BB:8:U:O4' | 2.11 | 0.50 |
| 25:DA:460:A:C2 | 25:DA:470:A:C4 | 2.99 | 0.50 |
| 6:CI:96:PRO:HB3 | 18:CU:30:ASP:CG | 2.32 | 0.50 |
| 25:DA:2393:A:P | 54:D8:30:ARG:HB2 | 2.52 | 0.50 |
| 54:D8:33:ASN:C | 54:D8:34:TRP:HD1 | 2.15 | 0.50 |
| 27:DD:35:LYS:NZ | 27:DD:64:ILE:O | 2.45 | 0.50 |
| 28:BE:23:VAL:CG1 | 28:BE:185:LYS:CA | 2.69 | 0.50 |
| 33:DM:38:HIS:CE1 | 33:DM:39:ARG:HG3 | 2.46 | 0.50 |
| 33:BM:47:ALA:CB | 33:BM:112:LEU:HD11 | 2.19 | 0.50 |
| 39:DR:22:PHE:HE2 | 39:DR:86:ILE:HD11 | 1.74 | 0.50 |
| 22:CB:21:A:C4' | 22:CB:22:G:OP1 | 2.60 | 0.50 |
| 47:DZ:89:GLU:HA | 47:DZ:93:GLU:HG3 | 1.93 | 0.50 |
| 36:BP:65:PHE:O | 36:BP:66:ILE:CG1 | 2.57 | 0.50 |
| 1:AA:975:A:H62 | 10:AM:60:ARG:HH12 | 1.58 | 0.50 |
| 44:DU:76:CYS:HB3 | 44:DU:96:ILE:HD11 | 1.94 | 0.50 |
| 31:BH:30:LYS:CD | 31:BH:81:GLU:H | 2.11 | 0.50 |
| 25:DA:1557:C:H5'' | 25:DA:1558:A:OP2 | 2.11 | 0.50 |
| 10:CM:30:SER:HB2 | 10:CM:81:THR:HG22 | 1.94 | 0.50 |
| 2:AE:5:ILE:HG13 | 2:AE:6:THR:N | 2.25 | 0.50 |
| 25:BA:2116:G:P | 25:BA:2165:G:N2 | 2.82 | 0.50 |
| 45:DV:108:PRO:HB3 | 45:DV:143:GLY:N | 2.26 | 0.50 |
| 25:BA:2893:G:H4' | 25:BA:2894:G:O4' | 2.11 | 0.50 |
| 25:BA:2135:A:H2' | 25:BA:2136:C:O5' | 2.11 | 0.50 |
| 27:BD:6:PHE:CE1 | 27:BD:18:VAL:CG2 | 2.94 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:437:U:C5' | 4:AG:155:LEU:HD22 | 2.40 | 0.50 |
| 36:DP:10:ARG:HE | 36:DP:10:ARG:HA | 1.75 | 0.50 |
| 25:BA:654(T):A:H2' | 25:BA:654(U):A:O4' | 2.12 | 0.50 |
| 29:DF:110:LEU:HD21 | 29:DF:181:LEU:HD22 | 1.94 | 0.50 |
| 25:BA:304:G:C2 | 25:BA:314:A:C2 | 3.00 | 0.50 |
| 22:CB:26:C:H5' | 22:CB:27:G:OP2 | 2.11 | 0.50 |
| 1:AA:156:G:H1 | 1:AA:165:C:N4 | 2.07 | 0.50 |
| 1:CA:1266:G:N2 | 1:CA:1269:A:OP2 | 2.44 | 0.50 |
| 44:BU:42:VAL:O | 44:BU:42:VAL:CG1 | 2.60 | 0.50 |
| 14:CQ:37:PHE:HE1 | 14:CQ:53:LEU:HD13 | 1.75 | 0.50 |
| 42:BS:70:TYR:HE2 | 42:BS:108:GLY:HA3 | 1.76 | 0.50 |
| 25:BA:1983:C:O2' | 25:BA:1984:G:H5' | 2.10 | 0.50 |
| 2:AE:87:ARG:NH1 | 2:AE:220:ASP:OD1 | 2.43 | 0.50 |
| 4:CG:9:CYS:CA | 4:CG:12:CYS:HB2 | 2.41 | 0.50 |
| 25:DA:2861:G:O2' | 25:DA:2862:G:H5' | 2.11 | 0.50 |
| 16:AS:58:TYR:C | 16:AS:58:TYR:CD1 | 2.84 | 0.50 |
| 20:CW:51:GLU:HA | 20:CW:54:LYS:HE3 | 1.93 | 0.50 |
| 1:CA:339:C:C2' | 1:CA:340:U:H5' | 2.41 | 0.50 |
| 16:CS:74:LEU:HD13 | 16:CS:79:VAL:HG21 | 1.92 | 0.50 |
| 46:D3:12:ASN:HA | 46:D3:14:ARG:HH21 | 1.76 | 0.50 |
| 16:AS:56:ALA:O | 16:AS:60:LEU:HD12 | 2.11 | 0.50 |
| 25:BA:2886:G:H2' | 25:BA:2887:U:H6 | 1.75 | 0.50 |
| 5:AH:147:ASP:N | 5:AH:147:ASP:OD2 | 2.45 | 0.50 |
| 3:AF:27:LYS:HZ3 | 3:AF:27:LYS:HA | 1.76 | 0.50 |
| 1:AA:750:G:N3 | 15:AR:23:GLY:HA3 | 2.26 | 0.50 |
| 1:CA:1403:C:O2' | 1:CA:1404:C:H5' | 2.11 | 0.50 |
| 28:DE:167:VAL:HG12 | 28:DE:170:LEU:HD11 | 1.93 | 0.50 |
| 1:AA:1160:G:O6 | 1:AA:1181:G:C6 | 2.64 | 0.50 |
| 25:DA:997:G:OP1 | 40:D1:93:LYS:HD2 | 2.12 | 0.50 |
| 27:BD:77:ALA:HB2 | 27:BD:97:TYR:HA | 1.94 | 0.50 |
| 29:DF:83:PHE:O | 29:DF:84:VAL:O | 2.30 | 0.50 |
| 28:DE:8:LYS:HE3 | 28:DE:188:VAL:O | 2.12 | 0.50 |
| 28:DE:8:LYS:HB3 | 28:DE:192:ASN:HA | 1.92 | 0.50 |
| 28:DE:51:PHE:O | 28:DE:74:PRO:HB2 | 2.10 | 0.50 |
| 1:CA:1227:A:OP1 | 19:CV:80:TYR:OH | 2.23 | 0.50 |
| 35:DO:65:ARG:O | 35:DO:66:GLY:O | 2.30 | 0.50 |
| 25:DA:2748:A:C2 | 25:DA:2749:A:C4 | 2.99 | 0.50 |
| 1:AA:1032(B):G:C6 | 1:AA:1033:G:C6 | 2.99 | 0.50 |
| 54:B8:29:LYS:CD | 54:B8:29:LYS:O | 2.59 | 0.50 |
| 29:DF:3:GLU:O | 29:DF:19:GLU:HB3 | 2.11 | 0.50 |
| 25:BA:1509:C:N4 | 25:BA:1511:A:N6 | 2.58 | 0.50 |
| 9:CL:4:TYR:HA | 9:CL:88:TYR:CE1 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 4:AG:12:CYS:HA | 4:AG:19:LEU:CD2 | 2.41 | 0.50 |
| 31:BH:4:ILE:HG21 | 31:BH:6:ARG:CZ | 2.40 | 0.50 |
| 26:DB:109:G:C6 | 26:DB:110:G:C5 | 2.99 | 0.50 |
| 1:CA:1238:A:N7 | 1:CA:1303:C:H1' | 2.27 | 0.50 |
| 54:B8:52:LYS:H | 54:B8:53:PRO:HD2 | 1.74 | 0.50 |
| 39:BR:56:GLY:O | 39:BR:59:THR:CG2 | 2.56 | 0.50 |
| 1:AA:1028(A):C:N4 | 1:AA:1028(B):C:H41 | 2.09 | 0.50 |
| 25:DA:654(B):C:C2 | 25:DA:654(T):A:H2 | 2.29 | 0.50 |
| 25:BA:1472:A:H2' | 25:BA:1473:G:O4' | 2.12 | 0.50 |
| 25:DA:864:G:O6 | 25:DA:865:C:N4 | 2.43 | 0.50 |
| 25:BA:1300:U:H4' | 25:BA:1301:A:H5' | 1.92 | 0.50 |
| 45:DV:10:ARG:HH21 | 45:DV:26:GLY:H | 1.60 | 0.50 |
| 25:DA:2211:G:H4' | 25:DA:2212:A:OP2 | 2.11 | 0.50 |
| 1:AA:464:G:C6 | 1:AA:466:C:H5' | 2.47 | 0.50 |
| 23:AD:60:A:H2' | 23:AD:61:U:H5' | 1.93 | 0.50 |
| 7:CJ:97:GLN:NE2 | 7:CJ:101:LEU:HD11 | 2.25 | 0.50 |
| 1:AA:352:C:O2' | 1:AA:354:G:OP1 | 2.25 | 0.50 |
| 3:CF:64:VAL:CG2 | 3:CF:66:VAL:HG23 | 2.41 | 0.50 |
| 36:BP:78:PRO:C | 36:BP:79:LEU:HD12 | 2.31 | 0.50 |
| 2:CE:121:LEU:O | 2:CE:121:LEU:HD23 | 2.12 | 0.50 |
| 10:CM:99:LYS:HD3 | 10:CM:100:THR:H | 1.77 | 0.50 |
| 25:BA:155:C:N4 | 25:BA:171:G:H1 | 2.09 | 0.50 |
| 25:DA:483:A:H4' | 44:DU:49:VAL:HA | 1.92 | 0.50 |
| 22:AB:24:C:H3' | 22:AB:24:C:H6 | 1.76 | 0.50 |
| 1:CA:953:G:H5' | 1:CA:965:A:H61 | 1.77 | 0.50 |
| 1:CA:57:G:C6 | 1:CA:58:C:N4 | 2.80 | 0.50 |
| 25:BA:2188:C:H2' | 25:BA:2189:U:O4' | 2.12 | 0.50 |
| 25:BA:974(A):C:H4' | 25:BA:975:G:O5' | 2.12 | 0.50 |
| 25:BA:302:C:H2' | 25:BA:303:U:H6 | 1.75 | 0.50 |
| 2:CE:5:ILE:CD1 | 2:CE:55:PHE:HB3 | 2.42 | 0.50 |
| 23:AD:67:C:N3 | 23:AD:68:C:C4 | 2.79 | 0.50 |
| 1:CA:1413:A:H2' | 1:CA:1414:U:O4' | 2.11 | 0.50 |
| 13:CP:10:PRO:HB2 | 13:CP:18:ALA:HB1 | 1.94 | 0.50 |
| 25:BA:826:U:H2' | 25:BA:828:U:O4' | 2.12 | 0.50 |
| 25:BA:236:C:H2' | 25:BA:237:C:H6 | 1.76 | 0.50 |
| 1:CA:340:U:H3 | 1:CA:349:A:H61 | 1.59 | 0.50 |
| 1:CA:309:G:O2' | 1:CA:607:A:N1 | 2.44 | 0.50 |
| 30:DG:32:PRO:HB2 | 30:DG:172:LEU:HD22 | 1.94 | 0.50 |
| 30:DG:25:TYR:HB3 | 30:DG:30:GLU:HB2 | 1.94 | 0.50 |
| 2:AE:100:GLY:O | 2:AE:104:ASN:N | 2.42 | 0.50 |
| 25:BA:2206:C:H2' | 25:BA:2207:C:H6 | 1.76 | 0.50 |
| 1:CA:1166:G:C2 | 1:CA:1171:G:C6 | 2.99 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 31:DH:74:ASN:ND2 | 31:DH:138:LYS:HG2 | 2.26 | 0.50 |
| 4:CG:120:LEU:HD22 | 4:CG:158:ILE:HD11 | 1.93 | 0.50 |
| 6:CI:76:ALA:HB1 | 6:CI:80:ARG:HH21 | 1.76 | 0.50 |
| 1:CA:672:U:O2 | 1:CA:672:U:H2' | 2.10 | 0.50 |
| 36:DP:138:ASP:O | 36:DP:138:ASP:OD2 | 2.29 | 0.50 |
| 25:DA:2833:G:H8 | 25:DA:2833:G:OP1 | 1.95 | 0.50 |
| 25:DA:947:G:H2' | 25:DA:948:G:C8 | 2.47 | 0.50 |
| 25:DA:57:C:H2' | 25:DA:58:G:O4' | 2.11 | 0.50 |
| 54:B8:39:LYS:O | 54:B8:43:GLN:HG3 | 2.12 | 0.50 |
| 41:D2:47:VAL:O | 41:D2:47:VAL:HG22 | 2.11 | 0.50 |
| 8:AK:16:ALA:HB2 | 8:AK:24:THR:HG21 | 1.92 | 0.50 |
| 36:DP:25:ASP:O | 36:DP:25:ASP:OD1 | 2.30 | 0.50 |
| 33:DM:38:HIS:ND1 | 33:DM:39:ARG:HG3 | 2.27 | 0.50 |
| 28:BE:51:PHE:O | 28:BE:52:LEU:O | 2.30 | 0.50 |
| 28:BE:80:GLU:C | 28:BE:82:ARG:N | 2.63 | 0.50 |
| 28:DE:171:GLU:O | 28:DE:184:VAL:HA | 2.12 | 0.50 |
| 30:BG:63:ILE:HD12 | 30:BG:141:PHE:CD2 | 2.47 | 0.50 |
| 25:DA:2401:U:C3' | 25:DA:2402:C:H5'' | 2.42 | 0.50 |
| 25:BA:2371:G:C1' | 52:B6:45:LYS:HG3 | 2.39 | 0.50 |
| 25:BA:259:G:HO2' | 25:BA:621:A:HO2' | 1.38 | 0.50 |
| 22:CB:41:G:H2' | 22:CB:42:U:H6 | 1.77 | 0.50 |
| 19:AV:68:GLY:HA2 | 50:B4:59:PHE:CE1 | 2.46 | 0.50 |
| 30:DG:61:ALA:HA | 30:DG:64:THR:CG2 | 2.41 | 0.50 |
| 40:B1:92:ARG:C | 40:B1:94:ASN:N | 2.64 | 0.50 |
| 25:BA:998:C:C2' | 25:BA:999:U:O5' | 2.60 | 0.50 |
| 2:AE:221:LEU:HD13 | 2:AE:221:LEU:O | 2.11 | 0.50 |
| 11:AN:41:THR:HG21 | 11:AN:71:LYS:CB | 2.41 | 0.50 |
| 25:DA:2156:G:C6 | 25:DA:2157:G:C2 | 3.00 | 0.50 |
| 25:BA:2173:A:H2' | 25:BA:2174:C:O4' | 2.12 | 0.50 |
| 25:DA:1464:C:HO2' | 25:DA:1528:A:H8 | 0.72 | 0.50 |
| 25:BA:572:A:H3' | 25:BA:573:G:O4' | 2.12 | 0.50 |
| 39:BR:50:ILE:HD11 | 39:BR:102:ILE:HD13 | 1.92 | 0.50 |
| 6:CI:61:LEU:HB3 | 6:CI:63:TYR:HE2 | 1.76 | 0.50 |
| 27:DD:186:HIS:HD2 | 27:DD:188:GLU:N | 2.05 | 0.50 |
| 1:AA:439:A:H2' | 1:AA:440:A:O5' | 2.12 | 0.50 |
| 4:AG:5:ILE:CG2 | 4:AG:6:GLY:N | 2.69 | 0.50 |
| 3:CF:14:ILE:CG1 | 3:CF:15:THR:H | 2.25 | 0.50 |
| 1:AA:219:C:H2' | 1:AA:220:G:O4' | 2.10 | 0.50 |
| 45:BV:111:VAL:HG11 | 45:BV:146:ILE:CB | 2.40 | 0.50 |
| 42:BS:79:GLY:HA3 | 42:BS:100:THR:CG2 | 2.42 | 0.50 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:H8 | 1.73 | 0.50 |
| 8:CK:82:HIS:CD2 | 8:CK:82:HIS:O | 2.63 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 7:AJ:38:LEU:HD12 | 7:AJ:38:LEU:O | 2.12 | 0.50 |
| 25:BA:754:C:H2' | 25:BA:755:C:C6 | 2.47 | 0.50 |
| 3:CF:21:ARG:HH11 | 3:CF:21:ARG:HB3 | 1.76 | 0.50 |
| 1:CA:6:G:H4' | 1:CA:298:A:H4' | 1.93 | 0.50 |
| 7:CJ:69:VAL:HG22 | 7:CJ:135:VAL:HG23 | 1.93 | 0.50 |
| 48:DW:47:ASN:ND2 | 48:DW:47:ASN:H | 2.09 | 0.50 |
| 1:CA:457:C:H2' | 1:CA:458:C:C6 | 2.46 | 0.50 |
| 37:D0:28:LEU:HD11 | 37:D0:114:VAL:HG12 | 1.94 | 0.50 |
| 6:CI:25:ILE:HG21 | 6:CI:82:ARG:HD2 | 1.93 | 0.50 |
| 25:DA:2462:U:H1' | 25:DA:2491:U:O4 | 2.11 | 0.50 |
| 2:CE:24:TRP:O | 2:CE:24:TRP:HD1 | 1.95 | 0.50 |
| 3:CF:188:LEU:N | 3:CF:188:LEU:HD22 | 2.27 | 0.50 |
| 27:DD:10:THR:OG1 | 27:DD:13:ARG:HB2 | 2.11 | 0.50 |
| 34:BN:75:SER:HB2 | 39:BR:75:ILE:O | 2.12 | 0.50 |
| 32:DK:84:GLY:O | 32:DK:85:GLU:HB3 | 2.11 | 0.50 |
| 25:DA:1879:C:H2' | 25:DA:1880:C:O4' | 2.12 | 0.50 |
| 15:AR:8:LYS:O | 15:AR:12:ILE:HG13 | 2.11 | 0.50 |
| 34:BN:98:VAL:HG13 | 34:BN:117:LEU:HB3 | 1.92 | 0.50 |
| 1:CA:145:G:H2' | 1:CA:146:G:O5' | 2.11 | 0.50 |
| 28:DE:204:ALA:O | 28:DE:205:ALA:HB3 | 2.11 | 0.50 |
| 25:DA:265:A:H1' | 25:DA:266:G:O4' | 2.12 | 0.50 |
| 25:BA:1205:U:H4' | 25:BA:1206:G:OP2 | 2.12 | 0.50 |
| 25:BA:207:A:H2' | 25:BA:208:C:O4' | 2.10 | 0.50 |
| 1:CA:19:C:H5'' | 5:CH:86:ALA:CB | 2.42 | 0.50 |
| 1:CA:763:G:H2' | 1:CA:764:C:H6 | 1.75 | 0.50 |
| 38:BQ:30:ARG:HG3 | 38:BQ:30:ARG:O | 2.11 | 0.50 |
| 25:BA:2301:C:H6 | 25:BA:2301:C:H3' | 1.76 | 0.50 |
| 1:CA:945:G:H2' | 1:CA:945:G:N3 | 2.26 | 0.50 |
| 25:BA:1691:C:H2' | 25:BA:1692:U:H5' | 1.93 | 0.50 |
| 30:BG:82:LEU:HA | 30:BG:86:MET:CE | 2.42 | 0.50 |
| 30:BG:57:ALA:HB2 | 30:BG:90:LEU:HD21 | 1.94 | 0.50 |
| 54:D8:22:VAL:O | 54:D8:49:VAL:HA | 2.12 | 0.50 |
| 28:BE:23:VAL:CG1 | 28:BE:173:VAL:HG21 | 2.32 | 0.50 |
| 25:BA:2310:A:H61 | 30:BG:79:ASN:ND2 | 2.08 | 0.50 |
| 28:BE:53:PRO:O | 28:BE:54:GLN:O | 2.30 | 0.50 |
| 1:CA:1026:G:C6 | 1:CA:1036:G:C2 | 2.99 | 0.50 |
| 29:DF:88:VAL:O | 29:DF:89:VAL:O | 2.30 | 0.50 |
| 1:CA:1226:C:P | 13:CP:91:ARG:HH22 | 2.35 | 0.50 |
| 1:CA:980:C:H5'' | 1:CA:981:U:C5 | 2.47 | 0.50 |
| 5:AH:126:ARG:NH1 | 5:AH:126:ARG:CG | 2.62 | 0.50 |
| 10:CM:57:LYS:O | 10:CM:58:ASP:O | 2.30 | 0.50 |
| 29:BF:197:ASP:O | 29:BF:198:ALA:CB | 2.60 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:2273:A:H2' | 25:DA:2274:A:C8 | 2.47 | 0.50 |
| 25:DA:2250:G:O2' | 25:DA:2496:C:OP1 | 2.18 | 0.50 |
| 2:AE:96:ARG:CD | 2:AE:96:ARG:H | 2.07 | 0.50 |
| 1:AA:1059:C:O2' | 10:AM:53:PRO:HD3 | 2.11 | 0.50 |
| 9:AL:114:TYR:HD2 | 9:AL:114:TYR:N | 2.10 | 0.50 |
| 10:AM:53:PRO:HA | 14:AQ:42:ILE:HD11 | 1.94 | 0.50 |
| 54:B8:31:HIS:O | 54:B8:32:LEU:O | 2.30 | 0.50 |
| 23:CD:59:A:C1' | 23:CD:61:U:H5 | 2.19 | 0.50 |
| 26:DB:3:C:N3 | 26:DB:117:G:N2 | 2.45 | 0.50 |
| 25:DA:2392:A:N1 | 25:DA:2424:C:N3 | 2.60 | 0.50 |
| 42:BS:91:GLY:O | 42:BS:92:ARG:O | 2.30 | 0.50 |
| 22:AB:86:C:H2' | 22:AB:87:A:C4 | 2.47 | 0.50 |
| 26:DB:15:A:H2' | 26:DB:16:G:OP1 | 2.11 | 0.50 |
| 23:AD:56:U:O4 | 23:AD:58:A:H5'' | 2.11 | 0.50 |
| 51:B5:40:LYS:HG2 | 51:B5:47:PRO:CD | 2.36 | 0.50 |
| 1:CA:452:A:H2' | 1:CA:453:A:H8 | 1.76 | 0.50 |
| 19:CV:49:ILE:HD12 | 19:CV:49:ILE:N | 2.27 | 0.50 |
| 25:BA:309:G:O2' | 25:BA:329:G:C8 | 2.63 | 0.50 |
| 29:DF:123:LEU:O | 29:DF:125:LEU:N | 2.45 | 0.50 |
| 29:DF:164:ARG:HH11 | 29:DF:177:ALA:HB2 | 1.77 | 0.50 |
| 29:DF:133:ASN:HB3 | 29:DF:135:LYS:H | 1.77 | 0.50 |
| 23:CC:44:A:O2' | 23:CC:45:A:H5' | 2.12 | 0.50 |
| 22:AB:54:G:N1 | 22:AB:55:G:O6 | 2.45 | 0.50 |
| 1:CA:860:A:H2' | 1:CA:861:G:O4' | 2.12 | 0.50 |
| 51:B5:42:PRO:CB | 51:B5:43:HIS:HD2 | 2.24 | 0.50 |
| 32:DK:79:ILE:HD12 | 32:DK:140:LEU:HD21 | 1.94 | 0.50 |
| 14:CQ:36:PHE:CD1 | 14:CQ:37:PHE:CD2 | 2.99 | 0.50 |
| 20:CW:49:ALA:HB2 | 20:CW:92:LEU:HD22 | 1.94 | 0.50 |
| 25:BA:1464:C:O2' | 25:BA:1528:A:H8 | 1.94 | 0.50 |
| 13:CP:7:VAL:CG2 | 30:DG:115:ARG:HB3 | 2.42 | 0.50 |
| 25:BA:1278:A:OP1 | 37:B0:36:THR:HG23 | 2.12 | 0.50 |
| 48:BW:24:LEU:HD13 | 48:BW:60:LEU:HD11 | 1.92 | 0.50 |
| 7:CJ:71:PRO:HD3 | 7:CJ:103:TRP:CZ3 | 2.47 | 0.50 |
| 1:CA:668:G:O2' | 15:CR:46:HIS:HB3 | 2.12 | 0.50 |
| 1:CA:1105:A:H2' | 1:CA:1106:G:H8 | 1.76 | 0.50 |
| 12:AO:77:LEU:HD21 | 12:AO:107:ALA:HA | 1.93 | 0.50 |
| 17:AT:18:THR:HG21 | 17:AT:69:LYS:HD2 | 1.93 | 0.50 |
| 31:DH:41:MET:HE2 | 31:DH:65:HIS:N | 2.26 | 0.50 |
| 25:DA:656:G:H2' | 25:DA:657:U:O4' | 2.12 | 0.50 |
| 1:CA:145:G:C2' | 1:CA:146:G:O5' | 2.60 | 0.50 |
| 25:BA:354:G:O2' | 25:BA:355:G:H5' | 2.12 | 0.50 |
| 25:BA:270(R):G:H2' | 25:BA:270(S):G:C8 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1014:A:H4' | 19:AV:14:HIS:CE1 | 2.47 | 0.50 |
| 25:DA:1509:C:O2 | 25:DA:1509:C:H2' | 2.12 | 0.50 |
| 28:DE:96:PHE:O | 28:DE:175:VAL:HG11 | 2.12 | 0.50 |
| 1:CA:879:C:C5 | 12:CO:6:THR:HG21 | 2.46 | 0.50 |
| 25:DA:1039:G:H1 | 25:DA:1116:C:H42 | 1.60 | 0.50 |
| 9:CL:73:GLN:O | 9:CL:76:ALA:HB3 | 2.12 | 0.50 |
| 30:BG:73:ALA:HB3 | 30:BG:83:ARG:O | 2.12 | 0.50 |
| 38:BQ:26:LEU:HD22 | 38:BQ:87:PHE:HD1 | 1.77 | 0.50 |
| 1:AA:1206:G:C6 | 1:AA:1207:G:C5 | 3.00 | 0.50 |
| 28:DE:5:LEU:HD22 | 28:DE:79:ARG:HG2 | 1.93 | 0.50 |
| 1:CA:1323:G:H4' | 1:CA:1362(A):C:N3 | 2.26 | 0.50 |
| 1:AA:1036:G:H3' | 1:AA:1037:C:C5 | 2.46 | 0.50 |
| 22:CB:85:C:N4 | 25:DA:2508:G:H5' | 2.27 | 0.50 |
| 13:CP:25:ILE:O | 13:CP:29:ARG:HB2 | 2.12 | 0.50 |
| 1:CA:1128:C:H4' | 9:CL:16:ARG:HH22 | 1.77 | 0.50 |
| 38:BQ:25:ARG:NH1 | 38:BQ:42:ASP:OD2 | 2.35 | 0.50 |
| 32:BK:100:ALA:O | 32:BK:102:SER:N | 2.44 | 0.50 |
| 26:DB:15:A:C2' | 26:DB:16:G:OP1 | 2.60 | 0.50 |
| 1:CA:1238:A:H62 | 1:CA:1301:U:H3 | 1.59 | 0.50 |
| 25:DA:2572:A:OP1 | 28:DE:144:ARG:HB2 | 2.11 | 0.50 |
| 25:DA:1408:C:C2 | 25:DA:1595:G:N2 | 2.80 | 0.50 |
| 25:DA:2298:A:N6 | 25:DA:2318:G:C8 | 2.80 | 0.50 |
| 7:CJ:23:VAL:HG13 | 7:CJ:43:PHE:HE2 | 1.76 | 0.50 |
| 29:BF:104:LYS:O | 29:BF:108:LYS:HB2 | 2.12 | 0.50 |
| 25:BA:2261:C:H1' | 25:BA:2388:A:N3 | 2.27 | 0.50 |
| 50:B4:37:SER:HB3 | 50:B4:42:PHE:HD1 | 1.73 | 0.50 |
| 8:CK:20:TYR:HA | 8:CK:65:TYR:CE2 | 2.46 | 0.50 |
| 8:CK:20:TYR:HD1 | 8:CK:65:TYR:CE2 | 2.30 | 0.50 |
| 36:BP:20:ALA:HB1 | 36:BP:99:PRO:HB2 | 1.94 | 0.50 |
| 1:AA:1318:A:C1' | 19:AV:37:ARG:HH21 | 2.23 | 0.50 |
| 25:BA:1264:G:C5' | 51:B5:11:THR:HG21 | 2.40 | 0.50 |
| 33:BM:57:ALA:O | 33:BM:58:ASP:CB | 2.60 | 0.50 |
| 45:DV:158:PRO:CB | 45:DV:159:PRO:HD2 | 2.42 | 0.50 |
| 9:CL:125:TYR:C | 9:CL:125:TYR:HD2 | 2.15 | 0.50 |
| 18:CU:22:VAL:CG2 | 18:CU:23:LYS:H | 2.25 | 0.50 |
| 26:DB:55:U:C2' | 26:DB:56:G:H5' | 2.41 | 0.50 |
| 1:CA:937:A:C5 | 1:CA:938:A:N7 | 2.80 | 0.50 |
| 25:BA:373:U:H1' | 25:BA:423:A:C2 | 2.47 | 0.50 |
| 1:CA:77:C:C3' | 1:CA:78:G:H5'' | 2.42 | 0.50 |
| 4:AG:162:LEU:HD11 | 4:AG:181:MET:HB3 | 1.94 | 0.50 |
| 30:BG:15:VAL:HG22 | 30:BG:175:LEU:CB | 2.41 | 0.50 |
| 28:BE:167:VAL:HG21 | 28:BE:187:ALA:HB1 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 37:D0:51:LEU:HD13 | 37:D0:70:LEU:HD21 | 1.94 | 0.50 |
| 1:AA:323:U:H2' | 1:AA:324:G:O4' | 2.12 | 0.50 |
| 25:DA:276:A:H2' | 25:DA:277:C:H6 | 1.77 | 0.50 |
| 27:BD:75:ILE:HD13 | 27:BD:99:ASP:OD1 | 2.10 | 0.50 |
| 1:CA:1107:C:O2 | 1:CA:1107:C:H2' | 2.11 | 0.50 |
| 26:BB:94:C:H2' | 26:BB:95:U:H6 | 1.76 | 0.50 |
| 40:D1:48:ALA:O | 40:D1:52:ARG:HG3 | 2.11 | 0.50 |
| 1:AA:568:G:H2' | 1:AA:568:G:N3 | 2.27 | 0.50 |
| 1:AA:567:G:H2' | 1:AA:568:G:O4' | 2.11 | 0.50 |
| 49:BX:28:LEU:HD23 | 49:BX:33:GLN:HG2 | 1.92 | 0.50 |
| 11:AN:61:ALA:HB1 | 11:AN:94:ALA:HB2 | 1.93 | 0.50 |
| 25:DA:1915:U:H2' | 25:DA:1916:A:O5' | 2.12 | 0.50 |
| 37:B0:60:LEU:HD23 | 37:B0:61:HIS:N | 2.27 | 0.50 |
| 35:BO:90:ARG:O | 35:BO:90:ARG:HG2 | 2.12 | 0.50 |
| 25:BA:2469:A:H62 | 25:BA:2481:G:N2 | 2.10 | 0.50 |
| 1:AA:1182:G:C4' | 1:AA:1183:A:H5' | 2.26 | 0.50 |
| 27:DD:61:LEU:O | 27:DD:63:ARG:NH1 | 2.43 | 0.50 |
| 38:DQ:87:PHE:O | 38:DQ:88:ASP:O | 2.30 | 0.50 |
| 27:BD:35:LYS:N | 27:BD:64:ILE:CG2 | 2.75 | 0.50 |
| 28:BE:61:ARG:H | 28:BE:62:PRO:HD2 | 1.77 | 0.50 |
| 25:DA:1257:C:O2' | 29:DF:83:PHE:O | 2.29 | 0.50 |
| 25:BA:2298:A:H2' | 25:BA:2299:G:O4' | 2.12 | 0.50 |
| 1:AA:1133:G:C4 | 1:AA:1134:G:C8 | 3.00 | 0.50 |
| 39:DR:54:ARG:HA | 39:DR:59:THR:HB | 1.93 | 0.50 |
| 53:D7:8:ASN:ND2 | 53:D7:11:LYS:HB2 | 2.26 | 0.50 |
| 1:CA:951:G:OP2 | 13:CP:102:ARG:NH2 | 2.44 | 0.50 |
| 31:BH:170:ARG:O | 31:BH:171:LEU:HB2 | 2.12 | 0.50 |
| 29:BF:101:LEU:O | 29:BF:106:ARG:NH1 | 2.38 | 0.50 |
| 25:DA:1071:G:OP2 | 25:DA:1097:U:H5' | 2.11 | 0.50 |
| 25:BA:879:G:OP2 | 25:BA:879:G:H8 | 1.95 | 0.50 |
| 25:DA:2133:G:H1' | 25:DA:2158:A:N6 | 2.27 | 0.50 |
| 25:DA:2168:G:N2 | 25:DA:2169:A:H3' | 2.26 | 0.50 |
| 25:BA:1312:U:H4' | 25:BA:1313:U:O5' | 2.12 | 0.50 |
| 25:DA:811:U:C4 | 35:DO:21:ARG:NH2 | 2.80 | 0.50 |
| 25:DA:39:C:O2 | 29:DF:46:ARG:NH2 | 2.44 | 0.50 |
| 5:AH:11:ILE:CD1 | 5:AH:31:LEU:HB3 | 2.41 | 0.50 |
| 25:BA:2646:C:OP2 | 25:BA:2732:G:O2' | 2.24 | 0.50 |
| 25:DA:1240:U:O2' | 25:DA:1241:A:H5' | 2.12 | 0.50 |
| 23:CC:43:G:H2' | 23:CC:44:A:C8 | 2.42 | 0.50 |
| 3:CF:59:ARG:HG3 | 3:CF:64:VAL:HA | 1.93 | 0.50 |
| 25:BA:2476:A:N3 | 25:BA:2476:A:H2' | 2.26 | 0.50 |
| 32:BK:25:TYR:CE2 | 32:BK:29:TYR:CD2 | 3.00 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:652:U:H1' | 1:AA:653:A:C2 | 2.47 | 0.50 |
| 31:DH:26:VAL:HB | 31:DH:75:ALA:HB1 | 1.93 | 0.50 |
| 1:AA:115:G:H4' | 1:AA:116:A:O5' | 2.12 | 0.50 |
| 25:BA:1486:A:H2' | 25:BA:1487:G:C8 | 2.44 | 0.50 |
| 34:DN:68:GLU:OE2 | 34:DN:78:ARG:NH1 | 2.45 | 0.50 |
| 23:CD:38:A:H2' | 23:CD:39:A:O4' | 2.11 | 0.50 |
| 1:CA:745:C:H2' | 1:CA:746:A:C8 | 2.46 | 0.50 |
| 25:BA:852:G:H2' | 25:BA:853:G:C8 | 2.46 | 0.50 |
| 25:DA:1955:U:O3' | 25:DA:1956:U:H6 | 1.95 | 0.50 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.47 | 0.50 |
| 25:DA:1915:U:C2' | 25:DA:1916:A:O5' | 2.60 | 0.50 |
| 7:CJ:152:ALA:O | 7:CJ:155:ARG:HB3 | 2.11 | 0.50 |
| 25:DA:1889:A:O2' | 25:DA:2087:G:H5' | 2.12 | 0.50 |
| 25:BA:835:A:H2' | 25:BA:836:G:O5' | 2.12 | 0.50 |
| 13:CP:27:LYS:HE3 | 13:CP:31:LYS:HE3 | 1.94 | 0.50 |
| 1:AA:1177:G:C8 | 1:AA:1178:G:N1 | 2.80 | 0.49 |
| 30:BG:77:ILE:O | 30:BG:78:SER:O | 2.30 | 0.49 |
| 41:D2:82:ARG:O | 41:D2:83:ARG:O | 2.30 | 0.49 |
| 52:D6:47:THR:O | 52:D6:48:VAL:O | 2.30 | 0.49 |
| 29:DF:83:PHE:C | 29:DF:84:VAL:HG12 | 2.33 | 0.49 |
| 1:AA:1053:G:C5 | 1:AA:1199:U:C6 | 3.00 | 0.49 |
| 39:DR:16:ARG:H | 39:DR:79:HIS:CD2 | 2.30 | 0.49 |
| 25:DA:1342:A:N6 | 25:DA:1397:U:C5 | 2.80 | 0.49 |
| 25:BA:2602:A:H4' | 25:BA:2603:G:O5' | 2.12 | 0.49 |
| 43:DT:43:VAL:HG22 | 43:DT:51:VAL:CG2 | 2.42 | 0.49 |
| 9:AL:114:TYR:N | 9:AL:114:TYR:CD2 | 2.78 | 0.49 |
| 10:AM:61:GLU:OE2 | 14:AQ:45:ARG:HD2 | 2.12 | 0.49 |
| 31:BH:83:TYR:CB | 31:BH:135:GLY:H | 2.13 | 0.49 |
| 1:CA:606:G:N2 | 1:CA:631:G:H2' | 2.26 | 0.49 |
| 25:BA:1011:G:H3' | 25:BA:1012:U:H5'' | 1.92 | 0.49 |
| 26:DB:44:G:C5' | 26:DB:45:A:OP1 | 2.60 | 0.49 |
| 1:AA:404:U:H2' | 1:AA:405:U:C6 | 2.47 | 0.49 |
| 1:AA:1301:U:C4 | 1:AA:1303:C:H1' | 2.47 | 0.49 |
| 27:BD:270:ILE:HG22 | 27:BD:271:ILE:H | 1.76 | 0.49 |
| 27:BD:270:ILE:C | 27:BD:271:ILE:HG12 | 2.25 | 0.49 |
| 5:CH:93:PRO:HG2 | 8:CK:105:ARG:CZ | 2.42 | 0.49 |
| 1:AA:1028(A):C:H2' | 1:AA:1028(B):C:C6 | 2.47 | 0.49 |
| 25:DA:2872:G:C6 | 25:DA:2873:A:N1 | 2.79 | 0.49 |
| 19:CV:22:LEU:HD12 | 19:CV:22:LEU:O | 2.12 | 0.49 |
| 25:DA:943:U:OP2 | 35:DO:36:LYS:CG | 2.59 | 0.49 |
| 25:DA:2318:G:N1 | 38:DQ:2:ALA:HA | 2.18 | 0.49 |
| 35:DO:38:GLN:O | 35:DO:41:ARG:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:1170:G:N2 | 25:BA:1180:C:C2 | 2.80 | 0.49 |
| 10:AM:96:ILE:HD13 | 10:AM:96:ILE:N | 2.27 | 0.49 |
| 3:CF:8:ILE:HG23 | 3:CF:16:ARG:HG2 | 1.93 | 0.49 |
| 1:CA:411:A:C5 | 1:CA:413:G:H1' | 2.47 | 0.49 |
| 42:BS:14:PRO:HB2 | 42:BS:18:ARG:HH21 | 1.77 | 0.49 |
| 15:AR:17:ARG:HG3 | 15:AR:17:ARG:NH1 | 2.26 | 0.49 |
| 28:DE:64:LYS:HG2 | 28:DE:65:GLY:H | 1.77 | 0.49 |
| 4:AG:30:LYS:C | 4:AG:32:ALA:H | 2.12 | 0.49 |
| 7:CJ:62:PHE:HA | 7:CJ:124:LEU:HD22 | 1.94 | 0.49 |
| 25:DA:2:G:O2' | 25:DA:3:U:H5' | 2.11 | 0.49 |
| 25:DA:2189:U:H2' | 25:DA:2190:G:H5' | 1.93 | 0.49 |
| 28:DE:30:PRO:HD3 | 28:DE:180:ASN:ND2 | 2.27 | 0.49 |
| 5:CH:107:ARG:CG | 5:CH:108:ALA:N | 2.74 | 0.49 |
| 1:CA:468:A:H2' | 1:CA:474:G:C5' | 2.42 | 0.49 |
| 20:AW:65:LYS:HG3 | 20:AW:68:LYS:HE2 | 1.92 | 0.49 |
| 25:DA:1499:C:H2' | 25:DA:1500:G:C8 | 2.46 | 0.49 |
| 8:CK:109:ILE:HG12 | 8:CK:110:ALA:N | 2.27 | 0.49 |
| 25:BA:1412:A:H2' | 25:BA:1413:G:H8 | 1.77 | 0.49 |
| 9:AL:99:LEU:HB3 | 9:AL:101:PHE:CD1 | 2.46 | 0.49 |
| 50:D4:48:ARG:HH12 | 50:D4:51:ASP:HA | 1.77 | 0.49 |
| 12:CO:50:SER:O | 12:CO:51:ALA:HB2 | 2.10 | 0.49 |
| 25:BA:2855:C:H2' | 25:BA:2856:C:H6 | 1.77 | 0.49 |
| 45:DV:121:HIS:HB3 | 45:DV:123:ASP:O | 2.12 | 0.49 |
| 1:AA:939:G:H2' | 1:AA:940:C:C6 | 2.47 | 0.49 |
| 25:DA:654(I):C:H42 | 25:DA:654(M):C:H42 | 1.60 | 0.49 |
| 25:DA:1657:C:H2' | 25:DA:1658:C:C6 | 2.47 | 0.49 |
| 1:AA:84:U:O2 | 1:AA:84:U:H2' | 2.12 | 0.49 |
| 25:DA:2054:A:H5'' | 25:DA:2055:C:O5' | 2.12 | 0.49 |
| 45:DV:5:LEU:HG | 45:DV:47:VAL:HG21 | 1.94 | 0.49 |
| 52:D6:10:LEU:O | 52:D6:11:LEU:HD13 | 2.12 | 0.49 |
| 40:D1:70:ARG:HH11 | 40:D1:70:ARG:HG2 | 1.78 | 0.49 |
| 29:DF:90:PHE:O | 29:DF:91:GLY:O | 2.30 | 0.49 |
| 1:CA:509:A:N3 | 1:CA:543:C:O2' | 2.41 | 0.49 |
| 25:DA:2748:A:N3 | 25:DA:2748:A:H2' | 2.27 | 0.49 |
| 25:DA:1056:G:H4' | 25:DA:1086:A:H1' | 1.94 | 0.49 |
| 25:BA:1141:U:OP2 | 33:BM:63:THR:HG23 | 2.12 | 0.49 |
| 30:DG:98:ARG:O | 30:DG:101:ILE:HG13 | 2.13 | 0.49 |
| 25:BA:1434:A:N6 | 25:BA:1558:A:H62 | 2.06 | 0.49 |
| 2:CE:118:LEU:HD13 | 2:CE:142:LEU:HB2 | 1.93 | 0.49 |
| 25:DA:2134:A:C2 | 25:DA:2159:G:H1' | 2.47 | 0.49 |
| 19:CV:23:ASN:HA | 19:CV:27:GLU:CD | 2.32 | 0.49 |
| 39:BR:50:ILE:CD1 | 39:BR:102:ILE:HD11 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 51:B5:40:LYS:HZ3 | 51:B5:46:CYS:C | 2.15 | 0.49 |
| 25:BA:1405:U:H2' | 25:BA:1406:U:H6 | 1.76 | 0.49 |
| 2:AE:61:LEU:HD23 | 2:AE:68:ILE:CD1 | 2.41 | 0.49 |
| 8:AK:49:GLU:HG2 | 8:AK:62:TYR:HE2 | 1.77 | 0.49 |
| 23:CD:42:C:H2' | 23:CD:43:G:C8 | 2.42 | 0.49 |
| 25:DA:1093:G:H5' | 31:DH:170:ARG:HH12 | 1.77 | 0.49 |
| 1:AA:1194:U:H2' | 1:AA:1195:C:H6 | 1.76 | 0.49 |
| 53:D7:19:ARG:HG2 | 53:D7:19:ARG:NH1 | 2.26 | 0.49 |
| 1:CA:947:G:H2' | 1:CA:948:C:C6 | 2.47 | 0.49 |
| 25:DA:960:A:C8 | 25:DA:962:G:C8 | 3.00 | 0.49 |
| 45:BV:151:HIS:HD2 | 45:BV:168:GLU:CG | 2.25 | 0.49 |
| 25:BA:1118:C:H2' | 25:BA:1119:C:H6 | 1.76 | 0.49 |
| 8:AK:88:LYS:CB | 8:AK:89:PRO:HD2 | 2.42 | 0.49 |
| 1:CA:474:G:OP1 | 16:CS:81:ARG:HB3 | 2.12 | 0.49 |
| 34:BN:7:TYR:CE1 | 34:BN:20:MET:HG3 | 2.46 | 0.49 |
| 13:AP:57:ARG:HB2 | 13:AP:57:ARG:NH1 | 2.27 | 0.49 |
| 29:DF:86:GLY:O | 29:DF:87:GLY:O | 2.30 | 0.49 |
| 25:DA:1763:G:OP1 | 25:DA:1763:G:H4' | 2.11 | 0.49 |
| 25:DA:729:G:O5' | 27:DD:208:LYS:NZ | 2.45 | 0.49 |
| 8:CK:14:ARG:O | 8:CK:18:ARG:HD3 | 2.12 | 0.49 |
| 40:D1:71:GLN:HA | 40:D1:71:GLN:NE2 | 2.26 | 0.49 |
| 1:CA:1248:A:H2' | 9:CL:70:LYS:NZ | 2.27 | 0.49 |
| 25:BA:1270:C:H5'' | 25:BA:1271:G:O5' | 2.12 | 0.49 |
| 27:DD:77:ALA:HB2 | 27:DD:97:TYR:CD2 | 2.47 | 0.49 |
| 25:DA:1265:A:O4' | 25:DA:1267:U:C6 | 2.65 | 0.49 |
| 8:CK:30:ARG:O | 8:CK:34:GLU:HG2 | 2.10 | 0.49 |
| 25:BA:863:A:H2' | 25:BA:864:G:H8 | 1.77 | 0.49 |
| 32:BK:85:GLU:OE2 | 32:BK:85:GLU:HA | 2.10 | 0.49 |
| 1:AA:182:U:O2 | 1:AA:182:U:H2' | 2.12 | 0.49 |
| 12:AO:28:LYS:O | 12:AO:28:LYS:CD | 2.60 | 0.49 |
| 3:CF:141:VAL:HG12 | 3:CF:141:VAL:O | 2.12 | 0.49 |
| 45:BV:35:ARG:HB3 | 45:BV:35:ARG:NH1 | 2.27 | 0.49 |
| 25:DA:764:A:O4' | 27:DD:213:ARG:HG3 | 2.12 | 0.49 |
| 25:BA:1077:A:N1 | 25:BA:1088:A:N6 | 2.59 | 0.49 |
| 38:DQ:24:LEU:N | 38:DQ:24:LEU:HD22 | 2.13 | 0.49 |
| 41:D2:38:LEU:HD12 | 41:D2:57:VAL:HG12 | 1.94 | 0.49 |
| 41:D2:75:PHE:CE2 | 41:D2:81:TYR:CD1 | 3.00 | 0.49 |
| 1:CA:1004:A:P | 1:CA:1025:U:O4 | 2.70 | 0.49 |
| 3:CF:180:ALA:HA | 3:CF:206:GLU:HB3 | 1.92 | 0.49 |
| 36:DP:63:LYS:O | 36:DP:63:LYS:CG | 2.58 | 0.49 |
| 29:DF:25:PRO:HG2 | 29:DF:26:ALA:N | 2.27 | 0.49 |
| 29:DF:3:GLU:O | 29:DF:3:GLU:HG2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:1827:C:H2' | 25:DA:1828:G:H5' | 1.94 | 0.49 |
| 30:DG:101:ILE:HB | 30:DG:105:LYS:HZ3 | 1.76 | 0.49 |
| 30:DG:64:THR:HG23 | 30:DG:65:GLY:N | 2.26 | 0.49 |
| 44:BU:52:SER:HB2 | 44:BU:53:PRO:HD3 | 1.94 | 0.49 |
| 9:CL:46:ALA:HA | 9:CL:78:LYS:NZ | 2.27 | 0.49 |
| 25:BA:783:A:H3' | 25:BA:783:A:C8 | 2.46 | 0.49 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:H62 | 1.60 | 0.49 |
| 16:CS:8:ARG:O | 16:CS:9:PHE:CD2 | 2.65 | 0.49 |
| 27:BD:27:THR:HG22 | 27:BD:28:GLU:H | 1.78 | 0.49 |
| 25:DA:2319:G:H4' | 25:DA:2320:A:O4' | 2.13 | 0.49 |
| 25:BA:2666:C:H5'' | 25:BA:2667:C:OP2 | 2.12 | 0.49 |
| 33:BM:131:GLN:HE21 | 33:BM:132:ALA:H | 1.58 | 0.49 |
| 30:DG:117:PHE:C | 30:DG:117:PHE:HD1 | 2.14 | 0.49 |
| 8:AK:87:SER:CB | 8:AK:93:VAL:HB | 2.41 | 0.49 |
| 25:DA:1405:U:H2' | 25:DA:1406:U:H6 | 1.70 | 0.49 |
| 12:CO:26:ALA:HA | 12:CO:98:TYR:CE2 | 2.44 | 0.49 |
| 12:CO:98:TYR:N | 12:CO:98:TYR:CD1 | 2.80 | 0.49 |
| 25:BA:1169:G:N2 | 25:BA:1181:C:O2 | 2.45 | 0.49 |
| 25:BA:1177:A:H5' | 25:BA:1178:C:C6 | 2.47 | 0.49 |
| 19:CV:30:LEU:HD12 | 19:CV:31:ILE:N | 2.27 | 0.49 |
| 54:B8:58:ILE:HA | 54:B8:61:LEU:CD1 | 2.42 | 0.49 |
| 25:DA:2331:G:H4' | 46:D3:43:THR:N | 2.27 | 0.49 |
| 1:AA:1226:C:H4' | 19:AV:80:TYR:OH | 2.13 | 0.49 |
| 37:D0:38:VAL:HG22 | 37:D0:112:ALA:HB2 | 1.95 | 0.49 |
| 22:AB:15:A:N1 | 22:AB:21:A:N6 | 2.60 | 0.49 |
| 25:DA:298:G:H5'' | 25:DA:299:A:OP1 | 2.11 | 0.49 |
| 23:CD:64:G:C2 | 23:CD:65:G:C6 | 3.00 | 0.49 |
| 13:CP:81:LEU:HD13 | 13:CP:88:ARG:HG2 | 1.92 | 0.49 |
| 6:AI:19:LEU:HD21 | 6:AI:59:TYR:CE2 | 2.47 | 0.49 |
| 10:CM:75:ILE:HG13 | 10:CM:76:ASN:H | 1.76 | 0.49 |
| 25:DA:602:G:O2' | 25:DA:655:A:N6 | 2.45 | 0.49 |
| 32:BK:131:LYS:HB3 | 32:BK:132:PRO:CA | 2.42 | 0.49 |
| 11:AN:29:ILE:HD12 | 11:AN:44:SER:HB3 | 1.94 | 0.49 |
| 25:DA:444:C:H4' | 29:DF:49:ALA:HB2 | 1.93 | 0.49 |
| 23:CC:66:C:H2' | 23:CC:67:C:O4' | 2.12 | 0.49 |
| 28:BE:167:VAL:HG21 | 28:BE:187:ALA:CB | 2.42 | 0.49 |
| 25:DA:278:A:H4' | 25:DA:279:C:OP1 | 2.12 | 0.49 |
| 25:BA:1278:A:O3' | 37:B0:34:ILE:HD12 | 2.13 | 0.49 |
| 25:DA:1472:A:H2' | 25:DA:1473:G:C5' | 2.42 | 0.49 |
| 25:BA:639:U:O2' | 25:BA:640:C:H5' | 2.11 | 0.49 |
| 23:CD:71:G:H2' | 23:CD:72:C:H5' | 1.94 | 0.49 |
| 25:DA:2648:C:H2' | 25:DA:2649:U:C6 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 20:CW:10:LEU:CD2 | 20:CW:10:LEU:C | 2.81 | 0.49 |
| 25:DA:593:G:H1' | 54:D8:4:MET:HE1 | 1.94 | 0.49 |
| 46:D3:50:ASN:ND2 | 46:D3:81:VAL:O | 2.46 | 0.49 |
| 25:DA:2746:U:H4' | 31:DH:138:LYS:HG3 | 1.94 | 0.49 |
| 34:BN:113:LYS:HE2 | 34:BN:117:LEU:HD11 | 1.94 | 0.49 |
| 19:AV:11:VAL:HG23 | 19:AV:38:SER:HB2 | 1.94 | 0.49 |
| 41:D2:58:VAL:HB | 41:D2:98:GLU:HB2 | 1.94 | 0.49 |
| 38:DQ:48:LEU:O | 38:DQ:49:VAL:HG23 | 2.13 | 0.49 |
| 25:BA:493:G:H2' | 25:BA:494:G:O4' | 2.12 | 0.49 |
| 1:CA:779:C:C2' | 1:CA:780:A:H5' | 2.43 | 0.49 |
| 31:BH:105:LEU:HD23 | 31:BH:105:LEU:H | 1.76 | 0.49 |
| 25:BA:2465:C:O2' | 25:BA:2466:C:H5' | 2.12 | 0.49 |
| 20:AW:10:LEU:HD23 | 20:AW:12:ALA:CA | 2.42 | 0.49 |
| 28:BE:35:GLN:CG | 28:BE:36:ARG:N | 2.69 | 0.49 |
| 28:DE:36:ARG:HH21 | 28:DE:88:GLY:CA | 2.21 | 0.49 |
| 1:CA:1226:C:H4' | 19:CV:80:TYR:CZ | 2.46 | 0.49 |
| 1:AA:1330:U:H4' | 13:AP:23:TYR:HE2 | 1.77 | 0.49 |
| 52:B6:45:LYS:O | 52:B6:46:HIS:O | 2.30 | 0.49 |
| 10:CM:54:PHE:CE1 | 10:CM:55:LYS:HE3 | 2.47 | 0.49 |
| 1:AA:1023:G:C6 | 1:AA:1024:G:C5 | 3.00 | 0.49 |
| 25:DA:1085:A:H1' | 25:DA:1086:A:O5' | 2.12 | 0.49 |
| 25:DA:1057:A:OP2 | 25:DA:1089:G:N2 | 2.45 | 0.49 |
| 1:AA:1446:A:C4' | 1:AA:1446:A:OP1 | 2.47 | 0.49 |
| 33:BM:62:VAL:HG22 | 33:BM:63:THR:N | 2.26 | 0.49 |
| 43:BT:83:VAL:HG13 | 43:BT:87:GLN:HB3 | 1.95 | 0.49 |
| 30:BG:104:GLU:CG | 50:B4:23:GLU:HG3 | 2.42 | 0.49 |
| 25:BA:2506:U:O2 | 25:BA:2506:U:H2' | 2.11 | 0.49 |
| 25:BA:1558:A:OP2 | 25:BA:1558:A:H3' | 2.12 | 0.49 |
| 25:BA:2170:A:H5'' | 25:BA:2171:A:OP2 | 2.12 | 0.49 |
| 38:DQ:3:ARG:CG | 38:DQ:4:LEU:N | 2.76 | 0.49 |
| 25:DA:1006:C:O2' | 33:DM:106:MET:O | 2.29 | 0.49 |
| 35:BO:39:LYS:HB2 | 35:BO:45:LEU:CD2 | 2.42 | 0.49 |
| 45:DV:28:MET:CG | 45:DV:37:VAL:HG11 | 2.40 | 0.49 |
| 26:DB:83:G:H1 | 26:DB:93:C:N4 | 2.04 | 0.49 |
| 23:CD:32:G:C6 | 23:CD:33:C:C2 | 3.01 | 0.49 |
| 48:BW:58:ALA:O | 48:BW:62:THR:CG2 | 2.60 | 0.49 |
| 8:AK:138:TRP:HE3 | 8:AK:138:TRP:OXT | 1.94 | 0.49 |
| 25:DA:171:G:H2' | 25:DA:172:C:H6 | 1.75 | 0.49 |
| 25:BA:2864:G:C2' | 25:BA:2865:U:H5' | 2.43 | 0.49 |
| 38:BQ:63:THR:HA | 38:BQ:97:ARG:HB3 | 1.93 | 0.49 |
| 1:AA:1103:C:H2' | 1:AA:1104:G:O4' | 2.13 | 0.49 |
| 25:DA:901:A:H2' | 25:DA:901:A:N3 | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1455:G:OP1 | 20:AW:35:THR:OG1 | 2.24 | 0.49 |
| 23:AD:29:C:H2' | 23:AD:30:G:C8 | 2.47 | 0.49 |
| 25:DA:1177:A:H5' | 25:DA:1178:C:OP1 | 2.12 | 0.49 |
| 25:DA:276:A:H2' | 25:DA:277:C:C6 | 2.48 | 0.49 |
| 25:DA:1392:A:C6 | 25:DA:1393:A:C6 | 3.01 | 0.49 |
| 12:AO:42:THR:HA | 12:AO:53:ARG:O | 2.12 | 0.49 |
| 25:DA:1956:U:C2' | 25:DA:1957:C:H5' | 2.43 | 0.49 |
| 12:AO:46:LYS:CG | 12:AO:47:LYS:N | 2.75 | 0.49 |
| 8:CK:99:GLU:C | 8:CK:100:ILE:HG13 | 2.33 | 0.49 |
| 13:CP:70:LEU:O | 13:CP:74:VAL:HG23 | 2.13 | 0.49 |
| 13:CP:65:LYS:HE3 | 50:D4:52:THR:OG1 | 2.13 | 0.49 |
| 3:AF:90:GLU:HA | 3:AF:93:LYS:HB2 | 1.94 | 0.49 |
| 50:D4:43:TYR:CG | 50:D4:43:TYR:O | 2.66 | 0.49 |
| 9:AL:26:VAL:HG13 | 9:AL:61:ALA:HB3 | 1.93 | 0.49 |
| 23:CC:51:U:H2' | 23:CC:52:C:C6 | 2.48 | 0.49 |
| 3:AF:14:ILE:HG13 | 3:AF:15:THR:N | 2.26 | 0.49 |
| 1:AA:958:A:C6 | 1:AA:959:A:C6 | 3.01 | 0.49 |
| 34:DN:85:VAL:HG11 | 34:DN:114:ILE:HD13 | 1.95 | 0.49 |
| 1:AA:1418:A:C2 | 1:AA:1483:A:C2 | 3.00 | 0.49 |
| 39:BR:42:ILE:H | 39:BR:42:ILE:HD12 | 1.77 | 0.49 |
| 38:DQ:67:ARG:CZ | 38:DQ:67:ARG:HB2 | 2.42 | 0.49 |
| 35:DO:61:ARG:O | 35:DO:62:LEU:O | 2.30 | 0.49 |
| 28:DE:101:ARG:CZ | 28:DE:171:GLU:HB2 | 2.41 | 0.49 |
| 1:CA:972:C:C3' | 10:CM:57:LYS:HG3 | 2.42 | 0.49 |
| 4:CG:19:LEU:O | 4:CG:21:LEU:HG | 2.12 | 0.49 |
| 34:BN:104:ARG:HH11 | 39:BR:36:GLU:CD | 2.15 | 0.49 |
| 25:DA:1826:G:H2' | 25:DA:1827:C:O5' | 2.12 | 0.49 |
| 25:DA:2273:A:O2' | 25:DA:2274:A:H5' | 2.13 | 0.49 |
| 25:DA:952:G:P | 36:DP:16:ARG:HH12 | 2.35 | 0.49 |
| 25:DA:1268:A:C2 | 25:DA:2013:A:C4 | 3.00 | 0.49 |
| 31:BH:59:ARG:NH1 | 31:BH:59:ARG:HG3 | 2.10 | 0.49 |
| 1:CA:1143:G:H2' | 1:CA:1144:G:C8 | 2.48 | 0.49 |
| 1:AA:266:G:H5'' | 1:AA:268:C:H41 | 1.75 | 0.49 |
| 44:BU:49:VAL:CG1 | 44:BU:50:ARG:H | 2.25 | 0.49 |
| 25:BA:2119:A:C5 | 25:BA:2171:A:H2 | 2.30 | 0.49 |
| 1:AA:1028(A):C:C4 | 1:AA:1028(B):C:N4 | 2.79 | 0.49 |
| 2:CE:185:ILE:HG12 | 2:CE:185:ILE:O | 2.13 | 0.49 |
| 25:BA:2629:A:N6 | 25:BA:2895:U:C2 | 2.81 | 0.49 |
| 1:AA:1223:C:P | 1:AA:1224:G:H2' | 2.53 | 0.49 |
| 25:DA:2335:A:O2' | 25:DA:2336:A:P | 2.70 | 0.49 |
| 25:BA:1299:G:H5'' | 25:BA:1300:U:OP1 | 2.11 | 0.49 |
| 2:CE:92:TYR:HD2 | 2:CE:92:TYR:O | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:273(F):C:H3' | 25:BA:274:G:C5' | 2.38 | 0.49 |
| 45:DV:8:TYR:HD1 | 45:DV:38:TYR:CE1 | 2.31 | 0.49 |
| 1:CA:273:A:N6 | 1:CA:274:A:C6 | 2.80 | 0.49 |
| 12:AO:24:VAL:HG11 | 12:AO:27:LEU:HD11 | 1.95 | 0.49 |
| 1:AA:1278:U:H3' | 1:AA:1278:U:H6 | 1.77 | 0.49 |
| 37:B0:87:TYR:HE1 | 37:B0:117:VAL:HG12 | 1.77 | 0.49 |
| 16:CS:48:TRP:HH2 | 16:CS:76:GLN:NE2 | 2.09 | 0.49 |
| 14:AQ:29:ARG:HG2 | 14:AQ:40:CYS:HB3 | 1.93 | 0.49 |
| 8:AK:26:VAL:CG2 | 8:AK:26:VAL:O | 2.60 | 0.49 |
| 25:BA:754:C:O2' | 25:BA:755:C:H5' | 2.12 | 0.49 |
| 25:BA:363(B):G:H2' | 25:BA:363(C):G:C8 | 2.47 | 0.49 |
| 25:BA:1575:C:H2' | 25:BA:1576:U:H6 | 1.78 | 0.49 |
| 45:DV:18:LEU:HB3 | 45:DV:23:LYS:O | 2.13 | 0.49 |
| 40:D1:25:TRP:C | 40:D1:25:TRP:CD1 | 2.85 | 0.49 |
| 38:DQ:38:GLN:HG3 | 38:DQ:47:THR:HG21 | 1.94 | 0.49 |
| 1:AA:914:A:C4 | 1:AA:915:A:C8 | 3.00 | 0.49 |
| 6:CI:22:GLU:O | 6:CI:26:ILE:HG13 | 2.11 | 0.49 |
| 25:BA:2584:U:H2' | 25:BA:2585:U:H2' | 1.95 | 0.49 |
| 32:BK:18:VAL:HG21 | 32:BK:44:LEU:HD11 | 1.95 | 0.49 |
| 25:BA:2512:C:H2' | 25:BA:2513:G:O4' | 2.12 | 0.49 |
| 2:AE:52:GLU:HG2 | 2:AE:56:ARG:HH21 | 1.77 | 0.49 |
| 36:BP:59:ARG:H | 36:BP:59:ARG:HD3 | 1.78 | 0.49 |
| 25:DA:613:U:O2 | 25:DA:613:U:O4' | 2.30 | 0.49 |
| 13:AP:47:ASP:O | 13:AP:48:LEU:HB3 | 2.13 | 0.49 |
| 32:DK:5:LEU:HD11 | 32:DK:19:VAL:CG1 | 2.42 | 0.49 |
| 25:DA:777:A:O2' | 25:DA:778:G:H5' | 2.12 | 0.49 |
| 28:BE:38:THR:O | 28:BE:42:ASP:OD2 | 2.30 | 0.49 |
| 28:BE:73:GLU:HG3 | 28:BE:74:PRO:HD2 | 1.94 | 0.49 |
| 35:BO:65:ARG:O | 35:BO:66:GLY:O | 2.30 | 0.49 |
| 33:BM:4:TYR:CD2 | 40:B1:100:VAL:HG11 | 2.48 | 0.49 |
| 9:AL:5:TYR:CE2 | 9:AL:16:ARG:HG2 | 2.40 | 0.49 |
| 28:DE:48:GLN:NE2 | 28:DE:78:LEU:CD1 | 2.72 | 0.49 |
| 45:DV:145:GLU:O | 45:DV:146:ILE:HB | 2.12 | 0.49 |
| 25:BA:1026:U:C1' | 25:BA:1027:A:O5' | 2.41 | 0.49 |
| 25:BA:2287:A:N6 | 25:BA:2344:U:N3 | 2.46 | 0.49 |
| 4:CG:13:ARG:NH1 | 4:CG:36:ARG:O | 2.46 | 0.49 |
| 31:BH:169:VAL:C | 31:BH:170:ARG:CG | 2.81 | 0.49 |
| 2:CE:16:HIS:ND1 | 2:CE:16:HIS:N | 2.60 | 0.49 |
| 25:DA:1142(A):A:C8 | 25:DA:1144:G:C5 | 3.01 | 0.49 |
| 25:BA:2055:C:H5' | 25:BA:2056:G:O5' | 2.13 | 0.49 |
| 48:DW:71:ASN:O | 48:DW:72:ALA:HB3 | 2.12 | 0.49 |
| 25:DA:1536:A:H3' | 25:DA:1537:C:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 40:B1:95:LEU:O | 40:B1:98:LEU:HB3 | 2.11 | 0.49 |
| 25:DA:885:C:N3 | 25:DA:890:A:C5 | 2.81 | 0.49 |
| 25:DA:2169:A:H2' | 25:DA:2169:A:N3 | 2.28 | 0.49 |
| 25:BA:811:U:P | 35:BO:21:ARG:O | 2.70 | 0.49 |
| 25:DA:2067:G:O2' | 25:DA:2069:G:H5'' | 2.13 | 0.49 |
| 35:DO:35:HIS:O | 35:DO:36:LYS:O | 2.30 | 0.49 |
| 51:B5:40:LYS:HE2 | 51:B5:47:PRO:HD2 | 1.95 | 0.49 |
| 45:BV:164:ALA:O | 45:BV:165:VAL:CG2 | 2.56 | 0.49 |
| 25:BA:2262:U:H4' | 25:BA:2328:A:C2 | 2.47 | 0.49 |
| 2:AE:178:ARG:NH1 | 2:AE:196:LEU:O | 2.42 | 0.49 |
| 45:DV:10:ARG:NH2 | 45:DV:25:PRO:HB3 | 2.27 | 0.49 |
| 29:DF:155:LEU:HD22 | 29:DF:185:ASP:O | 2.13 | 0.49 |
| 12:CO:83:VAL:HG13 | 12:CO:84:LEU:N | 2.27 | 0.49 |
| 25:BA:2688:U:C5 | 25:BA:2720:U:OP2 | 2.60 | 0.49 |
| 10:CM:47:PHE:CZ | 14:CQ:37:PHE:CE2 | 3.01 | 0.49 |
| 35:BO:57:THR:C | 35:BO:59:LEU:N | 2.61 | 0.49 |
| 14:CQ:43:CYS:O | 14:CQ:46:GLU:N | 2.45 | 0.49 |
| 51:B5:16:ARG:HG3 | 51:B5:17:ASP:N | 2.28 | 0.49 |
| 51:B5:16:ARG:O | 51:B5:20:ARG:HD2 | 2.12 | 0.49 |
| 1:AA:195:A:C6 | 1:AA:196:A:N1 | 2.81 | 0.49 |
| 1:AA:171:A:C6 | 1:AA:172:A:C6 | 3.00 | 0.49 |
| 25:BA:154:G:H2' | 25:BA:155:C:O4' | 2.12 | 0.49 |
| 1:CA:350:G:H5' | 1:CA:351:G:OP2 | 2.12 | 0.49 |
| 35:BO:140:ALA:O | 35:BO:141:ALA:HB3 | 2.12 | 0.49 |
| 23:AD:67:C:C4 | 23:AD:68:C:N4 | 2.81 | 0.49 |
| 8:CK:29:SER:HB2 | 8:CK:32:LYS:HD2 | 1.94 | 0.49 |
| 25:DA:21:A:C2' | 25:DA:22:C:H5' | 2.42 | 0.49 |
| 3:AF:27:LYS:HA | 3:AF:27:LYS:NZ | 2.28 | 0.49 |
| 25:DA:2746:U:O3' | 31:DH:138:LYS:HG3 | 2.12 | 0.49 |
| 34:BN:98:VAL:HG13 | 34:BN:117:LEU:CB | 2.43 | 0.49 |
| 12:AO:28:LYS:O | 12:AO:28:LYS:HD2 | 2.12 | 0.49 |
| 36:DP:18:LYS:O | 36:DP:19:GLY:O | 2.30 | 0.49 |
| 45:BV:1:MET:CE | 45:BV:135:GLU:HB3 | 2.43 | 0.49 |
| 42:DS:41:LYS:HD2 | 51:D5:25:LEU:HD11 | 1.94 | 0.49 |
| 25:BA:24:G:C2' | 25:BA:25:U:H5' | 2.43 | 0.49 |
| 1:AA:1000:A:O2' | 1:AA:1001:G:H5' | 2.12 | 0.49 |
| 25:BA:531:C:OP1 | 25:BA:561:G:N1 | 2.45 | 0.49 |
| 1:AA:585:G:O2' | 1:AA:879:C:H5'' | 2.13 | 0.49 |
| 15:CR:50:HIS:O | 15:CR:53:HIS:HB3 | 2.13 | 0.49 |
| 25:BA:2870:C:H5'' | 37:B0:65:LEU:HD21 | 1.94 | 0.49 |
| 1:CA:775:G:C2' | 1:CA:776:G:H5' | 2.43 | 0.49 |
| 29:BF:164:ARG:HG2 | 29:BF:175:THR:OG1 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:AO:59:ARG:HB2 | 12:AO:65:GLU:HG3 | 1.95 | 0.49 |
| 30:DG:21:ARG:HH11 | 30:DG:21:ARG:HG2 | 1.76 | 0.49 |
| 1:AA:1110:A:O5' | 1:AA:1110:A:H8 | 1.96 | 0.49 |
| 25:DA:1418:G:H8 | 25:DA:1418:G:O5' | 1.94 | 0.49 |
| 38:DQ:10:ARG:O | 38:DQ:14:VAL:HG12 | 2.13 | 0.49 |
| 28:BE:51:PHE:CE1 | 28:BE:52:LEU:HD21 | 2.47 | 0.49 |
| 28:BE:53:PRO:O | 28:BE:74:PRO:HA | 2.13 | 0.49 |
| 4:AG:10:ARG:HA | 4:AG:13:ARG:HG3 | 1.94 | 0.49 |
| 29:DF:51:THR:HB | 29:DF:88:VAL:HG11 | 1.95 | 0.49 |
| 1:CA:1199:U:H4' | 10:CM:54:PHE:CZ | 2.47 | 0.49 |
| 25:DA:1057:A:N1 | 25:DA:1081:U:C4 | 2.80 | 0.49 |
| 39:BR:41:ARG:NH1 | 39:BR:43:GLN:HB2 | 2.27 | 0.49 |
| 25:BA:442:G:C4 | 25:BA:444:C:C5 | 3.00 | 0.49 |
| 1:CA:1178:G:C8 | 1:CA:1180:A:OP2 | 2.65 | 0.49 |
| 31:BH:75:ALA:O | 31:BH:79:VAL:HG22 | 2.12 | 0.49 |
| 1:CA:1329:A:H2' | 1:CA:1330:U:O4' | 2.13 | 0.49 |
| 25:DA:1109:C:H5 | 25:DA:1110:G:C6 | 2.30 | 0.49 |
| 20:AW:63:ILE:HG22 | 20:AW:77:ALA:HB1 | 1.95 | 0.49 |
| 26:DB:15:A:C5' | 26:DB:16:G:H8 | 2.20 | 0.49 |
| 26:DB:70:C:H2' | 26:DB:71:C:H6 | 1.78 | 0.49 |
| 1:CA:1237:C:H5'' | 1:CA:1238:A:O4' | 2.13 | 0.49 |
| 1:CA:209:U:H1' | 1:CA:210:U:OP1 | 2.13 | 0.49 |
| 41:B2:44:LYS:HD2 | 41:B2:45:THR:N | 2.21 | 0.49 |
| 45:DV:24:LEU:HD12 | 45:DV:25:PRO:O | 2.13 | 0.49 |
| 1:CA:113:G:O4' | 1:CA:354:G:H4' | 2.12 | 0.49 |
| 1:CA:1266:G:N2 | 1:CA:1270:C:C4 | 2.81 | 0.49 |
| 23:CC:29:C:O2 | 23:CC:44:A:C2 | 2.65 | 0.49 |
| 13:CP:110:ARG:NH1 | 13:CP:110:ARG:HG2 | 2.28 | 0.49 |
| 36:DP:102:VAL:O | 36:DP:103:MET:C | 2.50 | 0.49 |
| 1:AA:1194:U:H5'' | 5:AH:22:GLY:O | 2.13 | 0.49 |
| 25:DA:2111:C:H41 | 25:DA:2147:G:N2 | 2.10 | 0.49 |
| 3:CF:18:TRP:HE3 | 3:CF:18:TRP:N | 2.11 | 0.49 |
| 5:AH:96:PRO:HA | 5:AH:117:ASP:CG | 2.32 | 0.49 |
| 1:AA:412:A:C1' | 1:AA:413:G:OP2 | 2.59 | 0.49 |
| 1:CA:266:G:H1' | 1:CA:267:C:OP2 | 2.12 | 0.49 |
| 1:AA:674:G:H2' | 1:AA:675:A:C8 | 2.47 | 0.49 |
| 1:AA:721:G:H4' | 1:AA:722:A:O4' | 2.13 | 0.49 |
| 3:AF:188:LEU:HD13 | 3:AF:195:VAL:CG1 | 2.43 | 0.49 |
| 25:DA:1665:A:C4' | 34:DN:67:LYS:HB2 | 2.43 | 0.49 |
| 25:BA:1336:A:H2' | 25:BA:1337:G:C8 | 2.48 | 0.49 |
| 10:CM:13:HIS:HB3 | 10:CM:68:HIS:CD2 | 2.48 | 0.49 |
| 46:B3:11:ARG:HB2 | 46:B3:11:ARG:NH1 | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:CK:29:SER:CB | 8:CK:32:LYS:HD2 | 2.42 | 0.49 |
| 1:CA:373:A:C2 | 1:CA:374:A:C8 | 3.00 | 0.49 |
| 21:AX:3:LYS:HB3 | 21:AX:14:TRP:CG | 2.47 | 0.49 |
| 1:CA:10:A:H2' | 1:CA:11:G:C8 | 2.47 | 0.49 |
| 50:D4:49:PHE:CD1 | 50:D4:50:VAL:HG13 | 2.47 | 0.49 |
| 1:CA:775:G:O2' | 1:CA:776:G:H5' | 2.13 | 0.49 |
| 1:CA:604:G:H2' | 1:CA:605:U:O4' | 2.12 | 0.49 |
| 10:CM:82:ILE:O | 10:CM:86:MET:HB2 | 2.12 | 0.49 |
| 5:AH:72:GLN:O | 5:AH:75:THR:HG22 | 2.13 | 0.49 |
| 26:BB:20:C:C2' | 26:BB:21:G:H5' | 2.43 | 0.49 |
| 25:DA:2097:C:H2' | 25:DA:2098:U:O4' | 2.12 | 0.49 |
| 20:CW:44:ALA:HB1 | 20:CW:91:LEU:HB2 | 1.95 | 0.49 |
| 25:DA:1167:U:C2 | 25:DA:1183:G:N2 | 2.81 | 0.49 |
| 1:CA:51:A:H4' | 1:CA:52:G:C5' | 2.42 | 0.49 |
| 25:DA:810:U:O5' | 25:DA:810:U:H6 | 1.94 | 0.49 |
| 25:DA:55:G:C2 | 25:DA:116:C:C2 | 3.01 | 0.49 |
| 12:AO:55:VAL:HG12 | 12:AO:69:TYR:HA | 1.92 | 0.49 |
| 1:AA:1156:G:C2' | 1:AA:1157:A:H5'' | 2.41 | 0.49 |
| 1:CA:543:C:OP1 | 4:CG:14:ARG:HD2 | 2.13 | 0.49 |
| 29:BF:178:PRO:HG2 | 29:BF:179:GLU:OE2 | 2.13 | 0.49 |
| 25:BA:619:G:H5'' | 25:BA:620:G:OP2 | 2.12 | 0.49 |
| 25:DA:2749:A:N6 | 25:DA:2750:A:H62 | 2.11 | 0.49 |
| 13:CP:49:THR:HB | 13:CP:52:GLU:OE1 | 2.12 | 0.49 |
| 30:DG:61:ALA:HA | 30:DG:64:THR:HG22 | 1.95 | 0.49 |
| 38:BQ:27:SER:HA | 38:BQ:88:ASP:HB3 | 1.95 | 0.49 |
| 5:CH:88:LYS:HB3 | 5:CH:123:LEU:HB2 | 1.94 | 0.49 |
| 25:BA:2402:C:H2' | 25:BA:2403:C:C5' | 2.41 | 0.49 |
| 31:BH:4:ILE:H | 31:BH:4:ILE:CD1 | 2.15 | 0.49 |
| 25:DA:2129:C:N4 | 25:DA:2130:U:H3 | 2.10 | 0.49 |
| 2:CE:80:ILE:HD12 | 2:CE:84:GLU:HG3 | 1.95 | 0.49 |
| 25:DA:141:A:C8 | 25:DA:1408:C:H1' | 2.48 | 0.49 |
| 43:DT:23:GLU:HG3 | 43:DT:24:GLY:N | 2.23 | 0.49 |
| 2:AE:165:VAL:HG23 | 2:AE:166:ASP:H | 1.78 | 0.49 |
| 37:D0:20:LEU:HD21 | 37:D0:40:LYS:HD3 | 1.93 | 0.49 |
| 25:DA:2805:G:H2' | 25:DA:2807:G:C8 | 2.48 | 0.49 |
| 1:CA:926:G:H5'' | 1:CA:927:G:O5' | 2.13 | 0.49 |
| 25:BA:2682:U:H5'' | 28:BE:11:MET:HB2 | 1.95 | 0.49 |
| 48:DW:17:SER:CB | 48:DW:18:PRO:HA | 2.42 | 0.49 |
| 13:CP:78:ILE:HD13 | 13:CP:92:HIS:CD2 | 2.48 | 0.49 |
| 5:AH:148:VAL:HG21 | 8:AK:107:LEU:CD2 | 2.41 | 0.49 |
| 28:DE:66:HIS:CE1 | 28:DE:73:GLU:OE1 | 2.65 | 0.49 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:H1' | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 9:AL:79:LEU:O | 9:AL:82:ALA:HB3 | 2.12 | 0.49 |
| 28:BE:182:LEU:HD12 | 28:BE:183:LEU:N | 2.26 | 0.49 |
| 4:AG:194:LEU:HD12 | 4:AG:195:ALA:N | 2.27 | 0.49 |
| 5:CH:105:VAL:HG21 | 5:CH:128:PRO:HB3 | 1.94 | 0.49 |
| 29:BF:123:LEU:HD12 | 29:BF:124:LEU:H | 1.76 | 0.49 |
| 25:BA:646:A:H2' | 25:BA:647:G:O5' | 2.12 | 0.49 |
| 1:AA:967:C:H4' | 9:AL:125:TYR:HE2 | 1.77 | 0.49 |
| 25:BA:814:C:O2' | 25:BA:815:C:H5' | 2.13 | 0.49 |
| 44:DU:89:PHE:HB2 | 44:DU:90:LEU:HD23 | 1.95 | 0.49 |
| 18:CU:29:PHE:CD1 | 18:CU:39:VAL:HG11 | 2.47 | 0.49 |
| 2:AE:200:ILE:N | 2:AE:200:ILE:HD12 | 2.28 | 0.49 |
| 31:DH:41:MET:O | 31:DH:42:ARG:HB3 | 2.13 | 0.49 |
| 35:BO:79:ARG:HB2 | 35:BO:110:TYR:CD1 | 2.47 | 0.49 |
| 25:DA:337:C:H2' | 25:DA:338:G:O4' | 2.12 | 0.49 |
| 25:BA:1914:C:H2' | 25:BA:1915:U:O4' | 2.13 | 0.49 |
| 1:CA:186(F):C:H2' | 1:CA:187:C:O4' | 2.12 | 0.49 |
| 34:DN:122:LEU:HD13 | 39:DR:72:VAL:HG11 | 1.93 | 0.49 |
| 41:D2:64:HIS:CD2 | 41:D2:92:THR:OG1 | 2.66 | 0.49 |
| 39:BR:122:ASP:O | 39:BR:126:ALA:HB3 | 2.13 | 0.49 |
| 1:AA:1402:C:H2' | 1:AA:1403:C:O4' | 2.13 | 0.49 |
| 42:BS:111:HIS:HD2 | 42:BS:112:GLY:H | 1.59 | 0.49 |
| 1:AA:223:U:H2' | 1:AA:224:C:H6 | 1.76 | 0.49 |
| 4:AG:112:VAL:HG12 | 4:AG:116:GLN:OE1 | 2.13 | 0.49 |
| 1:CA:1221:G:H4' | 19:CV:77:THR:HG21 | 1.94 | 0.49 |
| 25:DA:1773:A:H2 | 25:DA:1977:A:N1 | 2.11 | 0.49 |
| 25:BA:693:C:O2' | 25:BA:694:U:H5' | 2.13 | 0.49 |
| 40:D1:95:LEU:CD2 | 41:D2:13:ARG:HB2 | 2.43 | 0.49 |
| 52:D6:39:TYR:O | 52:D6:47:THR:O | 2.30 | 0.49 |
| 28:BE:35:GLN:HB2 | 28:BE:48:GLN:CG | 2.36 | 0.49 |
| 28:BE:81:ILE:N | 28:BE:81:ILE:HD13 | 2.27 | 0.49 |
| 28:DE:48:GLN:CG | 28:DE:78:LEU:HB3 | 2.42 | 0.49 |
| 28:DE:23:VAL:HA | 28:DE:184:VAL:O | 2.13 | 0.49 |
| 25:BA:1026:U:H1' | 25:BA:1027:A:C5' | 2.42 | 0.49 |
| 10:CM:54:PHE:CD1 | 10:CM:55:LYS:HE3 | 2.48 | 0.49 |
| 25:BA:607:U:O2 | 25:BA:621:A:N1 | 2.46 | 0.49 |
| 25:DA:1058:U:O2 | 25:DA:1080:A:N1 | 2.45 | 0.49 |
| 25:DA:1075:C:H2' | 25:DA:1076:C:C6 | 2.48 | 0.49 |
| 2:CE:19:HIS:CD2 | 2:CE:20:GLU:OE1 | 2.66 | 0.49 |
| 30:DG:7:LEU:O | 30:DG:7:LEU:HD23 | 2.13 | 0.49 |
| 1:CA:1143:G:H2' | 1:CA:1144:G:H8 | 1.77 | 0.49 |
| 9:CL:17:VAL:HA | 9:CL:63:ILE:HG12 | 1.94 | 0.49 |
| 43:BT:82:GLN:HE21 | 43:BT:83:VAL:N | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 30:BG:37:VAL:HG22 | 30:BG:159:VAL:HB | 1.95 | 0.49 |
| 17:CT:67:LYS:CA | 17:CT:70:ARG:HH12 | 2.23 | 0.49 |
| 9:CL:10:ARG:HD3 | 9:CL:75:ASP:HB3 | 1.94 | 0.49 |
| 54:B8:51:ALA:N | 54:B8:53:PRO:HD2 | 2.28 | 0.49 |
| 25:BA:2117:A:O2' | 25:BA:2118:U:C5 | 2.65 | 0.49 |
| 20:AW:100:ILE:CG1 | 20:AW:101:GLY:H | 2.25 | 0.49 |
| 27:BD:186:HIS:CD2 | 27:BD:188:GLU:HB2 | 2.48 | 0.49 |
| 26:DB:87:G:H3' | 26:DB:88:C:C5' | 2.43 | 0.49 |
| 36:DP:60:ARG:O | 36:DP:60:ARG:HG3 | 2.13 | 0.49 |
| 1:AA:1352:C:H42 | 1:AA:1370:G:H1 | 1.61 | 0.49 |
| 1:CA:1069:C:H5 | 1:CA:1094:G:O6 | 1.95 | 0.49 |
| 25:DA:2332:U:H5' | 46:D3:43:THR:HG21 | 1.94 | 0.49 |
| 25:BA:2702:U:H4' | 25:BA:2703:C:OP1 | 2.12 | 0.49 |
| 40:B1:78:THR:O | 40:B1:81:HIS:N | 2.46 | 0.49 |
| 17:AT:45:HIS:CD2 | 17:AT:65:ILE:HG12 | 2.48 | 0.49 |
| 1:CA:1400:C:N4 | 23:CC:35:C:H1' | 2.28 | 0.49 |
| 25:DA:945:A:C4 | 25:DA:2448:A:C2 | 3.01 | 0.49 |
| 23:CD:22:A:C2 | 23:CD:47:G:C8 | 3.00 | 0.49 |
| 13:CP:55:ARG:NH1 | 13:CP:55:ARG:HG3 | 2.26 | 0.49 |
| 26:DB:5:C:N4 | 26:DB:115:G:H1 | 2.09 | 0.49 |
| 40:B1:8:VAL:CG2 | 40:B1:11:ARG:HH21 | 2.25 | 0.49 |
| 26:BB:73:A:C3' | 26:BB:74:U:H5' | 2.43 | 0.49 |
| 37:B0:9:LYS:HA | 37:B0:17:ARG:HE | 1.76 | 0.49 |
| 25:BA:2849:U:O4 | 39:BR:23:ARG:NH2 | 2.43 | 0.49 |
| 23:CC:66:C:O2' | 23:CC:67:C:H5' | 2.13 | 0.49 |
| 25:BA:1761:C:N3 | 25:BA:1762:A:C6 | 2.81 | 0.49 |
| 1:AA:1455:G:C5' | 20:AW:32:ALA:HB2 | 2.43 | 0.49 |
| 1:AA:575:G:C5 | 1:AA:881:G:C2 | 3.01 | 0.49 |
| 1:AA:1047:G:H2' | 1:AA:1048:G:H5' | 1.94 | 0.49 |
| 20:CW:33:ILE:HD12 | 20:CW:63:ILE:HA | 1.94 | 0.49 |
| 2:CE:51:LEU:HG | 2:CE:201:ILE:HG23 | 1.94 | 0.49 |
| 25:BA:2741:A:H2' | 25:BA:2742:C:O4' | 2.13 | 0.49 |
| 25:BA:317:G:C2 | 25:BA:318:C:C2 | 3.01 | 0.49 |
| 25:DA:1800:C:OP2 | 27:DD:183:ARG:NH2 | 2.45 | 0.49 |
| 1:CA:191(A):G:C2' | 1:CA:191(B):G:H5' | 2.43 | 0.49 |
| 25:BA:2271:G:OP1 | 46:B3:18:ALA:HB1 | 2.13 | 0.49 |
| 25:BA:576:U:H2' | 25:BA:577:G:C8 | 2.48 | 0.49 |
| 45:DV:29:TYR:HA | 45:DV:33:LEU:O | 2.13 | 0.49 |
| 1:AA:132:C:C2 | 1:AA:231:G:N2 | 2.81 | 0.49 |
| 43:DT:18:TYR:HD1 | 43:DT:21:PHE:CE2 | 2.30 | 0.49 |
| 45:BV:69:THR:HG22 | 45:BV:90:VAL:HG22 | 1.92 | 0.49 |
| 25:BA:1088:A:N3 | 25:BA:1088:A:H3' | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 36:DP:29:PHE:CB | 36:DP:65:PHE:CD1 | 2.92 | 0.49 |
| 38:DQ:84:GLN:HA | 38:DQ:109:GLY:HA3 | 1.95 | 0.49 |
| 28:BE:54:GLN:O | 28:BE:55:ASN:HB2 | 2.12 | 0.49 |
| 1:CA:1035:A:H3' | 1:CA:1036:G:H5'' | 1.95 | 0.49 |
| 25:BA:1899:G:O2' | 25:BA:1900:A:P | 2.70 | 0.49 |
| 33:BM:35:ARG:O | 33:BM:35:ARG:CG | 2.61 | 0.49 |
| 28:DE:4:ILE:HD12 | 28:DE:28:ALA:CB | 2.42 | 0.49 |
| 28:DE:36:ARG:O | 28:DE:37:ARG:O | 2.30 | 0.49 |
| 41:D2:76:LYS:C | 41:D2:79:VAL:HG23 | 2.27 | 0.49 |
| 26:BB:42:C:O3' | 30:BG:67:LYS:NZ | 2.46 | 0.49 |
| 26:DB:75:G:H5' | 26:DB:75:G:C8 | 2.37 | 0.49 |
| 1:CA:973:G:C1' | 10:CM:55:LYS:HG3 | 2.42 | 0.49 |
| 25:DA:1062:G:N2 | 25:DA:1077:A:H1' | 2.28 | 0.49 |
| 2:AE:21:ARG:O | 2:AE:23:ARG:N | 2.46 | 0.49 |
| 25:DA:1012:U:C2 | 25:DA:1143:A:H2 | 2.21 | 0.49 |
| 29:DF:25:PRO:HG2 | 29:DF:26:ALA:H | 1.77 | 0.49 |
| 14:AQ:23:ARG:CG | 14:AQ:23:ARG:NH1 | 2.75 | 0.49 |
| 1:CA:1305:G:H5'' | 21:CX:4:GLY:HA3 | 1.94 | 0.49 |
| 4:AG:33:MET:CE | 4:AG:37:PRO:HA | 2.42 | 0.49 |
| 44:BU:44:ILE:HG13 | 44:BU:45:VAL:H | 1.78 | 0.49 |
| 2:CE:111:ARG:CG | 2:CE:111:ARG:HH11 | 2.13 | 0.49 |
| 1:AA:686:U:C2' | 1:AA:687:A:O5' | 2.60 | 0.49 |
| 1:CA:1297:C:C1' | 1:CA:1298:C:OP2 | 2.59 | 0.49 |
| 25:BA:443:A:N7 | 29:BF:45:ARG:CD | 2.71 | 0.49 |
| 25:BA:1534:G:C6 | 25:BA:1538:G:N2 | 2.80 | 0.49 |
| 25:DA:6:A:H4' | 33:DM:129:PRO:CB | 2.42 | 0.49 |
| 28:BE:120:TRP:CD2 | 28:BE:155:LYS:HD3 | 2.47 | 0.49 |
| 50:B4:56:VAL:HG13 | 50:B4:60:GLN:HG3 | 1.95 | 0.49 |
| 4:AG:119:GLN:CG | 4:AG:123:HIS:CD2 | 2.96 | 0.49 |
| 1:CA:411:A:N7 | 1:CA:429:U:C5 | 2.80 | 0.49 |
| 17:AT:65:ILE:HD12 | 17:AT:65:ILE:N | 2.27 | 0.49 |
| 25:DA:2224:G:H4' | 25:DA:2226:C:C2 | 2.47 | 0.49 |
| 4:AG:138:TYR:HD2 | 4:AG:139:ARG:N | 2.09 | 0.49 |
| 1:CA:1342:C:O2' | 1:CA:1343:G:H5' | 2.13 | 0.49 |
| 43:DT:10:ALA:HB1 | 43:DT:11:PRO:HD2 | 1.94 | 0.49 |
| 42:BS:40:ASN:O | 42:BS:41:LYS:HG2 | 2.13 | 0.49 |
| 1:CA:279:A:H5'' | 1:CA:281:G:H5' | 1.94 | 0.49 |
| 1:AA:411:A:C6 | 1:AA:429:U:C4 | 3.01 | 0.49 |
| 10:CM:33:GLN:CB | 10:CM:75:ILE:HG12 | 2.42 | 0.49 |
| 31:DH:10:PRO:HD2 | 31:DH:50:VAL:O | 2.13 | 0.49 |
| 24:A1:14:U:H2' | 24:A1:15:U:O4' | 2.13 | 0.49 |
| 1:CA:580:U:H2' | 1:CA:581:G:O4' | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 45:DV:148:ASP:OD2 | 45:DV:149:SER:O | 2.30 | 0.49 |
| 50:B4:24:THR:O | 50:B4:25:TYR:HB2 | 2.13 | 0.49 |
| 25:DA:2364:C:H2' | 25:DA:2365:G:H5' | 1.94 | 0.49 |
| 1:AA:1240:U:P | 7:AJ:116:ALA:HB2 | 2.52 | 0.49 |
| 22:AB:24:C:H3' | 22:AB:24:C:C6 | 2.48 | 0.49 |
| 25:DA:620:G:C5' | 25:DA:620:G:N3 | 2.76 | 0.49 |
| 1:CA:184:G:N2 | 1:CA:194:C:C2 | 2.81 | 0.49 |
| 18:CU:44:LEU:HD11 | 18:CU:70:ILE:HG21 | 1.95 | 0.49 |
| 6:CI:53:ALA:HB3 | 6:CI:86:ARG:HD3 | 1.95 | 0.49 |
| 25:BA:2365:G:O6 | 54:B8:39:LYS:HE3 | 2.12 | 0.49 |
| 25:DA:843:G:N2 | 25:DA:936:C:C2 | 2.81 | 0.49 |
| 25:BA:194:G:H2' | 25:BA:195:A:O4' | 2.12 | 0.49 |
| 2:CE:68:ILE:HD12 | 2:CE:222:ILE:HD11 | 1.95 | 0.49 |
| 47:DZ:23:LYS:O | 47:DZ:31:GLY:HA2 | 2.13 | 0.49 |
| 25:DA:2485:G:C2 | 25:DA:2486:G:C8 | 3.00 | 0.49 |
| 1:CA:380:G:C2 | 1:CA:384:G:C6 | 3.01 | 0.49 |
| 25:DA:648:G:O2' | 25:DA:649:G:H5' | 2.12 | 0.49 |
| 1:AA:123:C:OP2 | 1:AA:123:C:H6 | 1.95 | 0.49 |
| 3:AF:56:ASP:HB2 | 3:AF:67:THR:HB | 1.93 | 0.49 |
| 1:AA:20:U:C2' | 1:AA:21:G:H5' | 2.43 | 0.49 |
| 25:BA:2288:A:C2 | 25:BA:2325:G:C8 | 3.01 | 0.49 |
| 25:BA:1070:A:C3' | 25:BA:1071:G:H5'' | 2.43 | 0.48 |
| 35:BO:61:ARG:O | 35:BO:62:LEU:O | 2.30 | 0.48 |
| 52:D6:9:LEU:HD22 | 52:D6:11:LEU:CD2 | 2.43 | 0.48 |
| 52:D6:25:LYS:HE2 | 52:D6:27:LYS:NZ | 2.28 | 0.48 |
| 27:BD:181:GLU:HG3 | 27:BD:272:ALA:CB | 2.40 | 0.48 |
| 36:DP:65:PHE:O | 36:DP:66:ILE:O | 2.30 | 0.48 |
| 38:DQ:10:ARG:HH21 | 38:DQ:91:PRO:HB2 | 1.78 | 0.48 |
| 40:D1:91:ASP:C | 40:D1:93:LYS:N | 2.65 | 0.48 |
| 25:DA:2681:C:C2' | 25:DA:2681:C:O2 | 2.54 | 0.48 |
| 33:BM:38:HIS:O | 40:B1:67:ALA:HB1 | 2.12 | 0.48 |
| 25:BA:298:G:OP1 | 44:BU:84:ARG:HG2 | 2.12 | 0.48 |
| 52:B6:47:THR:CG2 | 52:B6:48:VAL:N | 2.49 | 0.48 |
| 25:BA:2346:A:O3' | 52:B6:39:TYR:OH | 2.31 | 0.48 |
| 1:CA:510:A:H5'' | 1:CA:511:C:P | 2.53 | 0.48 |
| 4:CG:8:VAL:HG11 | 4:CG:21:LEU:HB2 | 1.94 | 0.48 |
| 4:AG:65:ARG:HG2 | 4:AG:65:ARG:NH1 | 2.26 | 0.48 |
| 9:CL:18:PHE:HB2 | 9:CL:62:TYR:O | 2.12 | 0.48 |
| 25:DA:888:C:H4' | 25:DA:889:C:H5' | 1.95 | 0.48 |
| 46:B3:27:GLU:HG3 | 46:B3:69:PHE:H | 1.78 | 0.48 |
| 27:BD:27:THR:O | 27:BD:28:GLU:OE1 | 2.30 | 0.48 |
| 16:CS:3:LYS:O | 16:CS:21:VAL:HA | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 35:DO:83:VAL:HG12 | 35:DO:112:LEU:HD21 | 1.94 | 0.48 |
| 1:CA:1069:C:C5 | 1:CA:1094:G:O6 | 2.66 | 0.48 |
| 1:CA:1069:C:O2' | 1:CA:1192:C:H1' | 2.12 | 0.48 |
| 1:CA:1069:C:H4' | 1:CA:1192:C:O2 | 2.13 | 0.48 |
| 25:BA:1519:G:O2' | 25:BA:1520:U:H5' | 2.13 | 0.48 |
| 25:DA:320:A:H4' | 25:DA:322:A:C8 | 2.48 | 0.48 |
| 37:B0:70:LEU:O | 37:B0:72:ASP:N | 2.46 | 0.48 |
| 35:BO:56:SER:O | 35:BO:57:THR:O | 2.30 | 0.48 |
| 25:DA:2766:G:N3 | 25:DA:2766:G:H2' | 2.28 | 0.48 |
| 1:AA:49:U:O2' | 1:AA:50:A:H2' | 2.12 | 0.48 |
| 30:DG:16:ARG:N | 30:DG:17:PRO:HD2 | 2.27 | 0.48 |
| 31:BH:98:LEU:HD12 | 31:BH:102:ALA:O | 2.13 | 0.48 |
| 25:DA:877:U:C4' | 25:DA:878:A:OP1 | 2.61 | 0.48 |
| 1:AA:753:A:H4' | 1:AA:754:C:C5' | 2.43 | 0.48 |
| 25:BA:2248:C:H2' | 25:BA:2249:U:H5' | 1.95 | 0.48 |
| 25:BA:1517:G:H4' | 25:BA:1556:C:O2' | 2.13 | 0.48 |
| 1:AA:1140:C:H2' | 1:AA:1141:C:H6 | 1.78 | 0.48 |
| 25:DA:756:C:H2' | 25:DA:757:U:H5' | 1.95 | 0.48 |
| 26:BB:94:C:C2' | 26:BB:95:U:H5' | 2.44 | 0.48 |
| 1:CA:114:U:H2' | 1:CA:115:G:C8 | 2.48 | 0.48 |
| 25:BA:26:G:H1' | 25:BA:515:A:N6 | 2.27 | 0.48 |
| 10:CM:6:ILE:HG12 | 10:CM:72:VAL:O | 2.13 | 0.48 |
| 28:DE:203:LYS:O | 28:DE:204:ALA:CB | 2.59 | 0.48 |
| 25:BA:2003:G:H2' | 25:BA:2004:G:O5' | 2.13 | 0.48 |
| 45:BV:130:PRO:HA | 45:BV:133:ILE:HD11 | 1.93 | 0.48 |
| 15:CR:15:PHE:CE2 | 15:CR:84:LYS:HD2 | 2.47 | 0.48 |
| 1:CA:257:G:H2' | 1:CA:258:G:O4' | 2.13 | 0.48 |
| 1:CA:620:C:H2' | 1:CA:621:A:O4' | 2.13 | 0.48 |
| 16:AS:8:ARG:O | 16:AS:9:PHE:CD2 | 2.66 | 0.48 |
| 25:BA:107:C:H2' | 25:BA:108:U:H6 | 1.77 | 0.48 |
| 42:BS:73:ALA:HB3 | 42:BS:106:ILE:CD1 | 2.43 | 0.48 |
| 1:CA:949:A:C1' | 1:CA:1364:U:H3 | 2.26 | 0.48 |
| 39:DR:125:ARG:HB3 | 39:DR:129:ARG:NH2 | 2.27 | 0.48 |
| 39:DR:136:GLN:O | 39:DR:137:LYS:HD2 | 2.12 | 0.48 |
| 25:BA:1063:G:O2' | 25:BA:1064:C:H5' | 2.14 | 0.48 |
| 25:BA:1077:A:H3' | 25:BA:1078:U:H5'' | 1.90 | 0.48 |
| 38:BQ:106:ARG:N | 38:BQ:110:LEU:HD21 | 2.28 | 0.48 |
| 38:BQ:86:ALA:O | 38:BQ:87:PHE:HB3 | 2.14 | 0.48 |
| 40:D1:91:ASP:O | 40:D1:92:ARG:HG2 | 2.13 | 0.48 |
| 40:D1:92:ARG:CD | 40:D1:95:LEU:HD12 | 2.42 | 0.48 |
| 1:AA:1130:A:O5' | 1:AA:1131:G:P | 2.71 | 0.48 |
| 23:CC:62:C:H2' | 23:CC:63:C:C6 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 54:D8:47:LYS:O | 54:D8:48:PHE:CB | 2.61 | 0.48 |
| 35:DO:64:LYS:CB | 54:D8:25:MET:SD | 3.01 | 0.48 |
| 1:AA:1004:A:C8 | 1:AA:1036:G:N2 | 2.75 | 0.48 |
| 25:DA:1085:A:H4' | 25:DA:1086:A:OP1 | 2.13 | 0.48 |
| 43:DT:40:LYS:HG3 | 43:DT:51:VAL:CG1 | 2.44 | 0.48 |
| 36:DP:87:LYS:O | 36:DP:88:GLY:O | 2.30 | 0.48 |
| 30:DG:105:LYS:CE | 50:D4:26:SER:HB3 | 2.44 | 0.48 |
| 38:DQ:95:HIS:N | 38:DQ:99:LYS:HB2 | 2.28 | 0.48 |
| 30:BG:96:ARG:HA | 30:BG:99:MET:HG2 | 1.95 | 0.48 |
| 25:DA:1494:A:H2' | 25:DA:1495:A:C8 | 2.48 | 0.48 |
| 48:BW:15:LYS:H | 48:BW:67:LYS:NZ | 2.11 | 0.48 |
| 37:B0:104:ARG:NH1 | 37:B0:107:ASP:OD1 | 2.34 | 0.48 |
| 45:BV:113:ALA:N | 45:BV:114:GLY:CA | 2.74 | 0.48 |
| 5:CH:70:PRO:O | 5:CH:71:LEU:HD23 | 2.13 | 0.48 |
| 27:DD:70:TRP:CD1 | 27:DD:70:TRP:C | 2.86 | 0.48 |
| 39:BR:110:ILE:HD12 | 39:BR:110:ILE:O | 2.13 | 0.48 |
| 25:DA:172:C:H2' | 25:DA:173:G:C8 | 2.47 | 0.48 |
| 1:AA:659:U:O2 | 1:AA:660:G:C8 | 2.67 | 0.48 |
| 45:DV:19:ARG:HH11 | 45:DV:84:GLU:HB2 | 1.77 | 0.48 |
| 28:BE:25:VAL:HG13 | 28:BE:183:LEU:HG | 1.95 | 0.48 |
| 25:BA:1735:C:C2' | 25:BA:1741:C:H5' | 2.43 | 0.48 |
| 8:AK:41:ARG:NH1 | 8:AK:41:ARG:HG3 | 2.27 | 0.48 |
| 52:B6:34:LEU:O | 52:B6:51:GLU:HB3 | 2.13 | 0.48 |
| 25:BA:1586:A:H3' | 25:BA:1587:A:C8 | 2.47 | 0.48 |
| 1:AA:628:G:H2' | 1:AA:629:G:C8 | 2.48 | 0.48 |
| 1:AA:1098:C:H2' | 1:AA:1099:G:O4' | 2.13 | 0.48 |
| 7:CJ:95:ARG:NH2 | 7:CJ:99:LEU:HD11 | 2.28 | 0.48 |
| 25:DA:1638:C:O2 | 25:DA:2698:U:O2' | 2.27 | 0.48 |
| 25:DA:2065:C:H2' | 25:DA:2066:C:C6 | 2.47 | 0.48 |
| 10:CM:6:ILE:HG22 | 10:CM:98:ILE:CG2 | 2.42 | 0.48 |
| 4:CG:111:ALA:HB2 | 4:CG:120:LEU:CD1 | 2.43 | 0.48 |
| 20:CW:40:ALA:HB2 | 20:CW:55:ILE:HG22 | 1.94 | 0.48 |
| 25:BA:172:C:H2' | 25:BA:173:G:C8 | 2.48 | 0.48 |
| 25:BA:1341:U:O4 | 43:BT:16:LYS:HE2 | 2.13 | 0.48 |
| 25:DA:1106:G:H2' | 25:DA:1107:G:O4' | 2.13 | 0.48 |
| 25:BA:2492:U:H2' | 25:BA:2493:U:C6 | 2.48 | 0.48 |
| 1:CA:662:G:H2' | 1:CA:663:A:C8 | 2.47 | 0.48 |
| 44:DU:29:GLU:HB2 | 44:DU:38:ILE:HD12 | 1.94 | 0.48 |
| 18:CU:38:GLU:HA | 18:CU:38:GLU:OE2 | 2.12 | 0.48 |
| 32:DK:56:LYS:HG3 | 32:DK:57:ARG:N | 2.28 | 0.48 |
| 25:DA:1218:C:O2' | 25:DA:1219:G:H5' | 2.13 | 0.48 |
| 1:AA:539:A:H2' | 1:AA:540:G:C8 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 16:AS:16:HIS:O | 16:AS:17:TYR:O | 2.30 | 0.48 |
| 4:AG:14:ARG:C | 4:AG:14:ARG:HD3 | 2.33 | 0.48 |
| 41:D2:78:LYS:O | 41:D2:79:VAL:HG13 | 2.13 | 0.48 |
| 26:DB:74:U:C3' | 26:DB:75:G:H5'' | 2.44 | 0.48 |
| 36:DP:62:GLY:O | 36:DP:63:LYS:CB | 2.61 | 0.48 |
| 2:CE:213:LEU:O | 2:CE:213:LEU:HD23 | 2.13 | 0.48 |
| 25:DA:1012:U:C2 | 33:DM:25:ARG:NH1 | 2.81 | 0.48 |
| 45:BV:7:ALA:HB3 | 45:BV:61:LEU:HB2 | 1.95 | 0.48 |
| 25:DA:2272:U:C5' | 25:DA:2273:A:OP1 | 2.61 | 0.48 |
| 44:DU:101:LYS:HB3 | 44:DU:101:LYS:HE2 | 1.63 | 0.48 |
| 1:CA:1281:U:H4' | 1:CA:1282:C:OP2 | 2.13 | 0.48 |
| 30:DG:36:LYS:HG3 | 30:DG:93:THR:HG23 | 1.95 | 0.48 |
| 9:CL:26:VAL:HG21 | 9:CL:47:LEU:HD21 | 1.96 | 0.48 |
| 43:DT:49:VAL:HB | 43:DT:83:VAL:CG2 | 2.43 | 0.48 |
| 25:DA:2875:C:O2' | 39:DR:3:ARG:HG3 | 2.13 | 0.48 |
| 35:DO:146:VAL:HG22 | 35:DO:147:LEU:CD1 | 2.44 | 0.48 |
| 25:BA:654(S):G:C4' | 25:BA:654(T):A:OP1 | 2.60 | 0.48 |
| 45:BV:105:VAL:HG13 | 45:BV:140:ASP:HB3 | 1.95 | 0.48 |
| 32:DK:78:THR:CG2 | 32:DK:104:GLN:HE22 | 2.26 | 0.48 |
| 1:CA:1378:C:C5 | 1:CA:1379:G:N9 | 2.78 | 0.48 |
| 25:BA:1296:G:O2' | 25:BA:1297:C:H5' | 2.13 | 0.48 |
| 1:AA:451:A:N6 | 1:AA:480:U:H2' | 2.29 | 0.48 |
| 25:DA:872:A:C5 | 25:DA:906:G:N2 | 2.82 | 0.48 |
| 25:DA:581:C:H2' | 25:DA:582:G:C8 | 2.45 | 0.48 |
| 1:AA:87:A:H2' | 1:AA:88:C:H6 | 1.76 | 0.48 |
| 25:BA:753:C:O2' | 25:BA:754:C:H5' | 2.13 | 0.48 |
| 1:CA:1338:G:C6 | 1:CA:1339:A:N1 | 2.81 | 0.48 |
| 26:BB:1:U:H2' | 26:BB:2:C:C6 | 2.48 | 0.48 |
| 1:CA:115:G:H4' | 1:CA:116:A:O5' | 2.12 | 0.48 |
| 25:BA:2884:U:C2' | 25:BA:2885:C:H5' | 2.43 | 0.48 |
| 25:BA:1716:U:O2' | 25:BA:1717:G:H5' | 2.13 | 0.48 |
| 45:DV:6:LYS:HE3 | 45:DV:43:GLU:HG3 | 1.95 | 0.48 |
| 25:BA:2023:G:H5' | 25:BA:2617:C:H4' | 1.95 | 0.48 |
| 5:AH:87:SER:HB3 | 5:AH:125:SER:O | 2.13 | 0.48 |
| 22:AB:2:C:H2' | 22:AB:3:C:H6 | 1.78 | 0.48 |
| 25:BA:1856:G:H2' | 25:BA:1857:G:H5' | 1.94 | 0.48 |
| 39:DR:99:LEU:O | 39:DR:101:PHE:N | 2.46 | 0.48 |
| 22:CB:52:U:H3' | 22:CB:53:A:C8 | 2.48 | 0.48 |
| 39:DR:78:LEU:HD23 | 39:DR:78:LEU:O | 2.13 | 0.48 |
| 44:DU:43:ASN:N | 44:DU:43:ASN:HD22 | 2.12 | 0.48 |
| 7:CJ:131:LYS:NZ | 7:CJ:131:LYS:HB2 | 2.28 | 0.48 |
| 1:AA:651:C:O2 | 1:AA:651:C:H2' | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:978:G:C2 | 25:BA:986:C:C2 | 3.02 | 0.48 |
| 1:AA:1157:A:O2' | 1:AA:1158:C:H5'' | 2.13 | 0.48 |
| 41:D2:73:SER:HB2 | 41:D2:83:ARG:HA | 1.95 | 0.48 |
| 27:BD:35:LYS:CA | 27:BD:64:ILE:CG2 | 2.91 | 0.48 |
| 25:DA:2680:C:O2' | 25:DA:2681:C:H5' | 2.14 | 0.48 |
| 25:BA:1007:C:OP1 | 33:BM:35:ARG:NH1 | 2.46 | 0.48 |
| 36:DP:133:ARG:HD3 | 36:DP:133:ARG:O | 2.13 | 0.48 |
| 25:DA:1061:U:H4' | 25:DA:1070:A:C1' | 2.43 | 0.48 |
| 25:DA:1005:C:O4' | 25:DA:1143:A:H2 | 1.97 | 0.48 |
| 1:CA:1176:A:C6 | 1:CA:1177:G:C5 | 3.01 | 0.48 |
| 2:AE:96:ARG:HD2 | 2:AE:96:ARG:N | 2.12 | 0.48 |
| 1:AA:974:A:C2' | 1:AA:975:A:OP2 | 2.61 | 0.48 |
| 1:AA:974:A:OP2 | 14:AQ:41:ARG:NH1 | 2.46 | 0.48 |
| 30:DG:101:ILE:HD12 | 30:DG:102:PHE:N | 2.27 | 0.48 |
| 1:AA:404:U:H5' | 4:AG:122:ARG:HD2 | 1.94 | 0.48 |
| 40:B1:90:VAL:HG12 | 40:B1:91:ASP:N | 2.26 | 0.48 |
| 25:DA:2165:G:N3 | 25:DA:2165:G:H2' | 2.29 | 0.48 |
| 25:BA:2895:U:H6 | 25:BA:2895:U:O5' | 1.96 | 0.48 |
| 25:DA:141:A:H8 | 25:DA:1595:G:N2 | 2.03 | 0.48 |
| 22:AB:60:A:H61 | 22:AB:76:U:H3 | 1.60 | 0.48 |
| 35:DO:10:PRO:O | 35:DO:11:GLY:O | 2.30 | 0.48 |
| 33:DM:134:ARG:N | 33:DM:135:PRO:CD | 2.77 | 0.48 |
| 25:DA:598:G:C6 | 25:DA:599:G:C5 | 3.01 | 0.48 |
| 33:BM:130:HIS:HD2 | 33:BM:134:ARG:NH1 | 2.12 | 0.48 |
| 7:CJ:43:PHE:O | 7:CJ:47:CYS:HB2 | 2.13 | 0.48 |
| 11:AN:57:THR:HG22 | 11:AN:59:TYR:N | 2.21 | 0.48 |
| 1:AA:1501:C:OP2 | 1:AA:1504:G:H2' | 2.13 | 0.48 |
| 1:CA:428:G:O4' | 1:CA:430:A:C8 | 2.66 | 0.48 |
| 25:BA:2562:U:C1' | 34:BN:23:ARG:HH11 | 2.22 | 0.48 |
| 36:BP:30:GLY:HA3 | 36:BP:107:ALA:HB2 | 1.92 | 0.48 |
| 23:AD:8:U:C5 | 23:AD:13:C:C4 | 3.01 | 0.48 |
| 25:DA:322:A:H4' | 25:DA:323:G:OP2 | 2.13 | 0.48 |
| 25:BA:72:U:H1' | 48:BW:58:ALA:CB | 2.44 | 0.48 |
| 28:DE:60:ASN:H | 28:DE:60:ASN:ND2 | 2.11 | 0.48 |
| 35:DO:55:ARG:O | 35:DO:56:SER:C | 2.51 | 0.48 |
| 35:DO:56:SER:O | 35:DO:57:THR:O | 2.30 | 0.48 |
| 31:DH:10:PRO:CG | 31:DH:50:VAL:HG13 | 2.43 | 0.48 |
| 1:CA:946:A:H2' | 1:CA:947:G:H8 | 1.74 | 0.48 |
| 28:BE:183:LEU:N | 28:BE:183:LEU:CD1 | 2.77 | 0.48 |
| 31:DH:26:VAL:HG11 | 31:DH:33:LEU:HB2 | 1.95 | 0.48 |
| 25:BA:2580:U:H4' | 28:BE:130:GLY:CA | 2.42 | 0.48 |
| 1:AA:390:C:H2' | 1:AA:391:G:C8 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 8:AK:7:ALA:HB2 | 8:AK:85:ARG:CD | 2.43 | 0.48 |
| 25:BA:247:G:H4' | 25:BA:386:G:C5 | 2.48 | 0.48 |
| 11:AN:81:ASP:O | 11:AN:82:VAL:O | 2.31 | 0.48 |
| 2:CE:5:ILE:HG12 | 2:CE:55:PHE:HB3 | 1.94 | 0.48 |
| 33:BM:120:LEU:HD21 | 33:BM:122:VAL:HG23 | 1.95 | 0.48 |
| 25:DA:496:G:C2' | 25:DA:497:A:H5' | 2.44 | 0.48 |
| 1:AA:1164:G:O2' | 1:AA:1165:C:H5' | 2.13 | 0.48 |
| 1:CA:1213:A:C5 | 1:CA:1215:G:C4 | 3.01 | 0.48 |
| 25:BA:863:A:H2' | 25:BA:864:G:C8 | 2.48 | 0.48 |
| 31:BH:105:LEU:CD2 | 31:BH:105:LEU:H | 2.27 | 0.48 |
| 32:DK:5:LEU:HD11 | 32:DK:19:VAL:HG12 | 1.94 | 0.48 |
| 25:DA:1407:C:C2 | 25:DA:1596:A:C2 | 3.00 | 0.48 |
| 1:AA:1151:A:N6 | 1:AA:1152:A:N6 | 2.61 | 0.48 |
| 25:DA:1693:U:H4' | 25:DA:1694:C:OP2 | 2.13 | 0.48 |
| 41:B2:19:LYS:HG3 | 41:B2:95:LEU:HD23 | 1.94 | 0.48 |
| 15:AR:4:THR:OG1 | 15:AR:7:GLU:HB2 | 2.12 | 0.48 |
| 48:BW:42:GLY:O | 48:BW:44:LEU:N | 2.46 | 0.48 |
| 27:BD:158:ALA:O | 27:BD:159:ALA:C | 2.51 | 0.48 |
| 1:AA:601:C:H2' | 1:AA:602:A:C8 | 2.48 | 0.48 |
| 25:BA:818:G:H4' | 25:BA:838:C:O3' | 2.13 | 0.48 |
| 25:DA:2345:G:N3 | 25:DA:2381:C:H2' | 2.28 | 0.48 |
| 13:AP:11:ARG:HG2 | 13:AP:12:ASN:H | 1.77 | 0.48 |
| 46:B3:55:ARG:HG3 | 46:B3:55:ARG:HH11 | 1.78 | 0.48 |
| 39:DR:82:LEU:H | 39:DR:82:LEU:HD12 | 1.77 | 0.48 |
| 19:CV:64:GLU:H | 19:CV:64:GLU:CD | 2.17 | 0.48 |
| 1:AA:519:C:H2' | 1:AA:520:A:C8 | 2.48 | 0.48 |
| 1:CA:495:A:H4' | 1:CA:496:A:OP1 | 2.14 | 0.48 |
| 1:AA:392:G:P | 16:AS:12:LYS:HG3 | 2.53 | 0.48 |
| 25:DA:227:A:C2 | 25:DA:2407:G:H1' | 2.49 | 0.48 |
| 52:D6:27:LYS:NZ | 52:D6:28:ARG:HH12 | 2.10 | 0.48 |
| 25:DA:7:G:H1 | 25:DA:2896:C:N4 | 2.11 | 0.48 |
| 25:BA:2309:A:HO2' | 25:BA:2310:A:H5'' | 1.75 | 0.48 |
| 28:BE:82:ARG:C | 28:BE:84:PHE:H | 2.17 | 0.48 |
| 28:BE:82:ARG:C | 28:BE:84:PHE:N | 2.66 | 0.48 |
| 45:DV:175:VAL:CG1 | 45:DV:176:PRO:HD3 | 2.43 | 0.48 |
| 25:DA:270(R):G:H2' | 25:DA:270(S):G:C8 | 2.49 | 0.48 |
| 25:DA:1065:U:C4 | 25:DA:1066:U:C4 | 3.02 | 0.48 |
| 25:DA:1087:G:C8 | 25:DA:1089:G:H1' | 2.49 | 0.48 |
| 39:DR:23:ARG:HB2 | 39:DR:24:PRO:HD2 | 1.95 | 0.48 |
| 25:DA:1312:U:H4' | 25:DA:1313:U:O5' | 2.14 | 0.48 |
| 28:BE:101:ARG:C | 28:BE:201:THR:OG1 | 2.52 | 0.48 |
| 26:BB:29:A:H2' | 26:BB:30:C:C6 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 35:DO:85:LEU:HB3 | 35:DO:114:ILE:HD11 | 1.94 | 0.48 |
| 33:BM:127:ASP:OD1 | 33:BM:127:ASP:N | 2.46 | 0.48 |
| 50:D4:34:GLU:OE2 | 50:D4:35:VAL:HG23 | 2.14 | 0.48 |
| 46:B3:56:ASP:OD2 | 46:B3:58:THR:HB | 2.14 | 0.48 |
| 45:DV:27:VAL:CG1 | 45:DV:87:ASP:HB3 | 2.39 | 0.48 |
| 31:BH:131:VAL:CG1 | 31:BH:132:ARG:N | 2.76 | 0.48 |
| 9:AL:17:VAL:HG21 | 9:AL:80:GLY:HA3 | 1.94 | 0.48 |
| 5:AH:13:ILE:HD11 | 5:AH:55:VAL:HG22 | 1.96 | 0.48 |
| 25:BA:1049:C:C2' | 25:BA:1050:A:C5' | 2.91 | 0.48 |
| 25:DA:142:G:H5'' | 25:DA:1598:C:O2' | 2.14 | 0.48 |
| 1:AA:164:U:H2' | 1:AA:165:C:C5 | 2.49 | 0.48 |
| 31:BH:77:LYS:HE2 | 31:BH:138:LYS:HE2 | 1.95 | 0.48 |
| 30:BG:42:GLY:O | 30:BG:43:LEU:HD13 | 2.13 | 0.48 |
| 25:BA:589:C:H2' | 25:BA:590:A:C8 | 2.49 | 0.48 |
| 25:BA:2567:G:H2' | 25:BA:2568:C:C6 | 2.47 | 0.48 |
| 35:DO:55:ARG:HG3 | 35:DO:55:ARG:O | 2.13 | 0.48 |
| 25:BA:1079:C:N4 | 25:BA:1080:A:C6 | 2.80 | 0.48 |
| 25:DA:2291:U:H2' | 25:DA:2292:C:C6 | 2.49 | 0.48 |
| 10:CM:4:ILE:HB | 10:CM:74:ILE:CG1 | 2.43 | 0.48 |
| 1:CA:1375:A:H4' | 7:CJ:29:LYS:NZ | 2.28 | 0.48 |
| 2:CE:189:ASP:N | 2:CE:189:ASP:OD1 | 2.46 | 0.48 |
| 22:AB:25:A:H2' | 22:AB:25:A:N3 | 2.27 | 0.48 |
| 29:BF:118:ALA:HB2 | 29:BF:123:LEU:HD23 | 1.95 | 0.48 |
| 1:AA:271:C:H2' | 1:AA:272:C:C6 | 2.47 | 0.48 |
| 1:CA:953:G:C5' | 1:CA:965:A:H61 | 2.26 | 0.48 |
| 25:DA:2790:A:H4' | 25:DA:2791:C:OP2 | 2.13 | 0.48 |
| 25:DA:1338:G:N3 | 25:DA:1393:A:H2 | 2.12 | 0.48 |
| 10:AM:16:LEU:CD1 | 10:AM:70:ARG:HB2 | 2.43 | 0.48 |
| 31:DH:94:TYR:HA | 31:DH:106:THR:O | 2.13 | 0.48 |
| 35:BO:71:VAL:HG12 | 35:BO:72:PRO:HD3 | 1.94 | 0.48 |
| 5:CH:76:ILE:HG23 | 5:CH:77:PRO:HD2 | 1.95 | 0.48 |
| 30:BG:26:GLN:HG3 | 30:BG:27:ASN:N | 2.28 | 0.48 |
| 1:CA:756:C:H2' | 1:CA:757:U:O4' | 2.14 | 0.48 |
| 20:CW:36:LEU:HD12 | 20:CW:55:ILE:HG23 | 1.95 | 0.48 |
| 1:CA:527:G:C2' | 1:CA:528:C:H5' | 2.44 | 0.48 |
| 25:BA:1444:G:N2 | 25:BA:1548:C:C2 | 2.81 | 0.48 |
| 43:BT:11:PRO:HB3 | 43:BT:92:LEU:HD21 | 1.94 | 0.48 |
| 1:CA:216:G:O2' | 1:CA:217:C:O5' | 2.31 | 0.48 |
| 26:DB:20:C:O2' | 26:DB:21:G:H5' | 2.13 | 0.48 |
| 27:BD:127:VAL:HA | 27:BD:193:VAL:HG22 | 1.95 | 0.48 |
| 25:DA:491:G:O6 | 42:DS:49:LYS:HD3 | 2.13 | 0.48 |
| 5:CH:40:ARG:HH11 | 5:CH:40:ARG:HG2 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:693:G:H2' | 1:CA:694:A:O4' | 2.13 | 0.48 |
| 52:D6:9:LEU:HD22 | 52:D6:11:LEU:HD22 | 1.95 | 0.48 |
| 38:BQ:108:GLY:O | 38:BQ:110:LEU:HG | 2.13 | 0.48 |
| 25:DA:994:C:O2' | 25:DA:996:A:OP1 | 2.22 | 0.48 |
| 28:BE:61:ARG:HB2 | 28:BE:62:PRO:HD3 | 1.94 | 0.48 |
| 25:DA:2059:A:C2 | 25:DA:2062:A:N6 | 2.82 | 0.48 |
| 28:DE:47:VAL:C | 28:DE:80:GLU:HA | 2.29 | 0.48 |
| 25:DA:2401:U:H2' | 25:DA:2402:C:H6 | 1.79 | 0.48 |
| 1:AA:1023:G:H3' | 1:AA:1024:G:C5' | 2.42 | 0.48 |
| 19:AV:40:ILE:C | 19:AV:41:VAL:HG22 | 2.34 | 0.48 |
| 28:DE:135:HIS:N | 28:DE:135:HIS:ND1 | 2.60 | 0.48 |
| 39:DR:92:GLY:HA2 | 39:DR:117:ASP:H | 1.79 | 0.48 |
| 25:BA:1728:G:C3' | 25:BA:1729:A:C5' | 2.79 | 0.48 |
| 50:B4:49:PHE:O | 50:B4:50:VAL:HB | 2.13 | 0.48 |
| 10:AM:53:PRO:HA | 14:AQ:42:ILE:CD1 | 2.44 | 0.48 |
| 25:DA:1050:A:C4 | 25:DA:2751:G:N2 | 2.81 | 0.48 |
| 50:D4:12:ALA:H | 50:D4:24:THR:CG2 | 2.27 | 0.48 |
| 50:D4:2:LYS:HD2 | 50:D4:6:HIS:CE1 | 2.48 | 0.48 |
| 25:DA:2312:U:O2' | 30:DG:40:ASN:ND2 | 2.47 | 0.48 |
| 30:BG:104:GLU:HG2 | 50:B4:23:GLU:HG3 | 1.95 | 0.48 |
| 1:CA:1446:A:OP1 | 1:CA:1446:A:C4' | 2.61 | 0.48 |
| 44:BU:48:ALA:O | 44:BU:49:VAL:C | 2.52 | 0.48 |
| 4:AG:108:LEU:HD11 | 4:AG:174:LEU:HD22 | 1.94 | 0.48 |
| 31:BH:6:ARG:HE | 31:BH:54:ARG:HH12 | 1.60 | 0.48 |
| 45:DV:108:PRO:HB3 | 45:DV:142:SER:C | 2.34 | 0.48 |
| 16:AS:34:GLU:HG2 | 16:AS:35:LYS:H | 1.79 | 0.48 |
| 25:DA:2720:U:C2 | 25:DA:2721:A:C8 | 3.02 | 0.48 |
| 17:AT:76:LEU:HD12 | 17:AT:77:VAL:H | 1.78 | 0.48 |
| 35:DO:35:HIS:O | 35:DO:36:LYS:C | 2.51 | 0.48 |
| 33:DM:134:ARG:N | 33:DM:135:PRO:HD3 | 2.28 | 0.48 |
| 1:AA:920:U:O4' | 1:AA:1080:A:C2 | 2.67 | 0.48 |
| 2:CE:178:ARG:HH21 | 8:CK:74:PRO:HG3 | 1.79 | 0.48 |
| 9:CL:111:ARG:HD2 | 14:CQ:61:TRP:OXT | 2.13 | 0.48 |
| 45:DV:70:LEU:O | 45:DV:89:PHE:N | 2.41 | 0.48 |
| 1:CA:408:A:C4 | 1:CA:409:G:C8 | 3.02 | 0.48 |
| 25:BA:2734:A:C8 | 25:BA:2734:A:H5' | 2.47 | 0.48 |
| 34:BN:23:ARG:HG3 | 34:BN:24:VAL:N | 2.28 | 0.48 |
| 25:DA:298:G:N2 | 25:DA:339:U:C5 | 2.82 | 0.48 |
| 1:CA:860:A:N6 | 1:CA:861:G:C2 | 2.82 | 0.48 |
| 14:CQ:37:PHE:CE1 | 14:CQ:53:LEU:HD22 | 2.47 | 0.48 |
| 1:AA:1270:C:H2' | 1:AA:1271:G:C8 | 2.48 | 0.48 |
| 27:BD:120:GLY:O | 27:BD:123:ALA:CB | 2.62 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:AA:719:C:C5 | 1:AA:720:C:C4 | 3.00 | 0.48 |
| 25:BA:2579:C:H2' | 25:BA:2580:U:O4' | 2.14 | 0.48 |
| 1:AA:298:A:H2' | 1:AA:299:G:O4' | 2.13 | 0.48 |
| 1:CA:186:C:H1' | 20:CW:81:LYS:HZ3 | 1.78 | 0.48 |
| 12:AO:7:ILE:CD1 | 17:AT:32:TYR:HB3 | 2.44 | 0.48 |
| 25:DA:668:G:H2' | 25:DA:669:G:OP1 | 2.13 | 0.48 |
| 27:DD:31:LYS:NZ | 27:DD:31:LYS:HB2 | 2.28 | 0.48 |
| 1:AA:1086:U:C2' | 1:AA:1087:G:H5' | 2.43 | 0.48 |
| 34:DN:10:VAL:CG2 | 34:DN:16:ALA:O | 2.62 | 0.48 |
| 25:BA:2648:C:H2' | 25:BA:2649:U:H6 | 1.79 | 0.48 |
| 25:DA:1217:C:OP1 | 40:D1:15:LYS:HE3 | 2.13 | 0.48 |
| 33:BM:7:LYS:O | 33:BM:9:VAL:HG22 | 2.13 | 0.48 |
| 13:CP:73:GLU:O | 13:CP:77:ASN:HB2 | 2.14 | 0.48 |
| 1:AA:829:G:C2' | 1:AA:830:G:H5' | 2.43 | 0.48 |
| 1:CA:476:G:H2' | 1:CA:477:G:H8 | 1.77 | 0.48 |
| 25:DA:2199:A:C8 | 25:DA:2205:C:C5 | 3.02 | 0.48 |
| 25:BA:2615:U:H2' | 25:BA:2616:C:H6 | 1.79 | 0.48 |
| 25:DA:2406:U:H2' | 25:DA:2406:U:OP2 | 2.13 | 0.48 |
| 39:BR:89:VAL:O | 39:BR:89:VAL:HG23 | 2.12 | 0.48 |
| 11:AN:124:LYS:HG2 | 11:AN:125:PHE:CD1 | 2.49 | 0.48 |
| 1:AA:359:U:H2' | 1:AA:360:A:C8 | 2.49 | 0.48 |
| 25:BA:439:G:C2' | 25:BA:440:G:H5' | 2.43 | 0.48 |
| 54:D8:49:VAL:HG23 | 54:D8:50:LEU:H | 1.77 | 0.48 |
| 36:DP:29:PHE:HB3 | 36:DP:65:PHE:CZ | 2.46 | 0.48 |
| 41:D2:82:ARG:NH1 | 41:D2:82:ARG:CG | 2.47 | 0.48 |
| 25:BA:1568:G:OP2 | 27:BD:63:ARG:NH2 | 2.46 | 0.48 |
| 45:DV:115:GLY:HA2 | 45:DV:177:PRO:HD3 | 1.95 | 0.48 |
| 14:CQ:41:ARG:HG3 | 14:CQ:42:ILE:N | 2.29 | 0.48 |
| 25:DA:1071:G:C4 | 25:DA:1089:G:H2' | 2.49 | 0.48 |
| 25:DA:883:G:H2' | 25:DA:884:C:C5 | 2.48 | 0.48 |
| 1:AA:1203:C:H2' | 1:AA:1204:A:O4' | 2.14 | 0.48 |
| 1:CA:1305:G:H22 | 1:CA:1331:G:C2' | 2.26 | 0.48 |
| 54:B8:36:LYS:HD2 | 54:B8:40:GLU:HG2 | 1.95 | 0.48 |
| 25:DA:547:A:N7 | 25:DA:548:A:N6 | 2.60 | 0.48 |
| 25:DA:91:A:C2' | 25:DA:92:G:H5' | 2.44 | 0.48 |
| 11:AN:41:THR:CG2 | 11:AN:42:TRP:N | 2.77 | 0.48 |
| 25:DA:2168:G:C2 | 25:DA:2170:A:OP2 | 2.66 | 0.48 |
| 33:BM:130:HIS:CD2 | 33:BM:134:ARG:NH1 | 2.82 | 0.48 |
| 35:DO:81:GLN:HB3 | 35:DO:106:LEU:HD12 | 1.95 | 0.48 |
| 3:AF:68:VAL:HG12 | 3:AF:70:VAL:HG23 | 1.96 | 0.48 |
| 25:DA:587:C:N3 | 35:DO:33:ARG:HD2 | 2.29 | 0.48 |
| 25:BA:1606:G:H5'' | 25:BA:1607:C:OP1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 48:DW:17:SER:OG | 48:DW:18:PRO:HA | 2.13 | 0.48 |
| 25:BA:2687:U:C4 | 25:BA:2688:U:C5 | 3.02 | 0.48 |
| 28:DE:66:HIS:NE2 | 28:DE:73:GLU:OE1 | 2.46 | 0.48 |
| 25:DA:1288:U:C2 | 25:DA:1327:C:O2 | 2.66 | 0.48 |
| 25:DA:76:C:H2' | 25:DA:77:C:H6 | 1.78 | 0.48 |
| 25:DA:1388:G:O2' | 25:DA:1389:G:H5' | 2.13 | 0.48 |
| 25:DA:1146:C:H2' | 25:DA:1147:C:H5' | 1.95 | 0.48 |
| 49:BX:10:LYS:HZ3 | 49:BX:15:TYR:HH | 1.57 | 0.48 |
| 53:D7:35:ARG:CG | 53:D7:42:LEU:HD11 | 2.43 | 0.48 |
| 25:BA:1257:C:H4' | 29:BF:83:PHE:CE2 | 2.49 | 0.48 |
| 25:DA:2472:G:C4 | 25:DA:2475:C:N4 | 2.82 | 0.48 |
| 48:BW:16:LEU:CG | 48:BW:16:LEU:O | 2.62 | 0.48 |
| 25:BA:547:A:H3' | 25:BA:548:A:C8 | 2.48 | 0.48 |
| 45:BV:69:THR:HA | 45:BV:89:PHE:O | 2.14 | 0.48 |
| 3:AF:67:THR:HG23 | 3:AF:102:ASN:HB2 | 1.94 | 0.48 |
| 45:DV:1:MET:HG2 | 45:DV:2:GLU:H | 1.79 | 0.48 |
| 20:CW:69:GLY:O | 20:CW:73:HIS:CD2 | 2.67 | 0.48 |
| 25:BA:2758:A:C2 | 25:BA:2759:G:H1' | 2.49 | 0.48 |
| 25:DA:558:G:OP1 | 33:DM:111:PRO:HD2 | 2.13 | 0.48 |
| 25:DA:273(E):U:O2' | 25:DA:273(F):C:H5' | 2.13 | 0.48 |
| 1:AA:509:A:H3' | 1:AA:509:A:C8 | 2.48 | 0.48 |
| 25:DA:659:C:H4' | 29:DF:100:THR:O | 2.12 | 0.48 |
| 1:CA:1179:A:O3' | 9:CL:103:THR:HG23 | 2.13 | 0.48 |
| 25:BA:2184:G:C6 | 25:BA:2185:C:N4 | 2.82 | 0.48 |
| 54:D8:30:ARG:O | 54:D8:31:HIS:HB2 | 2.14 | 0.48 |
| 25:BA:2376:A:H2' | 25:BA:2377:A:O4' | 2.14 | 0.48 |
| 27:DD:62:TYR:CE1 | 27:DD:64:ILE:HA | 2.48 | 0.48 |
| 28:BE:48:GLN:HE22 | 28:BE:77:ILE:CD1 | 2.25 | 0.48 |
| 28:DE:53:PRO:HG2 | 28:DE:54:GLN:H | 1.79 | 0.48 |
| 28:DE:9:VAL:HG13 | 28:DE:26:ILE:O | 2.13 | 0.48 |
| 1:CA:1226:C:N4 | 13:CP:104:ARG:HD2 | 2.29 | 0.48 |
| 45:DV:175:VAL:O | 45:DV:177:PRO:CD | 2.52 | 0.48 |
| 25:DA:1057:A:H2 | 25:DA:1081:U:N3 | 2.01 | 0.48 |
| 1:CA:327:A:O2' | 1:CA:328:C:O4' | 2.22 | 0.48 |
| 29:DF:117:ARG:HH12 | 35:DO:1:MET:N | 2.12 | 0.48 |
| 25:DA:1826:G:H2' | 25:DA:1827:C:H6 | 1.78 | 0.48 |
| 25:DA:2276:G:P | 36:DP:84:GLY:HA2 | 2.54 | 0.48 |
| 32:BK:92:VAL:O | 32:BK:120:ILE:HG22 | 2.13 | 0.48 |
| 25:BA:1141:U:P | 33:BM:63:THR:HG21 | 2.54 | 0.48 |
| 1:CA:1133:G:N2 | 1:CA:1141:C:N3 | 2.60 | 0.48 |
| 25:DA:307:G:N1 | 25:DA:310:A:OP2 | 2.45 | 0.48 |
| 1:CA:1240:U:OP2 | 7:CJ:115:ARG:HA | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:1298:C:C6 | 7:CJ:114:ARG:NH1 | 2.82 | 0.48 |
| 45:DV:141:VAL:O | 45:DV:142:SER:O | 2.30 | 0.48 |
| 25:DA:2689:U:P | 25:DA:2719:G:H22 | 2.36 | 0.48 |
| 25:DA:2297:C:O2 | 25:DA:2298:A:C8 | 2.67 | 0.48 |
| 1:CA:503:C:C2' | 1:CA:504:C:H5' | 2.43 | 0.48 |
| 50:B4:56:VAL:CG1 | 50:B4:60:GLN:HG3 | 2.44 | 0.48 |
| 22:AB:19:G:H1' | 22:AB:20:U:OP1 | 2.14 | 0.48 |
| 25:BA:849:A:N1 | 49:BX:25:ALA:HB2 | 2.27 | 0.48 |
| 29:DF:8:GLN:HG2 | 29:DF:124:LEU:HD11 | 1.95 | 0.48 |
| 23:AC:1:C:O2' | 23:AC:2:G:OP2 | 2.32 | 0.48 |
| 25:BA:530:G:O4' | 25:BA:530:G:N3 | 2.45 | 0.48 |
| 9:CL:112:LYS:HD3 | 9:CL:113:LYS:O | 2.14 | 0.48 |
| 35:BO:38:GLN:O | 35:BO:41:ARG:HB2 | 2.13 | 0.48 |
| 4:CG:24:GLU:O | 4:CG:27:TYR:N | 2.42 | 0.48 |
| 5:AH:51:VAL:O | 5:AH:55:VAL:HG23 | 2.13 | 0.48 |
| 54:D8:61:LEU:O | 54:D8:62:LEU:C | 2.51 | 0.48 |
| 1:CA:353:A:C2' | 1:CA:354:G:OP2 | 2.62 | 0.48 |
| 1:AA:163:C:H2' | 1:AA:164:U:H6 | 1.78 | 0.48 |
| 1:CA:420:U:H2' | 1:CA:422:C:O2 | 2.14 | 0.48 |
| 8:AK:138:TRP:OXT | 8:AK:138:TRP:CE3 | 2.66 | 0.48 |
| 50:B4:61:ARG:O | 50:B4:65:ASP:OD1 | 2.31 | 0.48 |
| 25:BA:2863:C:O2' | 25:BA:2864:G:H5' | 2.13 | 0.48 |
| 52:B6:11:LEU:HD21 | 52:B6:51:GLU:HG3 | 1.96 | 0.48 |
| 25:BA:2820:A:C5 | 37:B0:4:LEU:HD21 | 2.49 | 0.48 |
| 25:DA:839:U:H2' | 25:DA:840:C:C6 | 2.49 | 0.48 |
| 25:BA:2099:U:O2 | 25:BA:2099:U:H2' | 2.14 | 0.48 |
| 1:CA:955:U:H2' | 1:CA:956:U:H6 | 1.78 | 0.48 |
| 8:CK:29:SER:HB3 | 8:CK:32:LYS:CB | 2.43 | 0.48 |
| 27:BD:36:PRO:HA | 27:BD:62:TYR:O | 2.13 | 0.48 |
| 1:CA:9:G:C8 | 5:CH:126:ARG:NH2 | 2.81 | 0.48 |
| 15:CR:43:LEU:HD11 | 15:CR:53:HIS:HA | 1.96 | 0.48 |
| 1:AA:829:G:O2' | 1:AA:830:G:H5' | 2.13 | 0.48 |
| 5:CH:12:LEU:O | 5:CH:30:ALA:HA | 2.14 | 0.48 |
| 23:AC:41:C:O2' | 23:AC:42:C:H5' | 2.14 | 0.48 |
| 36:BP:137:TYR:C | 36:BP:139:GLU:H | 2.15 | 0.48 |
| 25:BA:1578:U:H2' | 25:BA:1579:A:H5' | 1.95 | 0.48 |
| 39:BR:11:GLU:N | 39:BR:11:GLU:OE1 | 2.47 | 0.48 |
| 20:CW:58:LYS:O | 20:CW:58:LYS:HD3 | 2.13 | 0.48 |
| 3:CF:52:LEU:CD2 | 3:CF:52:LEU:H | 2.27 | 0.48 |
| 15:AR:3:ILE:HG13 | 15:AR:3:ILE:O | 2.13 | 0.48 |
| 25:BA:2406:U:OP2 | 25:BA:2406:U:H2' | 2.14 | 0.48 |
| 44:BU:68:HIS:O | 44:BU:71:LYS:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 52:D6:28:ARG:HG3 | 52:D6:31:PRO:HD2 | 1.95 | 0.48 |
| 1:AA:1159:U:O4' | 1:AA:1182:G:N2 | 2.47 | 0.48 |
| 54:D8:52:LYS:HD3 | 54:D8:52:LYS:N | 2.27 | 0.48 |
| 25:DA:997:G:O2' | 25:DA:998:C:H5' | 2.13 | 0.48 |
| 23:AC:20:G:O2' | 23:AC:21:U:H5 | 1.95 | 0.48 |
| 1:AA:1125:U:O4 | 10:AM:5:ARG:HD2 | 2.13 | 0.48 |
| 25:DA:1187:G:C4' | 41:D2:76:LYS:HZ2 | 2.23 | 0.48 |
| 1:CA:1226:C:OP2 | 13:CP:103:THR:HG21 | 2.14 | 0.48 |
| 26:DB:73:A:H5' | 26:DB:74:U:OP2 | 2.14 | 0.48 |
| 25:DA:1097:U:H2' | 25:DA:1098:A:O4' | 2.14 | 0.48 |
| 25:DA:363(B):G:H2' | 25:DA:363(C):G:C8 | 2.49 | 0.48 |
| 1:AA:1358:U:H5'' | 14:AQ:33:VAL:O | 2.14 | 0.48 |
| 25:BA:1021:A:H3' | 25:BA:1022:G:C5' | 2.32 | 0.48 |
| 1:AA:255:G:H1' | 17:AT:16:GLN:HE21 | 1.78 | 0.48 |
| 17:AT:67:LYS:HA | 17:AT:70:ARG:HH12 | 1.79 | 0.48 |
| 30:DG:67:LYS:H | 50:D4:6:HIS:HE2 | 1.61 | 0.48 |
| 25:DA:90:U:O2' | 25:DA:91:A:H5'' | 2.13 | 0.48 |
| 25:BA:997:G:O2' | 25:BA:998:C:H5' | 2.14 | 0.48 |
| 25:BA:2401:U:H5' | 52:B6:18:ARG:HD3 | 1.94 | 0.48 |
| 28:DE:197:ILE:CD1 | 28:DE:199:ARG:HH21 | 2.18 | 0.48 |
| 20:AW:50:GLU:HG3 | 20:AW:51:GLU:N | 2.29 | 0.48 |
| 25:DA:2872:G:C8 | 25:DA:2873:A:H2 | 2.28 | 0.48 |
| 25:DA:2298:A:C2 | 25:DA:2299:G:H1' | 2.49 | 0.48 |
| 33:BM:134:ARG:N | 33:BM:135:PRO:HD3 | 2.29 | 0.48 |
| 9:CL:95:LYS:HZ2 | 9:CL:96:LEU:CD1 | 2.27 | 0.48 |
| 32:BK:12:LEU:HD13 | 32:BK:12:LEU:N | 2.29 | 0.48 |
| 2:AE:18:GLY:H | 2:AE:42:ILE:CG2 | 2.22 | 0.48 |
| 25:BA:1385:G:O2' | 25:BA:1396:U:C6 | 2.66 | 0.48 |
| 1:AA:926:G:C6 | 1:AA:1505:G:C5 | 3.02 | 0.48 |
| 5:AH:32:VAL:HB | 5:AH:58:ALA:HB1 | 1.95 | 0.48 |
| 4:CG:208:SER:OG | 5:CH:101:ILE:HG22 | 2.14 | 0.48 |
| 45:BV:105:VAL:HG12 | 45:BV:139:VAL:O | 2.13 | 0.48 |
| 25:BA:1991:U:C2' | 25:BA:1992:G:H5'' | 2.41 | 0.48 |
| 30:BG:109:VAL:O | 30:BG:113:ARG:HG3 | 2.14 | 0.48 |
| 39:BR:55:ASN:HB3 | 39:BR:58:ASN:O | 2.14 | 0.48 |
| 3:CF:58:GLU:CB | 3:CF:65:ALA:HB3 | 2.44 | 0.48 |
| 13:CP:88:ARG:O | 13:CP:88:ARG:HG3 | 2.13 | 0.48 |
| 1:AA:659:U:N3 | 1:AA:660:G:N7 | 2.62 | 0.48 |
| 9:CL:21:PRO:HA | 9:CL:59:PHE:HA | 1.94 | 0.48 |
| 25:BA:2302:G:C6 | 25:BA:2315:G:C6 | 3.02 | 0.48 |
| 46:B3:72:ARG:CB | 46:B3:75:LEU:HB2 | 2.43 | 0.48 |
| 1:CA:947:G:O3' | 13:CP:109:THR:OG1 | 2.25 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 9:AL:83:ARG:HA | 9:AL:86:VAL:CG1 | 2.44 | 0.48 |
| 19:CV:41:VAL:HG13 | 50:D4:63:TYR:CE2 | 2.49 | 0.48 |
| 25:DA:2011:U:H2' | 25:DA:2012:G:H5' | 1.96 | 0.48 |
| 25:DA:2124:G:H2' | 25:DA:2125:G:H5' | 1.96 | 0.48 |
| 25:BA:2850:A:H5' | 25:BA:2868:A:C2 | 2.49 | 0.48 |
| 1:AA:1072:G:C6 | 1:AA:1073:U:C4 | 3.02 | 0.48 |
| 2:CE:28:PHE:CD1 | 2:CE:32:ILE:HG22 | 2.46 | 0.48 |
| 25:DA:1180:C:H2' | 25:DA:1181:C:C6 | 2.49 | 0.48 |
| 25:DA:1181:C:H2' | 25:DA:1182:A:C8 | 2.49 | 0.48 |
| 30:DG:96:ARG:HG3 | 30:DG:96:ARG:H | 1.26 | 0.48 |
| 22:CB:31:C:C2 | 22:CB:32:C:C5 | 3.01 | 0.48 |
| 36:BP:31:ASP:O | 36:BP:133:ARG:O | 2.32 | 0.48 |
| 41:B2:87:HIS:NE2 | 41:B2:89:GLN:NE2 | 2.61 | 0.48 |
| 10:AM:4:ILE:HD13 | 10:AM:100:THR:CG2 | 2.44 | 0.48 |
| 2:CE:55:PHE:HD1 | 2:CE:58:ILE:HD12 | 1.79 | 0.48 |
| 7:AJ:152:ALA:O | 7:AJ:155:ARG:HB3 | 2.13 | 0.48 |
| 37:D0:72:ASP:HB3 | 37:D0:75:LEU:HB3 | 1.96 | 0.48 |
| 1:AA:131:C:H2' | 1:AA:131:C:O2 | 2.14 | 0.48 |
| 26:DB:78:A:C2 | 26:DB:99:A:C4 | 3.02 | 0.48 |
| 23:AC:26:C:H2' | 23:AC:27:G:O4' | 2.14 | 0.48 |
| 12:AO:122:THR:HG22 | 12:AO:123:LYS:O | 2.12 | 0.48 |
| 25:BA:724:U:H2' | 25:BA:725:G:O4' | 2.14 | 0.48 |
| 10:AM:17:ASP:O | 10:AM:21:GLN:HB2 | 2.12 | 0.48 |
| 10:AM:34:VAL:CG1 | 10:AM:74:ILE:HG23 | 2.44 | 0.48 |
| 45:DV:102:LEU:HD11 | 45:DV:124:ILE:HB | 1.96 | 0.48 |
| 25:DA:2768:C:O2' | 33:DM:89:LYS:HE2 | 2.14 | 0.48 |
| 45:BV:120:ILE:HG21 | 45:BV:170:THR:HB | 1.96 | 0.48 |
| 34:DN:7:TYR:CE1 | 34:DN:20:MET:HG3 | 2.48 | 0.48 |
| 19:CV:51:VAL:O | 19:CV:58:VAL:HG22 | 2.13 | 0.48 |
| 1:AA:261:U:OP2 | 20:AW:79:ARG:NH2 | 2.47 | 0.48 |
| 25:BA:340:A:C2' | 25:BA:341:G:H5' | 2.44 | 0.48 |
| 52:D6:25:LYS:CE | 54:D8:34:TRP:HH2 | 2.25 | 0.48 |
| 25:DA:2378:A:C5 | 25:DA:2379:G:H1' | 2.48 | 0.48 |
| 1:AA:1054:C:O2' | 1:AA:1055:A:C5' | 2.62 | 0.48 |
| 28:DE:48:GLN:CG | 28:DE:78:LEU:CB | 2.89 | 0.48 |
| 28:DE:79:ARG:N | 28:DE:79:ARG:HD2 | 2.29 | 0.48 |
| 25:DA:2401:U:O2' | 25:DA:2402:C:C6 | 2.64 | 0.48 |
| 4:CG:8:VAL:O | 4:CG:11:LEU:N | 2.47 | 0.48 |
| 1:CA:1177:G:OP2 | 9:CL:97:LYS:NZ | 2.43 | 0.48 |
| 30:DG:161:THR:HG22 | 30:DG:162:THR:N | 2.29 | 0.48 |
| 54:B8:37:SER:HA | 54:B8:41:ILE:CG2 | 2.41 | 0.48 |
| 25:DA:529:A:H4' | 25:DA:530:G:H5' | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:548:A:H8 | 25:DA:548:A:O5' | 1.97 | 0.48 |
| 1:CA:260:G:N2 | 1:CA:265:G:N7 | 2.61 | 0.48 |
| 13:AP:108:ARG:N | 13:AP:108:ARG:HD2 | 2.29 | 0.48 |
| 25:DA:676:A:N1 | 25:DA:802:A:N1 | 2.62 | 0.48 |
| 27:DD:24:ILE:CD1 | 27:DD:91:ARG:HD3 | 2.38 | 0.48 |
| 25:DA:654(T):A:H2' | 25:DA:654(U):A:O4' | 2.13 | 0.48 |
| 19:CV:28:LYS:CE | 19:CV:29:ARG:H | 2.26 | 0.48 |
| 19:CV:30:LEU:CD1 | 19:CV:31:ILE:H | 2.27 | 0.48 |
| 25:BA:141:A:H8 | 25:BA:1408:C:H1' | 1.77 | 0.48 |
| 25:DA:861:A:C2 | 25:DA:917:A:C5 | 3.02 | 0.48 |
| 1:CA:1328:C:OP1 | 21:CX:21:TYR:OH | 2.22 | 0.48 |
| 23:AD:27:G:O6 | 23:AD:45:A:N6 | 2.46 | 0.48 |
| 38:DQ:59:LYS:HD3 | 38:DQ:60:GLY:H | 1.79 | 0.48 |
| 45:BV:76:LEU:N | 45:BV:76:LEU:CD2 | 2.74 | 0.48 |
| 28:BE:92:THR:O | 28:BE:95:ILE:CG1 | 2.61 | 0.48 |
| 1:AA:658:G:H2' | 1:AA:659:U:H6 | 1.78 | 0.48 |
| 25:DA:1171:G:O2' | 25:DA:1173:G:O5' | 2.30 | 0.48 |
| 10:CM:8:LEU:CD2 | 10:CM:20:ALA:HB2 | 2.43 | 0.48 |
| 22:CB:35:G:C2' | 22:CB:36:A:H5' | 2.44 | 0.48 |
| 2:AE:150:SER:OG | 2:AE:151:GLY:N | 2.46 | 0.48 |
| 18:CU:41:LYS:HD3 | 18:CU:41:LYS:O | 2.14 | 0.48 |
| 25:DA:1443:G:C2' | 25:DA:1444:G:H5' | 2.43 | 0.48 |
| 29:DF:187:VAL:HG12 | 35:DO:3:LEU:HG | 1.96 | 0.48 |
| 5:CH:100:VAL:HG22 | 5:CH:118:ILE:CG2 | 2.44 | 0.48 |
| 1:CA:194:C:H2' | 1:CA:195:A:H5'' | 1.95 | 0.48 |
| 34:BN:93:PRO:HG2 | 34:BN:113:LYS:HD3 | 1.95 | 0.48 |
| 1:CA:380:G:N2 | 1:CA:384:G:C5 | 2.82 | 0.48 |
| 25:DA:513:A:C2 | 25:DA:514:A:C5 | 3.02 | 0.48 |
| 16:CS:56:ALA:O | 16:CS:60:LEU:HG | 2.14 | 0.48 |
| 4:CG:75:PHE:HE1 | 4:CG:97:LEU:HD11 | 1.78 | 0.48 |
| 10:CM:44:VAL:HG22 | 10:CM:66:ARG:HG3 | 1.95 | 0.48 |
| 34:DN:108:GLU:HG2 | 34:DN:108:GLU:H | 1.46 | 0.48 |
| 1:AA:85:U:O2 | 1:AA:85:U:C2' | 2.62 | 0.48 |
| 37:D0:63:ARG:O | 37:D0:67:LEU:HB2 | 2.14 | 0.48 |
| 13:AP:4:ILE:HG22 | 13:AP:5:ALA:N | 2.28 | 0.48 |
| 13:AP:99:ARG:O | 13:AP:101:GLN:NE2 | 2.47 | 0.48 |
| 1:AA:1176:A:H2' | 1:AA:1177:G:C5' | 2.43 | 0.47 |
| 1:AA:1178:G:H5' | 9:AL:93:ARG:HH21 | 1.79 | 0.47 |
| 25:DA:1225:C:O3' | 41:D2:85:LYS:CA | 2.61 | 0.47 |
| 27:BD:102:LYS:C | 27:BD:103:ARG:HG2 | 2.34 | 0.47 |
| 25:BA:2784:C:H4' | 28:BE:41:LYS:O | 2.13 | 0.47 |
| 32:DK:83:ALA:O | 32:DK:89:TYR:CE2 | 2.67 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 51:D5:46:CYS:SG | 51:D5:47:PRO:HD2 | 2.54 | 0.47 |
| 25:BA:883:G:H2' | 25:BA:884:C:O4' | 2.14 | 0.47 |
| 14:AQ:41:ARG:HG2 | 14:AQ:41:ARG:NH1 | 2.26 | 0.47 |
| 31:DH:7:LEU:N | 31:DH:8:PRO:HD2 | 2.29 | 0.47 |
| 10:CM:80:LYS:O | 10:CM:83:GLU:HB3 | 2.14 | 0.47 |
| 43:DT:60:ARG:NH1 | 43:DT:60:ARG:CG | 2.67 | 0.47 |
| 33:BM:126:PRO:HB2 | 33:BM:127:ASP:OD1 | 2.14 | 0.47 |
| 8:AK:86:ILE:O | 8:AK:87:SER:C | 2.52 | 0.47 |
| 35:DO:97:PRO:HG3 | 35:DO:112:LEU:CB | 2.44 | 0.47 |
| 25:DA:654(B):C:N3 | 25:DA:654(T):A:C2 | 2.82 | 0.47 |
| 3:CF:117:ALA:HB2 | 3:CF:200:ALA:CB | 2.37 | 0.47 |
| 1:AA:438:G:HO2' | 1:AA:439:A:H5'' | 1.79 | 0.47 |
| 5:AH:110:LEU:CD1 | 5:AH:118:ILE:HD13 | 2.40 | 0.47 |
| 25:DA:1278:A:H2' | 25:DA:1279:G:C8 | 2.49 | 0.47 |
| 35:BO:112:LEU:HD22 | 35:BO:113:LYS:N | 2.29 | 0.47 |
| 25:DA:2212:A:H1' | 25:DA:2215:G:C5 | 2.49 | 0.47 |
| 1:CA:861:G:C5 | 1:CA:862:C:C5 | 3.01 | 0.47 |
| 36:DP:21:THR:HG23 | 36:DP:21:THR:O | 2.10 | 0.47 |
| 14:AQ:44:LEU:HD12 | 14:AQ:44:LEU:C | 2.35 | 0.47 |
| 30:BG:173:LEU:O | 30:BG:178:PHE:HB2 | 2.14 | 0.47 |
| 25:BA:404:C:O2' | 25:BA:405:U:OP2 | 2.27 | 0.47 |
| 1:CA:939:G:H2' | 1:CA:940:C:C6 | 2.49 | 0.47 |
| 25:DA:959:A:C6 | 25:DA:960:A:C2 | 3.03 | 0.47 |
| 1:AA:232:G:C5 | 1:AA:233:C:C5 | 3.01 | 0.47 |
| 25:BA:271(C):U:H2' | 25:BA:271:G:OP1 | 2.14 | 0.47 |
| 1:AA:93:U:H2' | 1:AA:95:G:C5' | 2.44 | 0.47 |
| 17:AT:31:LEU:HD23 | 17:AT:32:TYR:CZ | 2.49 | 0.47 |
| 30:DG:96:ARG:HH11 | 30:DG:96:ARG:CG | 2.25 | 0.47 |
| 25:DA:277:C:H3' | 25:DA:278:A:H8 | 1.79 | 0.47 |
| 36:BP:109:VAL:HG13 | 36:BP:113:GLN:HB2 | 1.95 | 0.47 |
| 10:AM:3:LYS:O | 10:AM:100:THR:HG22 | 2.14 | 0.47 |
| 25:DA:94:G:N3 | 48:DW:47:ASN:OD1 | 2.46 | 0.47 |
| 1:CA:1195:C:C4 | 1:CA:1197:G:C8 | 3.01 | 0.47 |
| 26:BB:1:U:H2' | 26:BB:2:C:H6 | 1.78 | 0.47 |
| 42:DS:92:ARG:NH1 | 42:DS:94:ASP:OD2 | 2.47 | 0.47 |
| 25:DA:1791:A:OP2 | 25:DA:1791:A:C8 | 2.67 | 0.47 |
| 25:DA:470:A:OP1 | 29:DF:59:TYR:HE2 | 1.97 | 0.47 |
| 1:CA:607:A:C2 | 16:CS:31:LYS:HB2 | 2.49 | 0.47 |
| 25:BA:725:G:C6 | 25:BA:726:G:N1 | 2.82 | 0.47 |
| 25:BA:184:C:H2' | 25:BA:185:U:C6 | 2.50 | 0.47 |
| 25:BA:2677:G:H2' | 25:BA:2678:C:C6 | 2.49 | 0.47 |
| 25:BA:2653:U:O2' | 31:BH:110:SER:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:1629:U:H2' | 25:DA:1630:G:C8 | 2.48 | 0.47 |
| 1:AA:303:A:H2' | 1:AA:304:U:O4' | 2.14 | 0.47 |
| 31:BH:167:GLU:H | 31:BH:167:GLU:HG2 | 1.36 | 0.47 |
| 29:DF:157:VAL:HB | 29:DF:194:MET:HB3 | 1.96 | 0.47 |
| 1:AA:706:A:H2' | 1:AA:707:C:H5' | 1.96 | 0.47 |
| 4:AG:84:LYS:N | 4:AG:84:LYS:HD2 | 2.29 | 0.47 |
| 1:AA:9:G:C2 | 1:AA:26:A:C2 | 3.01 | 0.47 |
| 1:AA:1159:U:N3 | 1:AA:1182:G:C6 | 2.82 | 0.47 |
| 40:D1:58:ARG:O | 40:D1:62:ILE:HD13 | 2.12 | 0.47 |
| 27:BD:35:LYS:CE | 27:BD:104:TYR:CD1 | 2.98 | 0.47 |
| 27:BD:35:LYS:H | 27:BD:64:ILE:HG23 | 1.79 | 0.47 |
| 27:BD:65:ILE:CG1 | 27:BD:67:PHE:CE1 | 2.96 | 0.47 |
| 26:BB:15:A:H3' | 26:BB:16:G:H5' | 1.96 | 0.47 |
| 39:DR:19:LEU:HD22 | 39:DR:86:ILE:HG23 | 1.96 | 0.47 |
| 25:DA:973:A:H5' | 25:DA:1188:U:H1' | 1.96 | 0.47 |
| 26:DB:73:A:C4 | 26:DB:104:A:C2 | 3.02 | 0.47 |
| 2:CE:18:GLY:O | 2:CE:19:HIS:ND1 | 2.40 | 0.47 |
| 29:DF:22:ALA:O | 29:DF:24:LEU:O | 2.32 | 0.47 |
| 45:BV:58:VAL:O | 45:BV:67:LEU:O | 2.32 | 0.47 |
| 1:AA:1351:U:O4 | 9:AL:118:LYS:HE3 | 2.14 | 0.47 |
| 14:AQ:21:TYR:HE2 | 14:AQ:23:ARG:HE | 1.61 | 0.47 |
| 1:CA:1133:G:H2' | 1:CA:1134:G:H8 | 1.78 | 0.47 |
| 30:DG:105:LYS:HE3 | 50:D4:26:SER:HB3 | 1.95 | 0.47 |
| 26:DB:44:G:H5'' | 26:DB:45:A:OP1 | 2.14 | 0.47 |
| 40:B1:91:ASP:O | 40:B1:92:ARG:C | 2.52 | 0.47 |
| 25:BA:2168:G:N2 | 25:BA:2170:A:O5' | 2.44 | 0.47 |
| 5:CH:103:GLY:N | 5:CH:106:PRO:HG2 | 2.29 | 0.47 |
| 41:B2:59:ALA:CB | 41:B2:96:ILE:HD13 | 2.36 | 0.47 |
| 25:DA:2032:G:N2 | 28:DE:146:THR:HG23 | 2.17 | 0.47 |
| 25:BA:2136:C:H2' | 25:BA:2137:C:O4' | 2.14 | 0.47 |
| 25:BA:1609:A:O2' | 25:BA:1610:A:H5' | 2.14 | 0.47 |
| 28:BE:111:ARG:HG2 | 37:B0:1:MET:CE | 2.44 | 0.47 |
| 39:BR:16:ARG:HD3 | 39:BR:19:LEU:CD1 | 2.38 | 0.47 |
| 1:AA:495:A:C2 | 1:AA:496:A:C5 | 3.02 | 0.47 |
| 19:CV:28:LYS:CG | 19:CV:29:ARG:H | 2.26 | 0.47 |
| 25:BA:593:G:O3' | 54:B8:61:LEU:HD13 | 2.14 | 0.47 |
| 1:AA:955:U:O2' | 19:AV:83:HIS:CD2 | 2.67 | 0.47 |
| 3:CF:16:ARG:HH11 | 3:CF:16:ARG:CA | 2.27 | 0.47 |
| 1:AA:1372:U:H2' | 1:AA:1373:G:O5' | 2.14 | 0.47 |
| 38:DQ:61:ASN:HB3 | 38:DQ:64:GLU:CB | 2.44 | 0.47 |
| 1:AA:658:G:C4 | 1:AA:659:U:C5 | 3.02 | 0.47 |
| 25:DA:753:C:C2 | 25:DA:754:C:C5 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 35:DO:52:GLU:OE2 | 35:DO:58:THR:N | 2.44 | 0.47 |
| 7:AJ:91:VAL:HG12 | 7:AJ:95:ARG:HB3 | 1.96 | 0.47 |
| 25:DA:825:C:O2 | 35:DO:55:ARG:NH2 | 2.46 | 0.47 |
| 35:BO:55:ARG:O | 35:BO:56:SER:C | 2.51 | 0.47 |
| 24:A1:14:U:C2' | 24:A1:15:U:O4' | 2.62 | 0.47 |
| 13:AP:84:ILE:HD11 | 19:AV:66:MET:HG2 | 1.95 | 0.47 |
| 43:BT:29:TRP:CZ3 | 43:BT:78:LYS:HG2 | 2.49 | 0.47 |
| 50:D4:38:LYS:C | 50:D4:40:HIS:H | 2.16 | 0.47 |
| 1:CA:1151:A:N6 | 1:CA:1152:A:N6 | 2.62 | 0.47 |
| 11:CN:78:GLN:O | 11:CN:103:LEU:HA | 2.14 | 0.47 |
| 27:DD:108:PRO:HG2 | 27:DD:111:LEU:HB2 | 1.95 | 0.47 |
| 25:BA:280:C:C2' | 25:BA:281:G:H5' | 2.44 | 0.47 |
| 25:DA:2564:A:OP1 | 25:DA:2648:C:H4' | 2.13 | 0.47 |
| 26:BB:79:C:O5' | 26:BB:79:C:H6 | 1.96 | 0.47 |
| 1:CA:1247:U:H1' | 1:CA:1291:G:N2 | 2.29 | 0.47 |
| 25:DA:17:G:H4' | 40:D1:25:TRP:CZ3 | 2.49 | 0.47 |
| 27:BD:158:ALA:HB3 | 27:BD:161:THR:CG2 | 2.44 | 0.47 |
| 25:BA:1531:C:O2' | 25:BA:1532:C:H5' | 2.13 | 0.47 |
| 1:CA:161:A:C6 | 1:CA:162:A:C6 | 3.02 | 0.47 |
| 25:DA:2093:G:N7 | 25:DA:2225:A:H2' | 2.29 | 0.47 |
| 1:AA:109:A:N7 | 1:AA:326:G:H2' | 2.29 | 0.47 |
| 41:D2:67:GLY:O | 41:D2:88:ARG:HD3 | 2.14 | 0.47 |
| 1:CA:31:G:O2' | 1:CA:48:C:N4 | 2.47 | 0.47 |
| 4:AG:158:ILE:HG22 | 4:AG:159:ARG:N | 2.30 | 0.47 |
| 41:D2:60:GLU:OE2 | 41:D2:97:LYS:HE3 | 2.14 | 0.47 |
| 23:CC:53:G:O2' | 23:CC:54:G:H5' | 2.15 | 0.47 |
| 20:AW:37:SER:O | 20:AW:41:ILE:HG12 | 2.14 | 0.47 |
| 1:CA:1480:G:C5 | 1:CA:1481:U:C5 | 3.02 | 0.47 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:C6 | 2.49 | 0.47 |
| 44:DU:85:VAL:O | 44:DU:85:VAL:HG12 | 2.14 | 0.47 |
| 22:CB:6:G:N2 | 22:CB:78:C:O2 | 2.47 | 0.47 |
| 25:BA:248:G:H5' | 25:BA:250:G:N7 | 2.28 | 0.47 |
| 35:BO:61:ARG:HB2 | 35:BO:61:ARG:CZ | 2.26 | 0.47 |
| 27:DD:35:LYS:HD3 | 27:DD:63:ARG:CA | 2.43 | 0.47 |
| 35:BO:15:ARG:O | 35:BO:16:ARG:C | 2.53 | 0.47 |
| 35:BO:65:ARG:CG | 35:BO:65:ARG:HH11 | 1.94 | 0.47 |
| 53:D7:8:ASN:ND2 | 53:D7:11:LYS:N | 2.36 | 0.47 |
| 25:BA:2287:A:N6 | 25:BA:2344:U:C2 | 2.82 | 0.47 |
| 1:CA:530:G:O6 | 24:C1:21:U:H1' | 2.14 | 0.47 |
| 28:DE:130:GLY:O | 28:DE:131:ALA:O | 2.32 | 0.47 |
| 25:BA:897:C:H2' | 25:BA:898:C:O5' | 2.14 | 0.47 |
| 25:BA:2056:G:H1 | 51:B5:4:HIS:CD2 | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|---------------------|-------------|----------|
| 25:DA:2712:U:O2' | 25:DA:2712(A):A:OP2 | 2.24 | 0.47 |
| 25:BA:1142(A):A:C4 | 25:BA:1144:G:N7 | 2.83 | 0.47 |
| 25:BA:905:U:C3' | 25:BA:906:G:H5'' | 2.45 | 0.47 |
| 19:CV:63:THR:HG23 | 19:CV:65:ASN:O | 2.14 | 0.47 |
| 33:BM:17:ASP:O | 33:BM:55:VAL:O | 2.32 | 0.47 |
| 50:D4:13:ARG:O | 50:D4:29:PRO:O | 2.33 | 0.47 |
| 1:CA:1068:G:N3 | 1:CA:1191:A:C2 | 2.82 | 0.47 |
| 25:DA:864:G:C6 | 25:DA:865:C:C4 | 3.02 | 0.47 |
| 1:CA:885:G:O2' | 1:CA:914:A:N1 | 2.36 | 0.47 |
| 25:DA:1839:G:C8 | 25:DA:1927:A:C1' | 2.96 | 0.47 |
| 29:BF:34:TRP:CE2 | 35:BO:8:PRO:HD3 | 2.49 | 0.47 |
| 35:BO:52:GLU:OE2 | 35:BO:58:THR:N | 2.44 | 0.47 |
| 1:CA:197:A:H1' | 1:CA:198:G:O4' | 2.13 | 0.47 |
| 41:D2:2:PHE:O | 41:D2:42:GLY:N | 2.47 | 0.47 |
| 25:BA:1449(A):G:H2' | 25:BA:1450:C:C6 | 2.49 | 0.47 |
| 25:DA:2820:A:O2' | 28:DE:191:PRO:HG3 | 2.14 | 0.47 |
| 4:AG:98:GLU:OE1 | 4:AG:194:LEU:CD2 | 2.62 | 0.47 |
| 25:BA:141(A):C:H2' | 25:BA:142:G:O4' | 2.15 | 0.47 |
| 25:DA:524:U:H2' | 25:DA:525:U:H6 | 1.79 | 0.47 |
| 25:BA:1155:A:O2' | 25:BA:1156:A:H2' | 2.14 | 0.47 |
| 6:CI:72:VAL:HG13 | 6:CI:73:ASN:N | 2.29 | 0.47 |
| 1:CA:552:U:H2' | 1:CA:553:A:H5' | 1.95 | 0.47 |
| 25:BA:822:U:O2' | 25:BA:823:G:H5' | 2.14 | 0.47 |
| 25:DA:78:A:C6 | 25:DA:79:G:C6 | 3.02 | 0.47 |
| 25:BA:394:A:C2' | 25:BA:395:U:H5' | 2.44 | 0.47 |
| 25:BA:301:G:H1' | 25:BA:302:C:C6 | 2.50 | 0.47 |
| 1:CA:787:A:C2 | 1:CA:796:C:N3 | 2.82 | 0.47 |
| 22:CB:51:A:OP1 | 22:CB:52:U:C5 | 2.67 | 0.47 |
| 1:AA:1152:A:C5 | 1:AA:1153:C:C5 | 3.02 | 0.47 |
| 34:DN:20:MET:HB2 | 34:DN:44:LYS:HG3 | 1.96 | 0.47 |
| 25:BA:2348:U:H4' | 52:B6:42:TRP:CD1 | 2.49 | 0.47 |
| 25:DA:1131:G:N2 | 25:DA:1132:A:C4 | 2.83 | 0.47 |
| 5:CH:6:PHE:HB3 | 5:CH:35:GLY:C | 2.34 | 0.47 |
| 1:AA:767:A:H2' | 1:AA:768:A:O4' | 2.14 | 0.47 |
| 48:BW:10:LEU:O | 48:BW:14:ARG:HG3 | 2.14 | 0.47 |
| 1:AA:778:G:O5' | 1:AA:778:G:H8 | 1.98 | 0.47 |
| 25:DA:2239:G:H5' | 27:DD:251:GLY:HA3 | 1.97 | 0.47 |
| 25:DA:1853:A:H2' | 25:DA:1854:A:C8 | 2.48 | 0.47 |
| 25:BA:1432:C:H2' | 25:BA:1433:U:O4' | 2.14 | 0.47 |
| 25:BA:2467:C:O2' | 25:BA:2468:G:H5'' | 2.15 | 0.47 |
| 27:DD:67:PHE:HB3 | 27:DD:153:ALA:H | 1.78 | 0.47 |
| 27:DD:34:VAL:C | 27:DD:35:LYS:HG3 | 2.35 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:1225:C:O2' | 41:D2:85:LYS:N | 2.46 | 0.47 |
| 28:BE:51:PHE:HD1 | 28:BE:52:LEU:HD21 | 1.71 | 0.47 |
| 1:CA:1037:C:H6 | 1:CA:1037:C:H3' | 1.79 | 0.47 |
| 28:DE:79:ARG:HA | 28:DE:79:ARG:NE | 2.28 | 0.47 |
| 25:DA:1188:U:H4' | 41:D2:79:VAL:HG12 | 1.96 | 0.47 |
| 14:CQ:16:PHE:HB2 | 14:CQ:18:VAL:HG23 | 1.95 | 0.47 |
| 25:BA:2347:C:H4' | 52:B6:39:TYR:HE2 | 1.78 | 0.47 |
| 1:AA:1004:A:C2 | 1:AA:1024:G:H2' | 2.50 | 0.47 |
| 1:AA:1039:C:H2' | 1:AA:1040:U:O4' | 2.13 | 0.47 |
| 50:B4:62:ARG:HG3 | 50:B4:62:ARG:O | 2.12 | 0.47 |
| 11:AN:17:GLY:HA3 | 11:AN:77:MET:HE1 | 1.91 | 0.47 |
| 36:BP:66:ILE:O | 36:BP:67:ARG:CB | 2.61 | 0.47 |
| 29:DF:24:LEU:HB3 | 29:DF:25:PRO:CD | 2.44 | 0.47 |
| 25:DA:2270:G:H2' | 25:DA:2271:G:H5' | 1.96 | 0.47 |
| 25:DA:953:A:O2' | 25:DA:954:G:H5' | 2.14 | 0.47 |
| 9:AL:112:LYS:C | 9:AL:112:LYS:HD3 | 2.34 | 0.47 |
| 20:AW:72:LEU:C | 20:AW:72:LEU:HD23 | 2.34 | 0.47 |
| 17:CT:68:ARG:N | 17:CT:70:ARG:NH1 | 2.63 | 0.47 |
| 35:BO:47:ASP:HA | 35:BO:48:PRO:HD3 | 1.55 | 0.47 |
| 2:AE:7:VAL:HG22 | 2:AE:8:LYS:O | 2.14 | 0.47 |
| 23:CD:57:C:C2 | 25:DA:2169:A:C8 | 3.02 | 0.47 |
| 9:CL:78:LYS:HB2 | 9:CL:78:LYS:HZ2 | 1.76 | 0.47 |
| 23:AD:57:C:H5' | 25:BA:2169:A:C1' | 2.45 | 0.47 |
| 25:DA:1952:A:C5 | 34:DN:22:ILE:CD1 | 2.92 | 0.47 |
| 45:DV:150:LEU:HD13 | 45:DV:150:LEU:O | 2.15 | 0.47 |
| 25:DA:958:U:O2 | 26:DB:89(A):A:H4' | 2.15 | 0.47 |
| 25:DA:2875:C:O2' | 39:DR:5:ALA:HB3 | 2.14 | 0.47 |
| 25:DA:2296:U:OP2 | 38:DQ:9:ARG:NH1 | 2.47 | 0.47 |
| 16:CS:22:THR:HA | 16:CS:33:ILE:HG12 | 1.95 | 0.47 |
| 1:CA:209:U:H2' | 1:CA:209:U:O2 | 2.14 | 0.47 |
| 30:DG:117:PHE:O | 30:DG:117:PHE:CD1 | 2.67 | 0.47 |
| 17:CT:59:ILE:HG23 | 17:CT:71:PHE:HB3 | 1.96 | 0.47 |
| 25:BA:606:U:OP1 | 29:BF:104:LYS:HD2 | 2.14 | 0.47 |
| 1:AA:965:A:C2 | 1:AA:969:A:N1 | 2.83 | 0.47 |
| 25:BA:529:A:C2' | 25:BA:529:A:N3 | 2.77 | 0.47 |
| 25:BA:529:A:H4' | 25:BA:530:G:H5' | 1.96 | 0.47 |
| 22:CB:28:C:H2' | 22:CB:29:U:O4' | 2.14 | 0.47 |
| 6:CI:100:ASN:ND2 | 18:CU:23:LYS:HD2 | 2.29 | 0.47 |
| 16:CS:1:MET:HB2 | 16:CS:1:MET:HE3 | 1.48 | 0.47 |
| 45:DV:93:ASP:O | 45:DV:94:GLU:HG3 | 2.15 | 0.47 |
| 25:BA:587:C:H4' | 25:BA:588:U:O5' | 2.14 | 0.47 |
| 1:CA:464:G:O6 | 1:CA:466:C:H5' | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:1288:A:H2' | 1:CA:1289:A:C8 | 2.50 | 0.47 |
| 13:AP:115:LYS:O | 13:AP:116:THR:C | 2.51 | 0.47 |
| 1:AA:1112:C:N4 | 3:AF:178:LEU:HD23 | 2.29 | 0.47 |
| 11:CN:56:GLY:O | 11:CN:89:ALA:HB3 | 2.14 | 0.47 |
| 34:BN:17:ARG:NE | 34:BN:47:ILE:HD13 | 2.30 | 0.47 |
| 1:AA:663:A:H2' | 1:AA:664:G:O4' | 2.14 | 0.47 |
| 1:AA:1083:U:H5 | 1:AA:1084:G:C6 | 2.32 | 0.47 |
| 34:BN:14:THR:HG22 | 34:BN:95:GLY:N | 2.29 | 0.47 |
| 17:AT:57:VAL:HG23 | 17:AT:58:GLU:N | 2.29 | 0.47 |
| 1:AA:529:G:O6 | 12:AO:49:ASN:ND2 | 2.48 | 0.47 |
| 4:CG:101:LEU:HD23 | 4:CG:121:VAL:HG11 | 1.96 | 0.47 |
| 6:CI:50:TYR:CE1 | 18:CU:74:ARG:O | 2.68 | 0.47 |
| 40:D1:110:VAL:O | 40:D1:113:ALA:HB3 | 2.15 | 0.47 |
| 31:DH:54:ARG:HB2 | 31:DH:55:PRO:HD2 | 1.96 | 0.47 |
| 1:AA:947:G:H2' | 1:AA:948:C:O4' | 2.14 | 0.47 |
| 1:AA:185:A:H2' | 1:AA:186:C:C6 | 2.49 | 0.47 |
| 1:AA:222:U:H2' | 1:AA:223:U:C6 | 2.49 | 0.47 |
| 1:AA:222:U:C2 | 1:AA:223:U:C5 | 3.02 | 0.47 |
| 20:CW:55:ILE:HA | 20:CW:55:ILE:HD13 | 1.77 | 0.47 |
| 3:AF:29:TYR:OH | 14:AQ:54:PRO:HD2 | 2.14 | 0.47 |
| 43:DT:64:LYS:HD3 | 43:DT:73:ARG:NE | 2.30 | 0.47 |
| 25:BA:2836:U:H2' | 25:BA:2837:G:C8 | 2.50 | 0.47 |
| 36:BP:106:VAL:HG21 | 36:BP:114:ALA:HB1 | 1.97 | 0.47 |
| 32:BK:128:LEU:O | 32:BK:138:ILE:HG22 | 2.14 | 0.47 |
| 35:BO:120:ALA:HB1 | 35:BO:138:LEU:HB3 | 1.96 | 0.47 |
| 25:BA:2860:A:C8 | 25:BA:2861:G:H1' | 2.49 | 0.47 |
| 25:BA:1588:C:H2' | 25:BA:1589:C:H6 | 1.79 | 0.47 |
| 1:CA:573:A:N3 | 1:CA:883:C:O2' | 2.37 | 0.47 |
| 25:DA:1829:A:N3 | 27:DD:15:PHE:HE1 | 2.12 | 0.47 |
| 25:DA:1215:G:O2' | 25:DA:1216:G:H5' | 2.14 | 0.47 |
| 38:DQ:110:LEU:HD13 | 38:DQ:111:GLU:H | 1.78 | 0.47 |
| 25:DA:996:A:O2' | 40:D1:92:ARG:NH2 | 2.48 | 0.47 |
| 40:B1:60:LEU:CD1 | 40:B1:64:ARG:HD2 | 2.44 | 0.47 |
| 1:CA:1200:C:H5' | 1:CA:1201:A:C5' | 2.45 | 0.47 |
| 1:CA:1222:G:OP1 | 1:CA:1321:C:O2 | 2.33 | 0.47 |
| 1:CA:1224:G:N2 | 1:CA:1322:C:H4' | 2.30 | 0.47 |
| 10:CM:54:PHE:CE1 | 10:CM:55:LYS:CE | 2.97 | 0.47 |
| 35:DO:15:ARG:O | 35:DO:16:ARG:C | 2.53 | 0.47 |
| 4:CG:31:CYS:C | 4:CG:33:MET:N | 2.68 | 0.47 |
| 25:DA:2747:G:H21 | 25:DA:2757:A:H62 | 1.61 | 0.47 |
| 1:AA:1005:A:N1 | 1:AA:1024:G:H8 | 2.11 | 0.47 |
| 25:DA:1088:A:H4' | 25:DA:1089:G:C8 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 43:DT:43:VAL:HG22 | 43:DT:51:VAL:HG21 | 1.97 | 0.47 |
| 54:B8:25:MET:O | 54:B8:47:LYS:NZ | 2.48 | 0.47 |
| 25:DA:2255:G:C2 | 36:DP:85:LYS:HE2 | 2.46 | 0.47 |
| 1:CA:631:G:O3' | 1:CA:632:A:H8 | 1.96 | 0.47 |
| 25:BA:2210:G:C3' | 25:BA:2211:G:N7 | 2.75 | 0.47 |
| 43:BT:49:VAL:CG1 | 43:BT:50:LYS:H | 2.24 | 0.47 |
| 1:CA:1442:G:N7 | 1:CA:1446:A:C2 | 2.82 | 0.47 |
| 2:CE:137:ARG:C | 2:CE:137:ARG:HD3 | 2.34 | 0.47 |
| 4:AG:11:LEU:O | 4:AG:12:CYS:C | 2.52 | 0.47 |
| 25:BA:780:G:C2 | 25:BA:783:A:N6 | 2.83 | 0.47 |
| 25:DA:856:C:HO2' | 25:DA:857:C:P | 2.37 | 0.47 |
| 33:BM:23:LEU:CD1 | 33:BM:99:LEU:HD23 | 2.44 | 0.47 |
| 25:BA:1534:G:H2' | 25:BA:1535:U:O4' | 2.15 | 0.47 |
| 7:AJ:120:ILE:O | 7:AJ:124:LEU:HD12 | 2.15 | 0.47 |
| 9:CL:85:LEU:HD12 | 9:CL:86:VAL:N | 2.28 | 0.47 |
| 25:BA:1784:A:H4' | 25:BA:1785:A:C5' | 2.44 | 0.47 |
| 51:B5:40:LYS:HD3 | 51:B5:46:CYS:HB3 | 1.94 | 0.47 |
| 25:DA:2154:G:O2' | 25:DA:2155:G:H5' | 2.14 | 0.47 |
| 7:CJ:13:GLN:O | 7:CJ:24:THR:HG21 | 2.15 | 0.47 |
| 50:D4:61:ARG:CG | 50:D4:62:ARG:HH21 | 2.27 | 0.47 |
| 28:DE:14:ILE:HB | 39:DR:14:TYR:CZ | 2.49 | 0.47 |
| 1:AA:955:U:H1' | 1:AA:1227:A:N6 | 2.29 | 0.47 |
| 35:BO:39:LYS:HB2 | 35:BO:45:LEU:HD22 | 1.97 | 0.47 |
| 38:DQ:56:LEU:O | 38:DQ:58:LEU:HD23 | 2.14 | 0.47 |
| 28:BE:13:ARG:CG | 39:BR:58:ASN:OD1 | 2.60 | 0.47 |
| 28:DE:10:GLY:O | 28:DE:24:THR:O | 2.33 | 0.47 |
| 25:DA:602:G:N2 | 25:DA:655:A:C8 | 2.79 | 0.47 |
| 25:BA:562:U:O4 | 25:BA:2036:C:H1' | 2.13 | 0.47 |
| 53:B7:48:LYS:O | 53:B7:49:ARG:HB2 | 2.14 | 0.47 |
| 2:AE:102:LEU:HB3 | 2:AE:180:LEU:HD12 | 1.96 | 0.47 |
| 43:BT:29:TRP:CE3 | 43:BT:78:LYS:HG2 | 2.49 | 0.47 |
| 28:BE:167:VAL:HG11 | 28:BE:187:ALA:O | 2.15 | 0.47 |
| 1:CA:522:C:OP2 | 12:CO:69:TYR:OH | 2.28 | 0.47 |
| 14:CQ:4:LYS:C | 14:CQ:6:LEU:N | 2.68 | 0.47 |
| 35:DO:113:LYS:HG2 | 35:DO:115:LEU:CD2 | 2.45 | 0.47 |
| 25:BA:1354:A:H2' | 25:BA:1355:G:O4' | 2.15 | 0.47 |
| 11:CN:66:LEU:CD2 | 11:CN:101:SER:HB3 | 2.44 | 0.47 |
| 25:BA:2751:G:N2 | 31:BH:3:ARG:HG2 | 2.30 | 0.47 |
| 22:CB:61:C:N4 | 22:CB:75:G:H1 | 2.12 | 0.47 |
| 23:CC:73:A:C6 | 23:CC:74:A:C6 | 3.02 | 0.47 |
| 1:CA:1137:C:H4' | 1:CA:1138:G:C2 | 2.50 | 0.47 |
| 1:CA:527:G:H2' | 1:CA:528:C:H5' | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:1480:G:H2' | 1:CA:1481:U:H6 | 1.78 | 0.47 |
| 1:AA:1281:U:H5'' | 1:AA:1282:C:OP2 | 2.15 | 0.47 |
| 25:DA:2728:U:O2' | 25:DA:2729:G:H5' | 2.14 | 0.47 |
| 4:AG:92:VAL:O | 4:AG:96:LEU:HD22 | 2.14 | 0.47 |
| 17:CT:10:VAL:HG13 | 17:CT:19:VAL:HB | 1.95 | 0.47 |
| 26:BB:39:A:C2 | 26:BB:44:G:C4 | 3.02 | 0.47 |
| 8:CK:38:ILE:HD11 | 8:CK:118:VAL:O | 2.15 | 0.47 |
| 25:BA:1505:C:H2' | 25:BA:1506:C:C6 | 2.49 | 0.47 |
| 49:BX:24:LYS:O | 49:BX:27:GLY:N | 2.46 | 0.47 |
| 25:DA:453:C:H4' | 25:DA:472:A:N6 | 2.28 | 0.47 |
| 25:DA:2654:A:H8 | 25:DA:2654:A:OP1 | 1.98 | 0.47 |
| 25:DA:2385:C:H4' | 25:DA:2385:C:OP2 | 2.15 | 0.47 |
| 25:BA:1063:G:C6 | 25:BA:1064:C:C4 | 3.02 | 0.47 |
| 52:D6:27:LYS:HB3 | 52:D6:27:LYS:NZ | 2.25 | 0.47 |
| 1:AA:1178:G:H5' | 9:AL:93:ARG:NH2 | 2.28 | 0.47 |
| 36:DP:33:GLY:O | 36:DP:118:LEU:HD13 | 2.15 | 0.47 |
| 40:D1:65:ILE:HD11 | 40:D1:96:ALA:HB1 | 1.94 | 0.47 |
| 40:D1:66:ASN:CB | 40:D1:76:TYR:HB2 | 2.44 | 0.47 |
| 27:BD:35:LYS:HZ3 | 27:BD:104:TYR:HD1 | 1.60 | 0.47 |
| 25:BA:2317:C:C2' | 25:BA:2318:G:C5' | 2.81 | 0.47 |
| 1:CA:983:A:H2 | 1:CA:984:C:C6 | 2.32 | 0.47 |
| 25:DA:2401:U:O2 | 25:DA:2402:C:H5 | 1.96 | 0.47 |
| 39:DR:90:GLN:HE22 | 39:DR:121:ILE:HD11 | 1.78 | 0.47 |
| 39:DR:90:GLN:HE21 | 39:DR:90:GLN:CA | 2.22 | 0.47 |
| 25:BA:889:C:H5'' | 25:BA:890:A:OP2 | 2.15 | 0.47 |
| 1:CA:1156:G:C3' | 1:CA:1157:A:H5'' | 2.44 | 0.47 |
| 1:CA:1162:C:O2' | 1:CA:1163:C:H5' | 2.15 | 0.47 |
| 45:BV:7:ALA:O | 45:BV:8:TYR:CD2 | 2.68 | 0.47 |
| 25:DA:1050:A:H2' | 25:DA:1051:G:O4' | 2.14 | 0.47 |
| 31:DH:4:ILE:CD1 | 31:DH:6:ARG:HG2 | 2.45 | 0.47 |
| 25:BA:1797:C:O2' | 27:BD:259:THR:HB | 2.15 | 0.47 |
| 30:BG:7:LEU:HD23 | 30:BG:100:TRP:CE3 | 2.49 | 0.47 |
| 1:CA:1446:A:C6 | 39:DR:118:ARG:CZ | 2.98 | 0.47 |
| 32:BK:99:GLU:O | 32:BK:102:SER:CB | 2.62 | 0.47 |
| 2:CE:114:ARG:HG3 | 2:CE:114:ARG:O | 2.14 | 0.47 |
| 25:BA:1266:G:C6 | 42:BS:16:LYS:HD2 | 2.50 | 0.47 |
| 25:BA:1372:U:H2' | 25:BA:1373:A:O4' | 2.14 | 0.47 |
| 25:BA:456:C:C4 | 43:BT:69:TYR:CE1 | 3.03 | 0.47 |
| 19:CV:66:MET:HE2 | 50:D4:56:VAL:N | 2.30 | 0.47 |
| 50:D4:56:VAL:HA | 50:D4:60:GLN:NE2 | 2.23 | 0.47 |
| 25:DA:2872:G:N9 | 25:DA:2873:A:C2 | 2.82 | 0.47 |
| 35:DO:38:GLN:O | 35:DO:41:ARG:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 38:DQ:35:ILE:O | 38:DQ:35:ILE:HG13 | 2.12 | 0.47 |
| 25:BA:2327:A:H2' | 25:BA:2328:A:H8 | 1.75 | 0.47 |
| 25:BA:636:G:N7 | 35:BO:113:LYS:HE2 | 2.30 | 0.47 |
| 1:AA:1091:U:O2 | 1:AA:1093:A:C8 | 2.68 | 0.47 |
| 42:BS:29:LEU:HD21 | 42:BS:33:ARG:NH2 | 2.28 | 0.47 |
| 1:AA:27:G:C4' | 4:AG:209:ARG:HG3 | 2.43 | 0.47 |
| 27:DD:68:LYS:HB2 | 27:DD:70:TRP:CE3 | 2.50 | 0.47 |
| 1:AA:198:G:C6 | 1:AA:220:G:C2 | 3.02 | 0.47 |
| 1:AA:465:A:N6 | 1:AA:467:G:C2 | 2.82 | 0.47 |
| 6:CI:100:ASN:HB2 | 18:CU:23:LYS:HD3 | 1.95 | 0.47 |
| 28:BE:11:MET:O | 28:BE:12:THR:HB | 2.13 | 0.47 |
| 31:DH:20:ALA:HB1 | 31:DH:21:PRO:CD | 2.45 | 0.47 |
| 25:DA:1671:U:O2' | 25:DA:1673:U:H5 | 1.96 | 0.47 |
| 25:DA:1000:A:C6 | 25:DA:1155:A:C8 | 3.03 | 0.47 |
| 4:CG:107:ARG:HG2 | 4:CG:107:ARG:NH1 | 2.30 | 0.47 |
| 1:AA:96:G:H2' | 1:AA:97:U:C5' | 2.44 | 0.47 |
| 5:AH:33:VAL:HB | 5:AH:112:LEU:HD12 | 1.97 | 0.47 |
| 22:AB:24:C:C5 | 22:AB:25:A:C8 | 3.02 | 0.47 |
| 22:AB:28:C:H2' | 22:AB:29:U:C6 | 2.50 | 0.47 |
| 29:BF:132:VAL:HG12 | 29:BF:163:VAL:HG22 | 1.95 | 0.47 |
| 11:CN:48:ILE:CG1 | 11:CN:63:LEU:HB2 | 2.44 | 0.47 |
| 1:AA:754:C:H3' | 1:AA:754:C:O2 | 2.14 | 0.47 |
| 45:BV:39:VAL:HG21 | 45:BV:44:PHE:HB2 | 1.96 | 0.47 |
| 25:BA:644:A:H4' | 25:BA:645:C:C5 | 2.49 | 0.47 |
| 25:DA:2646:C:O5' | 25:DA:2646:C:H6 | 1.96 | 0.47 |
| 25:DA:1657:C:H2' | 25:DA:1658:C:H6 | 1.79 | 0.47 |
| 20:CW:67:ALA:HA | 20:CW:73:HIS:H | 1.79 | 0.47 |
| 23:AD:37:U:H2' | 23:AD:38:A:O4' | 2.14 | 0.47 |
| 23:AC:52:C:H2' | 23:AC:53:G:O4' | 2.15 | 0.47 |
| 32:DK:10:GLU:OE2 | 32:DK:11:ASN:HB2 | 2.14 | 0.47 |
| 8:AK:73:ASP:OD2 | 8:AK:75:ARG:NE | 2.48 | 0.47 |
| 38:DQ:36:TYR:N | 38:DQ:36:TYR:CD1 | 2.83 | 0.47 |
| 26:DB:66:A:C2 | 26:DB:108:C:C4 | 3.03 | 0.47 |
| 1:AA:265:G:H5' | 17:AT:64:PRO:O | 2.14 | 0.47 |
| 1:AA:950:U:C5 | 13:AP:102:ARG:NH1 | 2.83 | 0.47 |
| 47:BZ:87:PRO:O | 47:BZ:88:LYS:C | 2.52 | 0.47 |
| 52:D6:28:ARG:CB | 52:D6:31:PRO:HD2 | 2.44 | 0.47 |
| 1:AA:1175:G:C6 | 1:AA:1176:A:N6 | 2.83 | 0.47 |
| 35:DO:19:VAL:HG13 | 35:DO:20:GLY:N | 2.30 | 0.47 |
| 36:DP:34:LEU:HD12 | 36:DP:130:LYS:O | 2.14 | 0.47 |
| 27:BD:35:LYS:CA | 27:BD:64:ILE:HG22 | 2.43 | 0.47 |
| 27:BD:30:GLU:CD | 27:BD:63:ARG:HH21 | 2.18 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|-------------------|-------------|----------|
| 27:BD:96:HIS:NE2 | 27:BD:102:LYS:HE2 | 2.30 | 0.47 |
| 28:BE:30:PRO:O | 28:BE:32:PRO:HD3 | 2.15 | 0.47 |
| 28:BE:80:GLU:O | 28:BE:81:ILE:C | 2.53 | 0.47 |
| 25:DA:674:G:C1' | 29:DF:74:ARG:HD3 | 2.43 | 0.47 |
| 28:DE:12:THR:O | 28:DE:23:VAL:HG22 | 2.14 | 0.47 |
| 31:DH:153:LYS:O | 31:DH:161:GLY:HA3 | 2.14 | 0.47 |
| 26:BB:42:C:H4' | 30:BG:67:LYS:HD3 | 1.95 | 0.47 |
| 1:CA:1223:C:OP2 | 1:CA:1224:G:H2' | 2.15 | 0.47 |
| 1:AA:10:A:OP2 | 5:AH:126:ARG:HD3 | 2.15 | 0.47 |
| 47:DZ:86:SER:N | 47:DZ:87:PRO:HD3 | 2.29 | 0.47 |
| 35:BO:9:ASN:CB | 35:BO:10:PRO:CD | 2.82 | 0.47 |
| 25:DA:1055:G:N3 | 25:DA:1085:A:C2 | 2.82 | 0.47 |
| 2:CE:73:THR:HG23 | 2:CE:170:GLU:OE2 | 2.14 | 0.47 |
| 1:CA:1159:U:O2 | 1:CA:1181:G:C6 | 2.67 | 0.47 |
| 29:DF:25:PRO:CG | 29:DF:26:ALA:N | 2.78 | 0.47 |
| 1:AA:1499:A:O2' | 1:AA:1520:G:H5' | 2.15 | 0.47 |
| 25:DA:1047:G:C2' | 25:DA:1110:G:H22 | 2.26 | 0.47 |
| 25:BA:1142(A):A:H4' | 25:BA:1143:A:OP1 | 2.14 | 0.47 |
| 36:DP:77:LYS:C | 36:DP:79:LEU:H | 2.17 | 0.47 |
| 25:BA:1435:G:H21 | 25:BA:1478:G:H5' | 1.80 | 0.47 |
| 35:BO:50:ARG:HH21 | 35:BO:50:ARG:CB | 2.28 | 0.47 |
| 35:BO:50:ARG:NH2 | 35:BO:50:ARG:HB2 | 2.30 | 0.47 |
| 2:CE:154:LEU:HB3 | 2:CE:155:LEU:H | 1.53 | 0.47 |
| 26:DB:110:G:H2' | 26:DB:111:U:O4' | 2.14 | 0.47 |
| 23:CD:57:C:H42 | 25:DA:2112:G:N2 | 1.99 | 0.47 |
| 23:CD:44:A:N1 | 23:CD:45:A:N6 | 2.63 | 0.47 |
| 33:BM:96:GLU:N | 33:BM:98:VAL:HG12 | 2.29 | 0.47 |
| 23:AD:57:C:H5' | 25:BA:2169:A:O4' | 2.14 | 0.47 |
| 33:BM:95:PRO:O | 33:BM:96:GLU:CD | 2.53 | 0.47 |
| 2:CE:237:ALA:N | 2:CE:239:VAL:H | 2.12 | 0.47 |
| 25:BA:2894:G:C2' | 25:BA:2895:U:OP2 | 2.63 | 0.47 |
| 19:CV:23:ASN:HA | 19:CV:27:GLU:HG3 | 1.97 | 0.47 |
| 25:BA:2032:G:H1' | 28:BE:145:LYS:HD3 | 1.97 | 0.47 |
| 35:DO:9:ASN:O | 35:DO:10:PRO:O | 2.33 | 0.47 |
| 35:DO:39:LYS:HD2 | 35:DO:45:LEU:HD21 | 1.94 | 0.47 |
| 33:DM:13:TRP:O | 33:DM:135:PRO:HD2 | 2.15 | 0.47 |
| 25:DA:2523:G:H8 | 25:DA:2523:G:C5' | 2.27 | 0.47 |
| 9:CL:95:LYS:HZ2 | 9:CL:96:LEU:HA | 1.80 | 0.47 |
| 35:DO:97:PRO:O | 35:DO:98:GLU:HB3 | 2.15 | 0.47 |
| 3:AF:134:ILE:HG22 | 3:AF:168:ALA:HB3 | 1.97 | 0.47 |
| 25:BA:2473:U:C3' | 25:BA:2474:C:H5'' | 2.44 | 0.47 |
| 25:BA:1519:G:H2' | 25:BA:1520:U:H5' | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:1116:C:H42 | 1:CA:1184:G:H1 | 1.62 | 0.47 |
| 1:AA:501:C:H1' | 1:AA:549:C:H1' | 1.96 | 0.47 |
| 2:AE:72:GLY:HA3 | 2:AE:165:VAL:CG2 | 2.44 | 0.47 |
| 22:AB:19:G:H4' | 22:AB:20:U:OP2 | 2.15 | 0.47 |
| 37:D0:37:THR:HG22 | 37:D0:39:PRO:HD2 | 1.95 | 0.47 |
| 26:BB:37:C:C3' | 26:BB:38:C:H5' | 2.43 | 0.47 |
| 45:DV:28:MET:HE1 | 45:DV:67:LEU:HD13 | 1.97 | 0.47 |
| 1:AA:1346:A:C5' | 9:AL:120:ARG:HH12 | 2.27 | 0.47 |
| 4:CG:24:GLU:C | 4:CG:27:TYR:H | 2.18 | 0.47 |
| 45:BV:99:TYR:HD1 | 45:BV:123:ASP:HB3 | 1.79 | 0.47 |
| 22:CB:44:G:H2' | 22:CB:45:U:H5' | 1.96 | 0.47 |
| 27:DD:70:TRP:HZ3 | 27:DD:146:GLU:OE2 | 1.97 | 0.47 |
| 1:CA:353:A:H5' | 1:CA:353:A:C8 | 2.42 | 0.47 |
| 25:DA:147:U:C2' | 25:DA:148:C:H5'' | 2.42 | 0.47 |
| 1:CA:859:A:N7 | 1:CA:860:A:C5 | 2.83 | 0.47 |
| 25:BA:1047:G:O2' | 25:BA:1048:A:C8 | 2.66 | 0.47 |
| 16:CS:1:MET:CE | 16:CS:65:GLN:HG2 | 2.44 | 0.47 |
| 1:AA:410:G:H5'' | 1:AA:411:A:OP1 | 2.14 | 0.47 |
| 28:DE:66:HIS:CE1 | 28:DE:73:GLU:HG3 | 2.49 | 0.47 |
| 1:AA:1374:A:C2' | 1:AA:1375:A:H5' | 2.43 | 0.47 |
| 1:CA:1072:G:C5 | 1:CA:1073:U:C5 | 3.03 | 0.47 |
| 31:DH:9:ILE:HG22 | 31:DH:51:ARG:HA | 1.96 | 0.47 |
| 2:AE:223:ILE:HG13 | 2:AE:229:VAL:HG22 | 1.96 | 0.47 |
| 6:AI:9:VAL:HB | 6:AI:87:ARG:HB2 | 1.97 | 0.47 |
| 1:CA:652:U:C5 | 1:CA:752:G:C4 | 3.03 | 0.47 |
| 25:DA:2365:G:H4' | 46:D3:60:PHE:CZ | 2.50 | 0.47 |
| 1:AA:586:C:O2' | 1:AA:878:G:H4' | 2.14 | 0.47 |
| 25:BA:1192:G:H2' | 25:BA:1193:G:H5' | 1.96 | 0.47 |
| 5:CH:107:ARG:O | 5:CH:110:LEU:N | 2.48 | 0.47 |
| 1:AA:960:U:N3 | 1:AA:1225:A:C4 | 2.82 | 0.47 |
| 25:BA:2303:G:O2' | 25:BA:2304:G:H5' | 2.15 | 0.47 |
| 25:DA:2517:C:C6 | 25:DA:2542:A:N1 | 2.82 | 0.47 |
| 32:BK:73:GLU:HG3 | 32:BK:137:PRO:CG | 2.44 | 0.47 |
| 1:CA:583:A:H2' | 1:CA:584:G:O4' | 2.14 | 0.47 |
| 25:DA:2389:G:H5'' | 25:DA:2390:U:C5' | 2.44 | 0.47 |
| 25:BA:2098:U:C4 | 25:BA:2099:U:C5 | 3.03 | 0.47 |
| 1:AA:256:U:P | 17:AT:17:LYS:HZ1 | 2.38 | 0.47 |
| 1:CA:792:A:H1' | 1:CA:794:A:N7 | 2.30 | 0.47 |
| 41:B2:22:VAL:HG12 | 41:B2:23:GLU:N | 2.30 | 0.47 |
| 27:BD:12:SER:HB2 | 27:BD:207:GLY:O | 2.15 | 0.47 |
| 1:AA:33:A:H5'' | 1:AA:364:A:H1' | 1.96 | 0.47 |
| 23:AD:50:G:N2 | 23:AD:67:C:O2 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 17:AT:58:GLU:O | 17:AT:74:LEU:N | 2.33 | 0.47 |
| 25:DA:107:C:H2' | 25:DA:108:U:C6 | 2.49 | 0.47 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:H8 | 1.79 | 0.47 |
| 1:CA:1056:U:H5' | 3:CF:163:ALA:HB2 | 1.97 | 0.47 |
| 5:AH:41:VAL:HG11 | 5:AH:113:ALA:HB2 | 1.97 | 0.47 |
| 53:B7:10:ARG:NH1 | 53:B7:14:LYS:HE2 | 2.29 | 0.47 |
| 25:BA:1691:C:C2' | 25:BA:1692:U:H5' | 2.45 | 0.47 |
| 1:AA:939:G:C6 | 1:AA:940:C:N4 | 2.83 | 0.47 |
| 34:DN:98:VAL:HG11 | 34:DN:114:ILE:HG23 | 1.97 | 0.47 |
| 25:BA:172:C:H2' | 25:BA:173:G:H8 | 1.80 | 0.47 |
| 25:DA:1104:C:H2' | 25:DA:1105:U:C6 | 2.49 | 0.47 |
| 25:BA:2182:G:H2' | 25:BA:2183:C:C6 | 2.50 | 0.47 |
| 25:DA:696:G:H2' | 25:DA:697:C:H6 | 1.79 | 0.47 |
| 27:DD:71:ASP:CG | 27:DD:103:ARG:HH22 | 2.17 | 0.47 |
| 18:CU:19:LYS:HD3 | 18:CU:20:ALA:H | 1.78 | 0.47 |
| 21:AX:9:ARG:O | 21:AX:13:ILE:HG13 | 2.14 | 0.47 |
| 40:D1:17:ILE:HD12 | 40:D1:32:PHE:HE2 | 1.79 | 0.47 |
| 44:BU:21:LYS:HB3 | 44:BU:21:LYS:HE2 | 1.56 | 0.47 |
| 25:BA:1150:C:H2' | 25:BA:1151:G:O4' | 2.14 | 0.47 |
| 30:BG:56:ALA:HB2 | 30:BG:153:ARG:HE | 1.79 | 0.47 |
| 1:AA:936:C:H2' | 1:AA:937:A:O4' | 2.15 | 0.47 |
| 25:BA:1376:C:H2' | 25:BA:1377:G:O5' | 2.14 | 0.47 |
| 25:BA:2599:G:O2' | 25:BA:2600:A:H5' | 2.15 | 0.47 |
| 25:BA:53:A:H2' | 25:BA:54:G:O4' | 2.14 | 0.47 |
| 29:DF:111:ALA:HB2 | 29:DF:206:ILE:HG21 | 1.97 | 0.47 |
| 40:B1:38:THR:O | 40:B1:41:ALA:HB3 | 2.15 | 0.47 |
| 25:DA:1454:U:C5 | 25:DA:2702:U:O4 | 2.68 | 0.47 |
| 25:BA:488:G:H1' | 25:BA:492:A:N6 | 2.30 | 0.47 |
| 1:CA:109:A:C6 | 1:CA:326:G:C6 | 3.03 | 0.47 |
| 39:DR:11:GLU:OE1 | 39:DR:11:GLU:N | 2.48 | 0.47 |
| 40:B1:30:LYS:N | 40:B1:30:LYS:HD3 | 2.29 | 0.47 |
| 25:BA:600:G:N2 | 25:BA:605:C:O3' | 2.48 | 0.47 |
| 27:BD:74:GLY:O | 27:BD:76:PRO:HD3 | 2.15 | 0.47 |
| 25:BA:1056:G:N2 | 25:BA:1103:A:C5 | 2.82 | 0.47 |
| 25:BA:1057:A:C8 | 25:BA:1086:A:C4 | 3.03 | 0.47 |
| 25:DA:996:A:N3 | 25:DA:997:G:C8 | 2.83 | 0.47 |
| 25:DA:2059:A:H2 | 25:DA:2062:A:N6 | 2.13 | 0.47 |
| 41:D2:76:LYS:C | 41:D2:79:VAL:CG2 | 2.83 | 0.47 |
| 1:CA:545:C:H2' | 1:CA:546:G:H5' | 1.96 | 0.47 |
| 22:CB:18:G:O2' | 22:CB:19:G:O5' | 2.26 | 0.47 |
| 22:CB:21:A:H4' | 22:CB:22:G:OP1 | 2.15 | 0.47 |
| 1:AA:1004:A:N3 | 1:AA:1025:U:C2 | 2.83 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:1342:A:N1 | 25:DA:1397:U:C2 | 2.83 | 0.47 |
| 39:DR:24:PRO:HA | 39:DR:49:VAL:HG13 | 1.97 | 0.47 |
| 1:CA:1497:G:C2' | 1:CA:1498:U:C5' | 2.91 | 0.47 |
| 25:BA:1141:U:C6 | 33:BM:63:THR:OG1 | 2.55 | 0.47 |
| 1:CA:1127:G:C8 | 1:CA:1127:G:OP2 | 2.67 | 0.47 |
| 1:AA:266:G:N2 | 1:AA:269:C:C5 | 2.83 | 0.47 |
| 38:BQ:88:ASP:OD1 | 38:BQ:89:ARG:N | 2.48 | 0.47 |
| 25:BA:1496:A:C8 | 25:BA:1577:C:O2' | 2.51 | 0.47 |
| 31:BH:4:ILE:C | 31:BH:6:ARG:N | 2.69 | 0.47 |
| 25:DA:2794:C:H2' | 25:DA:2795:G:O4' | 2.15 | 0.47 |
| 1:CA:1297:C:H4' | 1:CA:1298:C:O5' | 2.15 | 0.47 |
| 5:CH:80:ILE:HG13 | 5:CH:80:ILE:O | 2.15 | 0.47 |
| 54:B8:34:TRP:O | 54:B8:35:GLN:OE1 | 2.32 | 0.47 |
| 30:BG:112:PRO:CB | 50:B4:37:SER:HB2 | 2.44 | 0.47 |
| 25:BA:973:A:H8 | 25:BA:973:A:OP1 | 1.98 | 0.47 |
| 1:AA:1500:A:OP2 | 1:AA:1505:G:OP1 | 2.33 | 0.47 |
| 25:BA:528:A:N1 | 25:BA:2043:C:H5' | 2.30 | 0.47 |
| 27:DD:70:TRP:O | 27:DD:73:VAL:CG2 | 2.63 | 0.47 |
| 25:BA:197:A:H62 | 25:BA:2430:A:H2' | 1.80 | 0.47 |
| 25:DA:323:G:H5' | 29:DF:169:ASN:HD21 | 1.79 | 0.47 |
| 1:AA:447:G:H2' | 1:AA:485:G:N2 | 2.30 | 0.47 |
| 25:BA:1799:G:C5' | 25:BA:1819:A:N6 | 2.78 | 0.47 |
| 35:BO:58:THR:CG2 | 35:BO:58:THR:O | 2.62 | 0.47 |
| 31:BH:20:ALA:HB3 | 31:BH:23:ARG:HD2 | 1.95 | 0.47 |
| 25:DA:872:A:C4 | 25:DA:906:G:C2 | 3.02 | 0.47 |
| 25:BA:754:C:H2' | 25:BA:755:C:H6 | 1.79 | 0.47 |
| 25:BA:822:U:C2' | 25:BA:823:G:H5' | 2.45 | 0.47 |
| 7:AJ:17:VAL:HB | 7:AJ:44:TYR:OH | 2.14 | 0.47 |
| 35:BO:106:LEU:O | 35:BO:107:LYS:HB2 | 2.13 | 0.47 |
| 25:DA:244:A:H2' | 25:DA:245:G:O4' | 2.15 | 0.47 |
| 25:DA:2836:U:H2' | 25:DA:2837:G:C8 | 2.50 | 0.47 |
| 25:BA:354:G:C2' | 25:BA:355:G:H5' | 2.45 | 0.47 |
| 1:AA:84:U:H6 | 1:AA:84:U:OP1 | 1.98 | 0.47 |
| 3:AF:12:LEU:O | 3:AF:14:ILE:N | 2.47 | 0.47 |
| 45:BV:1:MET:HE2 | 45:BV:135:GLU:HB3 | 1.96 | 0.47 |
| 10:AM:34:VAL:HG13 | 10:AM:74:ILE:HG23 | 1.96 | 0.47 |
| 4:CG:75:PHE:CE1 | 4:CG:93:PHE:HZ | 2.33 | 0.47 |
| 25:BA:2348:U:O4 | 25:BA:2382:G:C2 | 2.67 | 0.47 |
| 31:BH:67:LEU:O | 31:BH:71:LEU:HB2 | 2.15 | 0.47 |
| 25:BA:2876:G:H5' | 39:BR:2:ASN:HB3 | 1.96 | 0.47 |
| 2:CE:37:ASN:O | 2:CE:39:ILE:HG13 | 2.15 | 0.47 |
| 1:CA:1371:G:OP1 | 9:CL:11:LYS:HG2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:1758:G:C2 | 25:BA:2696:U:H5' | 2.50 | 0.47 |
| 44:BU:2:ARG:HG2 | 44:BU:3:VAL:HG23 | 1.97 | 0.47 |
| 1:CA:853:G:O2' | 1:CA:854:G:H5' | 2.15 | 0.47 |
| 41:D2:68:LYS:HA | 41:D2:68:LYS:HD3 | 1.69 | 0.47 |
| 25:BA:2238:G:N3 | 25:BA:2238:G:H2' | 2.29 | 0.47 |
| 7:CJ:85:TYR:CE1 | 7:CJ:154:TYR:CE1 | 3.03 | 0.47 |
| 16:CS:25:ARG:HG3 | 16:CS:25:ARG:HH11 | 1.80 | 0.47 |
| 11:AN:105:VAL:O | 11:AN:105:VAL:HG23 | 2.15 | 0.47 |
| 11:CN:26:ASN:O | 11:CN:27:ASN:HB2 | 2.15 | 0.47 |
| 42:DS:18:ARG:HG3 | 42:DS:76:VAL:HG13 | 1.97 | 0.47 |
| 34:DN:31:LYS:HB3 | 34:DN:32:TYR:CD1 | 2.50 | 0.47 |
| 25:BA:1056:G:O4' | 25:BA:1086:A:C8 | 2.65 | 0.47 |
| 38:BQ:106:ARG:CB | 38:BQ:110:LEU:HD21 | 2.44 | 0.47 |
| 54:D8:49:VAL:C | 54:D8:50:LEU:CG | 2.78 | 0.47 |
| 38:DQ:88:ASP:O | 38:DQ:89:ARG:CB | 2.48 | 0.47 |
| 25:DA:996:A:H4' | 40:D1:92:ARG:CZ | 2.45 | 0.47 |
| 27:BD:35:LYS:CE | 27:BD:65:ILE:HG22 | 2.45 | 0.47 |
| 27:BD:35:LYS:HA | 27:BD:64:ILE:CG2 | 2.41 | 0.47 |
| 25:BA:2415:G:O3' | 35:BO:66:GLY:CA | 2.59 | 0.47 |
| 45:DV:146:ILE:HG23 | 45:DV:147:GLY:N | 2.29 | 0.47 |
| 9:CL:114:TYR:C | 9:CL:116:LYS:H | 2.18 | 0.47 |
| 1:CA:545:C:C2' | 1:CA:546:G:H5' | 2.45 | 0.47 |
| 2:CE:166:ASP:CG | 2:CE:169:LYS:HB2 | 2.35 | 0.47 |
| 25:BA:994:C:H5'' | 25:BA:995:C:P | 2.55 | 0.47 |
| 36:DP:87:LYS:HG3 | 36:DP:88:GLY:N | 2.27 | 0.47 |
| 1:CA:1176:A:N6 | 1:CA:1177:G:N1 | 2.63 | 0.47 |
| 1:CA:1157:A:N6 | 1:CA:1178:G:N2 | 2.63 | 0.47 |
| 13:CP:15:VAL:O | 13:CP:19:LEU:HD23 | 2.15 | 0.47 |
| 23:CD:48:U:H2' | 23:CD:49:C:OP1 | 2.15 | 0.47 |
| 25:DA:1535:U:H5' | 25:DA:1536:A:OP2 | 2.15 | 0.47 |
| 1:CA:634:C:H3' | 1:CA:634:C:H6 | 1.79 | 0.47 |
| 30:DG:36:LYS:HG2 | 30:DG:38:VAL:HG23 | 1.96 | 0.47 |
| 25:DA:310:A:P | 44:DU:18:GLY:HA2 | 2.54 | 0.47 |
| 35:BO:50:ARG:HH21 | 35:BO:50:ARG:HB2 | 1.79 | 0.47 |
| 25:DA:857:C:H2' | 25:DA:858:U:H6 | 1.80 | 0.47 |
| 1:AA:1028(A):C:H2' | 1:AA:1028(B):C:H6 | 1.79 | 0.47 |
| 25:BA:10:G:C2 | 25:BA:2629:A:C2 | 3.03 | 0.47 |
| 28:BE:115:GLY:O | 28:BE:119:ARG:HB2 | 2.15 | 0.47 |
| 28:BE:111:ARG:CD | 28:BE:160:TYR:CE1 | 2.93 | 0.47 |
| 25:DA:990:A:H5' | 25:DA:990:A:C8 | 2.34 | 0.47 |
| 1:CA:1243:C:OP1 | 21:CX:8:THR:HG21 | 2.15 | 0.47 |
| 52:D6:51:GLU:HG2 | 52:D6:52:VAL:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 35:BO:100:LEU:HD23 | 35:BO:112:LEU:HD11 | 1.96 | 0.47 |
| 23:AC:1:C:O4' | 23:AC:1:C:P | 2.73 | 0.47 |
| 1:CA:1187:G:P | 9:CL:113:LYS:NZ | 2.87 | 0.47 |
| 8:CK:69:ARG:HD3 | 8:CK:75:ARG:O | 2.15 | 0.47 |
| 1:CA:1286:A:H2 | 21:CX:18:TYR:HH | 1.56 | 0.47 |
| 1:CA:1325:C:C4' | 21:CX:17:THR:HG21 | 2.43 | 0.47 |
| 45:BV:152:ALA:CB | 45:BV:167:PRO:O | 2.60 | 0.47 |
| 13:CP:110:ARG:HG2 | 13:CP:110:ARG:HH11 | 1.80 | 0.47 |
| 20:CW:49:ALA:HA | 20:CW:52:ALA:CB | 2.43 | 0.47 |
| 32:BK:21:VAL:HG22 | 32:BK:22:LYS:N | 2.30 | 0.47 |
| 53:B7:9:ARG:HH21 | 53:B7:48:LYS:HG3 | 1.79 | 0.47 |
| 9:AL:79:LEU:HD22 | 9:AL:83:ARG:CG | 2.45 | 0.47 |
| 1:CA:1352:C:H2' | 1:CA:1353:G:C8 | 2.49 | 0.47 |
| 25:BA:1079:C:N4 | 25:BA:1080:A:N6 | 2.63 | 0.47 |
| 39:BR:23:ARG:HG3 | 39:BR:120:ARG:NH1 | 2.30 | 0.47 |
| 28:DE:89:ASP:O | 28:DE:90:THR:C | 2.53 | 0.47 |
| 25:DA:581:C:C2 | 25:DA:582:G:C8 | 3.02 | 0.47 |
| 38:BQ:48:LEU:HD22 | 38:BQ:82:ILE:HD11 | 1.96 | 0.47 |
| 45:BV:142:SER:HB3 | 45:BV:143:GLY:CA | 2.45 | 0.47 |
| 1:AA:1234:C:O2' | 1:AA:1235:U:H5' | 2.15 | 0.47 |
| 1:CA:1194:U:H4' | 5:CH:22:GLY:O | 2.15 | 0.47 |
| 12:AO:89:ARG:HG3 | 12:AO:89:ARG:HH11 | 1.80 | 0.47 |
| 25:DA:881:G:C6 | 25:DA:895:U:O2 | 2.68 | 0.47 |
| 46:D3:48:GLY:HA3 | 46:D3:80:HIS:ND1 | 2.30 | 0.47 |
| 5:AH:39:GLY:HA2 | 5:AH:113:ALA:O | 2.15 | 0.47 |
| 26:DB:11:C:OP2 | 26:DB:12:C:H5 | 1.98 | 0.47 |
| 1:AA:939:G:H2' | 1:AA:940:C:H6 | 1.79 | 0.47 |
| 23:CC:51:U:H2' | 23:CC:52:C:H6 | 1.80 | 0.47 |
| 32:DK:5:LEU:HD12 | 32:DK:5:LEU:H | 1.79 | 0.47 |
| 23:AD:37:U:O4 | 23:AD:38:A:N6 | 2.48 | 0.47 |
| 45:BV:10:ARG:HD3 | 45:BV:18:LEU:CD2 | 2.44 | 0.47 |
| 25:DA:1174:A:C6 | 25:DA:1175:U:O2' | 2.68 | 0.47 |
| 25:BA:2243:U:H2' | 25:BA:2244:U:C6 | 2.50 | 0.47 |
| 14:AQ:12:ARG:C | 14:AQ:14:PRO:HD2 | 2.35 | 0.47 |
| 33:DM:10:GLU:HG3 | 33:DM:11:PRO:HD2 | 1.97 | 0.47 |
| 22:CB:67:C:O2 | 22:CB:67:C:H2' | 2.13 | 0.47 |
| 1:CA:589:C:H42 | 1:CA:650:G:H1 | 1.62 | 0.47 |
| 1:CA:784:C:H4' | 25:DA:1837:C:OP1 | 2.15 | 0.47 |
| 8:AK:94:TYR:HE1 | 8:AK:132:GLU:HB2 | 1.79 | 0.47 |
| 25:DA:85:G:P | 44:DU:30:VAL:HB | 2.55 | 0.47 |
| 25:DA:2289:G:H1' | 25:DA:2346:A:H2 | 1.80 | 0.47 |
| 25:DA:2895:U:H2' | 25:DA:2896:C:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:2308:G:H3' | 25:BA:2310:A:OP2 | 2.15 | 0.47 |
| 25:DA:993:G:H1' | 41:D2:87:HIS:CE1 | 2.49 | 0.47 |
| 27:BD:65:ILE:HG13 | 27:BD:67:PHE:CE1 | 2.50 | 0.47 |
| 28:DE:48:GLN:O | 28:DE:49:LEU:HD12 | 2.15 | 0.47 |
| 1:AA:1331:G:OP2 | 13:AP:23:TYR:CD2 | 2.68 | 0.47 |
| 2:AE:21:ARG:HB2 | 2:AE:39:ILE:N | 2.30 | 0.47 |
| 2:CE:166:ASP:OD2 | 2:CE:169:LYS:HB2 | 2.15 | 0.47 |
| 25:DA:1034:G:H2' | 25:DA:1035:U:O4' | 2.15 | 0.47 |
| 44:DU:94:LYS:O | 44:DU:101:LYS:HB2 | 2.14 | 0.47 |
| 3:CF:119:ARG:HA | 3:CF:122:GLU:OE2 | 2.15 | 0.47 |
| 25:DA:1042:G:H2' | 25:DA:1043:C:O4' | 2.15 | 0.47 |
| 25:DA:528:A:C2 | 25:DA:2042:A:H2' | 2.50 | 0.47 |
| 25:DA:2314:C:H5' | 30:DG:38:VAL:HG11 | 1.96 | 0.47 |
| 43:BT:24:GLY:HA3 | 43:BT:82:GLN:HE22 | 1.80 | 0.47 |
| 25:DA:2131:G:H22 | 25:DA:2158:A:H2' | 1.80 | 0.47 |
| 1:AA:1321:C:C3' | 1:AA:1322:C:H5'' | 2.37 | 0.47 |
| 5:CH:79:GLU:OE1 | 8:CK:104:ARG:HA | 2.15 | 0.47 |
| 16:CS:8:ARG:CG | 16:CS:8:ARG:NH1 | 2.58 | 0.47 |
| 13:CP:53:VAL:HG12 | 13:CP:57:ARG:HH21 | 1.80 | 0.47 |
| 2:CE:97:TRP:CE3 | 2:CE:98:LEU:O | 2.68 | 0.47 |
| 1:AA:1251:A:H2' | 1:AA:1252:A:C8 | 2.50 | 0.47 |
| 35:DO:101:VAL:HG21 | 35:DO:108:LYS:H | 1.80 | 0.47 |
| 49:DX:5:LYS:HE3 | 49:DX:59:VAL:HG21 | 1.97 | 0.47 |
| 25:BA:330:A:H2 | 25:BA:1210:A:C2' | 2.28 | 0.47 |
| 40:B1:69:CYS:SG | 40:B1:79:PHE:CD1 | 3.02 | 0.47 |
| 29:DF:125:LEU:HD12 | 29:DF:196:LEU:CD2 | 2.45 | 0.47 |
| 23:AD:53:G:C4 | 23:AD:64:G:N2 | 2.83 | 0.47 |
| 1:AA:129(A):G:H5' | 1:AA:191(A):G:H5' | 1.97 | 0.47 |
| 22:CB:44:G:C6 | 22:CB:45:U:C2 | 3.02 | 0.47 |
| 1:AA:727:G:N1 | 1:AA:731:G:C6 | 2.83 | 0.47 |
| 32:BK:29:TYR:C | 32:BK:32:PRO:HD2 | 2.35 | 0.47 |
| 10:CM:4:ILE:HD13 | 10:CM:100:THR:HG22 | 1.97 | 0.47 |
| 3:CF:50:ALA:O | 3:CF:70:VAL:HG13 | 2.15 | 0.47 |
| 1:CA:689:C:H2' | 1:CA:690:G:C5' | 2.45 | 0.47 |
| 1:AA:448:A:C4 | 1:AA:487:A:C2 | 3.03 | 0.47 |
| 8:AK:91:ARG:HB2 | 12:AO:7:ILE:HG21 | 1.97 | 0.47 |
| 44:DU:57:GLN:HB3 | 44:DU:58:GLY:H | 1.58 | 0.47 |
| 27:BD:70:TRP:O | 27:BD:73:VAL:HG23 | 2.15 | 0.47 |
| 25:BA:646:A:C2' | 25:BA:647:G:O5' | 2.63 | 0.47 |
| 23:AD:50:G:N2 | 23:AD:66:C:O2 | 2.47 | 0.47 |
| 18:CU:44:LEU:HD21 | 18:CU:79:LEU:HD13 | 1.97 | 0.47 |
| 1:AA:813:U:OP2 | 1:AA:813:U:H6 | 1.98 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 26:BB:7:G:H5' | 26:BB:7:G:H8 | 1.79 | 0.47 |
| 25:BA:1206:G:C6 | 25:BA:1207:C:C4 | 3.03 | 0.47 |
| 1:AA:959:A:C2 | 1:AA:1222:G:O4' | 2.68 | 0.47 |
| 1:CA:692:U:O2 | 1:CA:695:A:C8 | 2.67 | 0.47 |
| 33:DM:111:PRO:HA | 33:DM:114:ARG:NH1 | 2.30 | 0.47 |
| 1:CA:1118:C:H1' | 1:CA:1179:A:C4 | 2.50 | 0.47 |
| 25:DA:2076:U:O5' | 25:DA:2076:U:H6 | 1.97 | 0.47 |
| 38:BQ:41:ASP:OD2 | 38:BQ:44:LYS:HD2 | 2.15 | 0.47 |
| 1:AA:918:A:H2' | 1:AA:919:A:C8 | 2.50 | 0.47 |
| 25:BA:2027:G:C5 | 25:BA:2028:U:C5 | 3.02 | 0.47 |
| 25:BA:557:U:H2' | 25:BA:558:G:H8 | 1.80 | 0.47 |
| 35:DO:68:GLN:HG2 | 54:D8:12:LYS:HD3 | 1.97 | 0.47 |
| 25:BA:2620:C:OP1 | 28:BE:152:LYS:O | 2.33 | 0.47 |
| 25:BA:484:C:H2' | 25:BA:485:C:C6 | 2.50 | 0.47 |
| 30:DG:72:ARG:HD2 | 30:DG:85:GLY:O | 2.15 | 0.47 |
| 25:BA:2355:C:O2 | 46:B3:39:ARG:NH2 | 2.47 | 0.47 |
| 31:DH:25:LYS:HG3 | 31:DH:25:LYS:O | 2.15 | 0.47 |
| 4:AG:154:ASN:OD1 | 4:AG:154:ASN:N | 2.48 | 0.47 |
| 41:B2:32:THR:CG2 | 41:B2:58:VAL:HG13 | 2.45 | 0.47 |
| 30:BG:82:LEU:HA | 30:BG:86:MET:HE3 | 1.96 | 0.46 |
| 54:D8:30:ARG:HD2 | 54:D8:30:ARG:HA | 1.57 | 0.46 |
| 27:BD:35:LYS:HG2 | 27:BD:64:ILE:CG2 | 2.43 | 0.46 |
| 40:B1:60:LEU:HD13 | 40:B1:64:ARG:HD2 | 1.97 | 0.46 |
| 25:BA:2383:G:C2' | 25:BA:2384:G:H5' | 2.45 | 0.46 |
| 4:AG:65:ARG:HG2 | 4:AG:65:ARG:HH11 | 1.80 | 0.46 |
| 1:CA:1158:C:C4 | 1:CA:1160:G:N7 | 2.82 | 0.46 |
| 48:DW:10:LEU:O | 48:DW:14:ARG:N | 2.36 | 0.46 |
| 1:AA:1058:G:C6 | 1:AA:1059:C:N3 | 2.83 | 0.46 |
| 1:CA:253:U:H2' | 1:CA:254:G:C8 | 2.49 | 0.46 |
| 1:AA:875:C:C4 | 1:AA:876:G:N7 | 2.83 | 0.46 |
| 25:DA:889:C:H2' | 25:DA:890:A:H4' | 1.96 | 0.46 |
| 45:BV:27:VAL:HG22 | 45:BV:28:MET:N | 2.30 | 0.46 |
| 54:B8:52:LYS:H | 54:B8:53:PRO:CD | 2.28 | 0.46 |
| 46:B3:27:GLU:CG | 46:B3:68:GLU:HA | 2.41 | 0.46 |
| 50:D4:56:VAL:CA | 50:D4:60:GLN:HE21 | 2.24 | 0.46 |
| 33:BM:18:ALA:HA | 33:BM:21:LYS:HG3 | 1.97 | 0.46 |
| 30:DG:109:VAL:HG13 | 50:D4:33:VAL:HG11 | 1.96 | 0.46 |
| 1:CA:686:U:O4 | 1:CA:703:G:H1' | 2.15 | 0.46 |
| 28:BE:179:GLU:O | 28:BE:180:ASN:HB2 | 2.14 | 0.46 |
| 43:DT:54:VAL:O | 43:DT:55:ASN:ND2 | 2.36 | 0.46 |
| 25:DA:2335:A:C8 | 25:DA:2337:G:N7 | 2.83 | 0.46 |
| 25:BA:671:C:O2' | 25:BA:672:C:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:1299:G:C5 | 25:BA:1639:U:C5 | 3.03 | 0.46 |
| 1:AA:954:G:C2 | 1:AA:955:U:C2 | 3.03 | 0.46 |
| 25:DA:2552:U:H2' | 25:DA:2554:U:H5'' | 1.97 | 0.46 |
| 41:B2:35:LEU:C | 41:B2:37:VAL:H | 2.16 | 0.46 |
| 8:CK:4:ASP:OD2 | 8:CK:7:ALA:HB2 | 2.15 | 0.46 |
| 31:BH:115:VAL:O | 31:BH:115:VAL:CG1 | 2.59 | 0.46 |
| 3:CF:63:ASN:CB | 3:CF:98:ASN:HB3 | 2.42 | 0.46 |
| 7:CJ:76:ARG:NH1 | 7:CJ:76:ARG:HG2 | 2.27 | 0.46 |
| 1:AA:618:C:H3' | 1:AA:619:U:C5' | 2.45 | 0.46 |
| 35:BO:55:ARG:O | 35:BO:55:ARG:HG3 | 2.14 | 0.46 |
| 1:CA:1207:G:C5 | 1:CA:1208:C:C5 | 3.03 | 0.46 |
| 1:AA:160:A:C6 | 1:AA:161:A:C2 | 3.03 | 0.46 |
| 1:AA:720:C:N4 | 1:AA:721:G:C2 | 2.82 | 0.46 |
| 25:DA:2187:G:C6 | 25:DA:2188:C:N3 | 2.83 | 0.46 |
| 5:CH:110:LEU:HA | 5:CH:110:LEU:HD23 | 1.74 | 0.46 |
| 25:DA:296:C:C2' | 25:DA:297:C:H5' | 2.45 | 0.46 |
| 1:CA:468:A:C2' | 1:CA:474:G:H5' | 2.44 | 0.46 |
| 33:DM:67:LEU:O | 33:DM:88:GLU:HG3 | 2.14 | 0.46 |
| 32:BK:110:ASP:HB3 | 32:BK:112:LYS:N | 2.30 | 0.46 |
| 18:AU:26:LEU:HD13 | 18:AU:39:VAL:HG13 | 1.96 | 0.46 |
| 30:BG:94:LEU:N | 30:BG:94:LEU:HD23 | 2.29 | 0.46 |
| 25:BA:991:C:H2' | 25:BA:992:C:H6 | 1.81 | 0.46 |
| 25:DA:1473:G:H2' | 25:DA:1474:C:O4' | 2.16 | 0.46 |
| 48:BW:24:LEU:HD13 | 48:BW:60:LEU:CD1 | 2.46 | 0.46 |
| 1:AA:928:G:C2 | 1:AA:1390:U:O2 | 2.68 | 0.46 |
| 25:BA:705:A:H2' | 25:BA:706:A:O4' | 2.15 | 0.46 |
| 44:BU:63:LYS:HD2 | 44:BU:64:GLU:H | 1.80 | 0.46 |
| 1:CA:358:U:C4 | 1:CA:359:U:C5 | 3.03 | 0.46 |
| 38:DQ:67:ARG:NH1 | 38:DQ:67:ARG:HB2 | 2.30 | 0.46 |
| 4:AG:23:GLY:HA2 | 4:AG:112:VAL:HG22 | 1.97 | 0.46 |
| 22:AB:2:C:H2' | 22:AB:3:C:C6 | 2.50 | 0.46 |
| 38:DQ:29:PHE:CD2 | 38:DQ:30:ARG:N | 2.83 | 0.46 |
| 27:DD:176:ARG:HA | 27:DD:181:GLU:O | 2.15 | 0.46 |
| 31:DH:71:LEU:HD12 | 31:DH:71:LEU:HA | 1.81 | 0.46 |
| 35:DO:107:LYS:O | 35:DO:109:GLY:N | 2.46 | 0.46 |
| 1:CA:547:A:H4' | 1:CA:548:G:O5' | 2.15 | 0.46 |
| 8:AK:8:ASP:O | 8:AK:12:ARG:HG3 | 2.15 | 0.46 |
| 27:DD:130:ALA:C | 27:DD:131:LEU:HD12 | 2.35 | 0.46 |
| 51:D5:57:VAL:HG12 | 51:D5:58:LEU:O | 2.14 | 0.46 |
| 18:CU:43:PHE:O | 18:CU:51:LEU:HD12 | 2.15 | 0.46 |
| 25:BA:498:G:C6 | 25:BA:499:U:C4 | 3.03 | 0.46 |
| 25:DA:2773:C:H5'' | 28:DE:164:ARG:HG2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 9:AL:89:ASN:N | 9:AL:89:ASN:OD1 | 2.47 | 0.46 |
| 29:BF:33:LEU:HA | 29:BF:33:LEU:HD12 | 1.76 | 0.46 |
| 19:CV:74:PHE:CD2 | 19:CV:74:PHE:N | 2.83 | 0.46 |
| 25:BA:1065:U:C5 | 25:BA:1066:U:C6 | 3.00 | 0.46 |
| 16:AS:22:THR:OG1 | 16:AS:31:LYS:O | 2.33 | 0.46 |
| 44:BU:78:ALA:CB | 44:BU:81:LYS:HZ1 | 2.22 | 0.46 |
| 13:AP:10:PRO:HB2 | 13:AP:18:ALA:HB1 | 1.97 | 0.46 |
| 1:CA:544:G:C6 | 1:CA:545:C:C4 | 3.03 | 0.46 |
| 4:CG:31:CYS:HB3 | 4:CG:33:MET:HB2 | 1.97 | 0.46 |
| 19:AV:40:ILE:HG12 | 19:AV:41:VAL:CG1 | 2.42 | 0.46 |
| 25:DA:1056:G:H5'' | 25:DA:1057:A:C5' | 2.43 | 0.46 |
| 25:DA:883:G:C6 | 25:DA:884:C:N4 | 2.83 | 0.46 |
| 29:BF:29:ASN:CB | 29:BF:112:MET:HE1 | 2.45 | 0.46 |
| 54:B8:36:LYS:HB2 | 54:B8:40:GLU:CB | 2.45 | 0.46 |
| 26:DB:45:A:H1' | 30:DG:95:ARG:CZ | 2.44 | 0.46 |
| 25:BA:2439:A:H3' | 25:BA:2439:A:P | 2.55 | 0.46 |
| 26:BB:28:C:O2' | 26:BB:29:A:H5' | 2.14 | 0.46 |
| 7:CJ:16:LEU:CD1 | 9:CL:45:ALA:HB2 | 2.37 | 0.46 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:C5' | 2.45 | 0.46 |
| 1:CA:1300:G:HO2' | 1:CA:1301:U:P | 2.35 | 0.46 |
| 25:BA:2171:A:H2' | 25:BA:2172:U:C6 | 2.45 | 0.46 |
| 25:DA:675:A:N6 | 25:DA:676:A:N6 | 2.64 | 0.46 |
| 25:BA:1140:C:OP1 | 33:BM:23:LEU:HB3 | 2.15 | 0.46 |
| 25:BA:574:C:N3 | 28:BE:145:LYS:NZ | 2.45 | 0.46 |
| 2:CE:144:ARG:CD | 2:CE:148:TYR:HE2 | 2.27 | 0.46 |
| 29:DF:136:THR:HG23 | 29:DF:166:ALA:O | 2.15 | 0.46 |
| 35:DO:106:LEU:HD13 | 35:DO:112:LEU:HD23 | 1.97 | 0.46 |
| 1:CA:152:A:N6 | 1:CA:170:U:C2 | 2.84 | 0.46 |
| 25:BA:1188:U:C5' | 41:B2:79:VAL:HG22 | 2.45 | 0.46 |
| 25:BA:819:A:C4 | 25:BA:1189:A:C2 | 3.03 | 0.46 |
| 40:B1:76:TYR:CZ | 40:B1:80:ILE:HG13 | 2.51 | 0.46 |
| 9:AL:17:VAL:CG1 | 9:AL:81:ILE:HD13 | 2.44 | 0.46 |
| 25:BA:654(R):C:C2' | 25:BA:654(S):G:H5' | 2.46 | 0.46 |
| 21:CX:6:ARG:CD | 21:CX:15:ARG:HH21 | 2.29 | 0.46 |
| 42:BS:14:PRO:CB | 42:BS:18:ARG:HH21 | 2.27 | 0.46 |
| 4:AG:138:TYR:HD2 | 4:AG:139:ARG:H | 1.61 | 0.46 |
| 32:DK:100:ALA:O | 32:DK:104:GLN:HB3 | 2.14 | 0.46 |
| 25:BA:612:G:N2 | 25:BA:616:A:O2' | 2.48 | 0.46 |
| 4:AG:25:ARG:O | 4:AG:28:SER:N | 2.43 | 0.46 |
| 14:CQ:29:ARG:HE | 14:CQ:40:CYS:HB2 | 1.80 | 0.46 |
| 25:BA:2330:G:H2' | 25:BA:2331:G:O4' | 2.15 | 0.46 |
| 1:CA:1289:A:P | 21:CX:9:ARG:HH22 | 2.38 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 20:CW:26:ASN:HB3 | 20:CW:71:THR:OG1 | 2.15 | 0.46 |
| 1:CA:77:C:N4 | 1:CA:92:G:H1 | 2.12 | 0.46 |
| 45:DV:114:GLY:C | 45:DV:116:VAL:N | 2.68 | 0.46 |
| 10:CM:99:LYS:CE | 10:CM:100:THR:H | 2.27 | 0.46 |
| 25:BA:2850:A:C2 | 25:BA:2851:A:C4 | 3.04 | 0.46 |
| 1:AA:299:G:H2' | 1:AA:300:A:C8 | 2.50 | 0.46 |
| 25:DA:2846:G:H2' | 25:DA:2847:U:C6 | 2.50 | 0.46 |
| 11:CN:59:TYR:CZ | 11:CN:63:LEU:HD21 | 2.50 | 0.46 |
| 25:DA:1688:U:H1' | 25:DA:1701:A:C6 | 2.49 | 0.46 |
| 14:CQ:7:ILE:HG22 | 14:CQ:23:ARG:CD | 2.46 | 0.46 |
| 45:BV:117:LEU:HD13 | 45:BV:118:GLN:H | 1.80 | 0.46 |
| 43:DT:26:TYR:OH | 43:DT:88:LYS:HB2 | 2.15 | 0.46 |
| 25:BA:1162:G:O4' | 41:B2:23:GLU:HG3 | 2.15 | 0.46 |
| 28:DE:120:TRP:CD2 | 28:DE:155:LYS:HD3 | 2.50 | 0.46 |
| 1:AA:342:C:N3 | 1:AA:348:G:C2 | 2.83 | 0.46 |
| 25:DA:1638:C:H5'' | 25:DA:2710:C:O2' | 2.16 | 0.46 |
| 24:C1:15:U:H2' | 24:C1:16:A:C8 | 2.51 | 0.46 |
| 12:AO:89:ARG:HG3 | 12:AO:89:ARG:NH1 | 2.30 | 0.46 |
| 37:D0:84:ALA:N | 37:D0:85:PRO:CD | 2.78 | 0.46 |
| 45:BV:10:ARG:HD3 | 45:BV:18:LEU:HD22 | 1.97 | 0.46 |
| 25:DA:1163:G:H2' | 25:DA:1164:G:H8 | 1.81 | 0.46 |
| 17:AT:100:LYS:O | 17:AT:101:ARG:HB2 | 2.14 | 0.46 |
| 20:AW:21:LYS:O | 20:AW:25:ARG:HB2 | 2.16 | 0.46 |
| 26:DB:24:G:H4' | 26:DB:25:A:C8 | 2.50 | 0.46 |
| 8:AK:42:GLU:HG3 | 8:AK:109:ILE:HD12 | 1.97 | 0.46 |
| 25:BA:1324:G:C4 | 25:BA:1328:G:O6 | 2.69 | 0.46 |
| 25:DA:830:G:H4' | 25:DA:831:G:OP2 | 2.15 | 0.46 |
| 25:DA:1007:C:OP1 | 33:DM:37:LYS:NZ | 2.45 | 0.46 |
| 39:BR:94:ALA:O | 39:BR:95:ARG:CB | 2.63 | 0.46 |
| 25:DA:1578:U:O2 | 25:DA:1578:U:H2' | 2.15 | 0.46 |
| 27:DD:145:VAL:HG11 | 27:DD:175:LEU:HD11 | 1.98 | 0.46 |
| 25:BA:1344:G:H4' | 25:BA:1384:A:C5 | 2.49 | 0.46 |
| 27:DD:30:GLU:HG3 | 27:DD:63:ARG:CZ | 2.45 | 0.46 |
| 27:BD:77:ALA:HB1 | 27:BD:96:HIS:O | 2.15 | 0.46 |
| 16:AS:20:VAL:CG2 | 16:AS:32:TYR:CB | 2.93 | 0.46 |
| 28:BE:59:VAL:CG1 | 28:BE:63:LEU:CB | 2.94 | 0.46 |
| 23:CC:20:G:HO2' | 23:CC:21:U:H6 | 1.63 | 0.46 |
| 31:DH:109:PHE:CZ | 31:DH:152:ARG:HD3 | 2.50 | 0.46 |
| 44:BU:76:CYS:CB | 44:BU:77:PRO:HD3 | 2.45 | 0.46 |
| 1:CA:1060:C:O2' | 1:CA:1061:G:H5' | 2.15 | 0.46 |
| 1:AA:1003:G:N2 | 1:AA:1004:A:O2' | 2.48 | 0.46 |
| 22:CB:37:G:C4 | 22:CB:38:G:C8 | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:2507:C:H2' | 25:DA:2508:G:O4' | 2.15 | 0.46 |
| 13:CP:29:ARG:HB3 | 13:CP:64:TRP:CZ2 | 2.50 | 0.46 |
| 25:DA:529:A:C2' | 25:DA:529:A:N3 | 2.79 | 0.46 |
| 25:DA:2312:U:O2' | 25:DA:2313:C:H5' | 2.16 | 0.46 |
| 26:DB:43:C:H4' | 30:DG:66:GLN:NE2 | 2.30 | 0.46 |
| 30:DG:86:MET:O | 30:DG:88:ILE:HG22 | 2.14 | 0.46 |
| 25:BA:1478:G:O2' | 25:BA:1558:A:C2 | 2.68 | 0.46 |
| 25:BA:1480:G:C6 | 25:BA:1482:U:N3 | 2.83 | 0.46 |
| 1:AA:872:A:N3 | 1:AA:872:A:H2' | 2.30 | 0.46 |
| 4:AG:114:ARG:HG3 | 4:AG:114:ARG:NH1 | 2.31 | 0.46 |
| 29:DF:122:LYS:HG3 | 29:DF:191:ARG:HG2 | 1.97 | 0.46 |
| 3:AF:150:LYS:HE3 | 3:AF:152:ILE:HD11 | 1.98 | 0.46 |
| 1:AA:475:G:H2' | 1:AA:476:G:H8 | 1.80 | 0.46 |
| 1:AA:1317:C:H5'' | 1:AA:1318:A:OP2 | 2.16 | 0.46 |
| 1:CA:410:G:OP2 | 4:CG:25:ARG:HB2 | 2.16 | 0.46 |
| 25:DA:2212:A:H1' | 25:DA:2215:G:C4 | 2.50 | 0.46 |
| 42:BS:18:ARG:CG | 42:BS:76:VAL:HG13 | 2.45 | 0.46 |
| 25:DA:148:C:C5' | 25:DA:148:C:C6 | 2.91 | 0.46 |
| 25:DA:2611:U:H5' | 25:DA:2611:U:C6 | 2.44 | 0.46 |
| 44:BU:42:VAL:HB | 44:BU:67:LEU:HD11 | 1.96 | 0.46 |
| 31:DH:169:VAL:O | 31:DH:170:ARG:HG2 | 2.16 | 0.46 |
| 14:CQ:37:PHE:CZ | 14:CQ:56:VAL:HG21 | 2.48 | 0.46 |
| 45:DV:130:PRO:HA | 45:DV:133:ILE:HD11 | 1.96 | 0.46 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:O4' | 2.15 | 0.46 |
| 37:D0:107:ASP:OD2 | 37:D0:107:ASP:C | 2.53 | 0.46 |
| 32:BK:29:TYR:CD2 | 32:BK:30:LEU:HD23 | 2.50 | 0.46 |
| 50:B4:12:ALA:HB2 | 50:B4:29:PRO:HA | 1.97 | 0.46 |
| 30:BG:39:ILE:HG13 | 30:BG:94:LEU:HD21 | 1.96 | 0.46 |
| 1:CA:641:U:O3' | 1:CA:642:A:H8 | 1.98 | 0.46 |
| 1:AA:1086:U:O2' | 1:AA:1087:G:H5' | 2.14 | 0.46 |
| 25:DA:1146:C:O2' | 25:DA:1147:C:H5' | 2.15 | 0.46 |
| 8:AK:53:VAL:HB | 8:AK:58:TYR:CE1 | 2.50 | 0.46 |
| 25:BA:1429:G:H2' | 25:BA:1430:C:C6 | 2.50 | 0.46 |
| 25:DA:1668:A:C8 | 25:DA:1674:G:C6 | 3.03 | 0.46 |
| 25:DA:592:G:O2' | 54:D8:4:MET:HB2 | 2.16 | 0.46 |
| 12:AO:47:LYS:CA | 12:AO:49:ASN:H | 2.28 | 0.46 |
| 2:CE:24:TRP:O | 2:CE:24:TRP:CD1 | 2.69 | 0.46 |
| 25:BA:27:G:N2 | 25:BA:512:G:H1' | 2.29 | 0.46 |
| 9:AL:22:GLY:HA3 | 9:AL:60:ASP:OD2 | 2.15 | 0.46 |
| 1:CA:763:G:H2' | 1:CA:764:C:C6 | 2.51 | 0.46 |
| 49:BX:59:VAL:HG22 | 49:BX:60:GLU:H | 1.80 | 0.46 |
| 41:D2:21:ARG:HG3 | 41:D2:21:ARG:HH11 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:1291:G:O2' | 1:AA:1292:U:H5' | 2.15 | 0.46 |
| 1:CA:275:G:H5' | 17:CT:14:LYS:HB3 | 1.97 | 0.46 |
| 15:AR:78:TYR:O | 15:AR:79:ARG:C | 2.54 | 0.46 |
| 25:DA:1479:G:N2 | 25:DA:1480:G:H1' | 2.30 | 0.46 |
| 25:BA:1847:A:H4' | 25:BA:1848:A:OP2 | 2.16 | 0.46 |
| 1:CA:833:U:H2' | 1:CA:834:C:H6 | 1.80 | 0.46 |
| 25:BA:851:U:H5' | 49:BX:46:ASN:ND2 | 2.31 | 0.46 |
| 1:CA:683:G:H2' | 1:CA:684:A:O4' | 2.15 | 0.46 |
| 45:DV:13:GLU:HA | 45:DV:14:LYS:HZ3 | 1.79 | 0.46 |
| 4:AG:58:LEU:O | 4:AG:58:LEU:HD22 | 2.15 | 0.46 |
| 45:BV:122:ARG:HE | 45:BV:122:ARG:HB2 | 1.60 | 0.46 |
| 25:DA:2167:U:H6 | 25:DA:2167:U:P | 2.38 | 0.46 |
| 23:CC:68:C:H2' | 23:CC:69:C:C6 | 2.50 | 0.46 |
| 25:BA:1071:G:O6 | 25:BA:1091:G:O6 | 2.34 | 0.46 |
| 25:DA:2287:A:N1 | 25:DA:2346:A:H2 | 2.10 | 0.46 |
| 25:DA:847:U:O4 | 25:DA:933:A:N1 | 2.49 | 0.46 |
| 27:DD:32:SER:HA | 27:DD:36:PRO:HD2 | 1.98 | 0.46 |
| 30:BG:80:PHE:O | 30:BG:81:LYS:C | 2.54 | 0.46 |
| 29:DF:67:GLN:O | 29:DF:68:LYS:HB2 | 2.14 | 0.46 |
| 50:B4:6:HIS:HD1 | 50:B4:7:PRO:HD2 | 1.81 | 0.46 |
| 1:AA:1305:G:OP2 | 1:AA:1305:G:H8 | 1.98 | 0.46 |
| 1:CA:1053:G:C5 | 1:CA:1199:U:C6 | 3.02 | 0.46 |
| 1:CA:963:G:O2' | 10:CM:54:PHE:HZ | 1.95 | 0.46 |
| 4:CG:30:LYS:H | 4:CG:30:LYS:HE2 | 1.80 | 0.46 |
| 22:CB:17:U:C5' | 22:CB:18:G:C8 | 2.96 | 0.46 |
| 11:AN:17:GLY:O | 11:AN:80:VAL:HA | 2.15 | 0.46 |
| 2:CE:165:VAL:HG23 | 2:CE:166:ASP:H | 1.80 | 0.46 |
| 25:BA:654(L):G:H2' | 25:BA:654(M):C:O4' | 2.15 | 0.46 |
| 25:BA:676:A:N1 | 25:BA:802:A:N1 | 2.63 | 0.46 |
| 1:CA:1124:G:O2' | 1:CA:1145:C:C4 | 2.62 | 0.46 |
| 1:CA:1147:C:O2 | 9:CL:16:ARG:NE | 2.49 | 0.46 |
| 17:AT:70:ARG:C | 17:AT:71:PHE:HD2 | 2.18 | 0.46 |
| 25:DA:547:A:C5 | 25:DA:548:A:N6 | 2.83 | 0.46 |
| 25:DA:2303:G:C2 | 25:DA:2314:C:N3 | 2.84 | 0.46 |
| 30:DG:102:PHE:CE2 | 30:DG:141:PHE:CE1 | 3.00 | 0.46 |
| 25:BA:507:A:H5'' | 25:BA:508:G:H5' | 1.98 | 0.46 |
| 32:BK:77:LEU:HD12 | 32:BK:140:LEU:HB2 | 1.97 | 0.46 |
| 25:DA:2116:G:P | 25:DA:2165:G:H22 | 2.38 | 0.46 |
| 26:BB:31:C:C2' | 26:BB:32:C:H5' | 2.45 | 0.46 |
| 1:AA:397:A:C6 | 1:AA:548:G:N7 | 2.83 | 0.46 |
| 28:BE:181:LEU:HD11 | 39:BR:7:ILE:HD13 | 1.97 | 0.46 |
| 45:DV:131:ARG:N | 45:DV:131:ARG:HD2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:BA:1332:G:N2 | 25:BA:1609:A:HO2' | 2.10 | 0.46 |
| 13:AP:44:ARG:N | 13:AP:44:ARG:HD3 | 2.31 | 0.46 |
| 27:DD:17:THR:O | 27:DD:211:ARG:NH2 | 2.49 | 0.46 |
| 25:BA:1406:U:H2' | 25:BA:1407:C:C6 | 2.50 | 0.46 |
| 25:BA:900:A:N3 | 25:BA:900:A:H2' | 2.30 | 0.46 |
| 25:DA:1486:A:C4 | 25:DA:1487:G:C8 | 3.04 | 0.46 |
| 45:DV:24:LEU:C | 45:DV:24:LEU:HD12 | 2.35 | 0.46 |
| 1:AA:1169:A:N6 | 1:AA:1170:A:N1 | 2.63 | 0.46 |
| 12:AO:24:VAL:HG11 | 12:AO:27:LEU:CD1 | 2.45 | 0.46 |
| 21:CX:3:LYS:O | 21:CX:14:TRP:CE3 | 2.69 | 0.46 |
| 25:BA:953:A:O2' | 25:BA:2266:A:OP2 | 2.26 | 0.46 |
| 22:AB:42:U:H3' | 22:AB:43:A:C8 | 2.50 | 0.46 |
| 11:AN:81:ASP:O | 11:AN:82:VAL:C | 2.53 | 0.46 |
| 10:CM:13:HIS:CD2 | 10:CM:13:HIS:C | 2.88 | 0.46 |
| 45:BV:109:ALA:HB1 | 45:BV:144:LEU:HB2 | 1.96 | 0.46 |
| 25:DA:218:A:C2 | 25:DA:235:U:H4' | 2.50 | 0.46 |
| 25:BA:633:A:H2' | 25:BA:634:C:H5' | 1.98 | 0.46 |
| 1:AA:929:G:N2 | 1:AA:1389:C:C2 | 2.84 | 0.46 |
| 45:BV:132:ASN:ND2 | 45:BV:132:ASN:N | 2.62 | 0.46 |
| 34:BN:35:VAL:CG2 | 34:BN:69:ILE:HG12 | 2.45 | 0.46 |
| 1:CA:1363:A:H1' | 1:CA:1365:G:N7 | 2.31 | 0.46 |
| 1:AA:328:C:O2 | 1:AA:328:C:H2' | 2.15 | 0.46 |
| 8:CK:29:SER:HB3 | 8:CK:32:LYS:CG | 2.45 | 0.46 |
| 3:AF:69:HIS:CD2 | 3:AF:69:HIS:N | 2.83 | 0.46 |
| 5:CH:63:ARG:HA | 5:CH:66:MET:HE2 | 1.96 | 0.46 |
| 20:CW:54:LYS:HA | 20:CW:57:ARG:NH2 | 2.31 | 0.46 |
| 25:BA:2860:A:N7 | 25:BA:2861:G:H1' | 2.30 | 0.46 |
| 25:DA:2729:G:H1' | 28:DE:187:ALA:HB3 | 1.98 | 0.46 |
| 25:BA:2695:C:H2' | 25:BA:2696:U:C6 | 2.51 | 0.46 |
| 25:BA:850:C:H5'' | 49:BX:18:ASP:HB2 | 1.96 | 0.46 |
| 1:CA:437:U:C5' | 4:CG:155:LEU:HD21 | 2.46 | 0.46 |
| 50:D4:36:CYS:HB3 | 50:D4:41:PRO:CD | 2.45 | 0.46 |
| 25:DA:2180:U:H2' | 25:DA:2181:G:O4' | 2.15 | 0.46 |
| 42:BS:24:ILE:HG21 | 42:BS:36:LEU:HD21 | 1.96 | 0.46 |
| 35:BO:34:GLY:O | 35:BO:35:HIS:HB2 | 2.14 | 0.46 |
| 25:BA:1655:A:H3' | 25:BA:1656:C:C6 | 2.50 | 0.46 |
| 25:DA:2567:G:H2' | 25:DA:2568:C:C6 | 2.49 | 0.46 |
| 25:BA:224:G:C6 | 25:BA:225:A:C5 | 3.02 | 0.46 |
| 27:BD:183:ARG:HG2 | 27:BD:269:PHE:O | 2.16 | 0.46 |
| 25:DA:553:U:C4 | 25:DA:554:U:C4 | 3.04 | 0.46 |
| 40:B1:13:LYS:H | 40:B1:13:LYS:HG2 | 1.61 | 0.46 |
| 40:B1:13:LYS:HE3 | 40:B1:13:LYS:HB3 | 1.72 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:492:A:C2' | 25:DA:493:G:H5' | 2.45 | 0.46 |
| 25:DA:829:A:N7 | 25:DA:2248:C:H5' | 2.31 | 0.46 |
| 47:BZ:87:PRO:O | 47:BZ:90:ILE:N | 2.48 | 0.46 |
| 52:D6:10:LEU:C | 52:D6:11:LEU:HD22 | 2.36 | 0.46 |
| 25:DA:2360:A:OP1 | 54:D8:50:LEU:HA | 2.15 | 0.46 |
| 33:DM:4:TYR:O | 40:D1:64:ARG:NH1 | 2.46 | 0.46 |
| 13:AP:23:TYR:HD1 | 13:AP:67:GLU:HA | 1.80 | 0.46 |
| 36:DP:31:ASP:O | 36:DP:133:ARG:O | 2.33 | 0.46 |
| 25:BA:880:G:C6 | 25:BA:881:G:N7 | 2.84 | 0.46 |
| 10:AM:55:LYS:O | 10:AM:56:HIS:CD2 | 2.68 | 0.46 |
| 9:AL:111:ARG:HH22 | 10:AM:62:HIS:CE1 | 2.32 | 0.46 |
| 14:AQ:21:TYR:CE2 | 14:AQ:23:ARG:NE | 2.80 | 0.46 |
| 25:BA:1797:C:H2' | 25:BA:1798:U:H5' | 1.96 | 0.46 |
| 25:BA:1803:A:O3' | 27:BD:259:THR:HG23 | 2.15 | 0.46 |
| 1:AA:267:C:OP1 | 17:AT:67:LYS:HB2 | 2.15 | 0.46 |
| 1:CA:265:G:O3' | 17:CT:66:SER:HA | 2.16 | 0.46 |
| 2:AE:204:ASN:HD22 | 2:AE:204:ASN:C | 2.18 | 0.46 |
| 29:DF:31:HIS:ND1 | 35:DO:9:ASN:OD1 | 2.47 | 0.46 |
| 25:BA:1313:U:H2' | 25:BA:1610:A:C2 | 2.50 | 0.46 |
| 49:DX:59:VAL:CG1 | 49:DX:60:GLU:H | 2.21 | 0.46 |
| 25:DA:910:A:N7 | 36:DP:12:GLN:HB2 | 2.30 | 0.46 |
| 39:BR:90:GLN:HE21 | 39:BR:116:ALA:HA | 1.81 | 0.46 |
| 25:DA:2337:G:N3 | 25:DA:2337:G:H2' | 2.31 | 0.46 |
| 4:AG:209:ARG:NE | 4:AG:209:ARG:HA | 2.31 | 0.46 |
| 5:CH:147:ASP:O | 5:CH:151:LEU:HG | 2.15 | 0.46 |
| 8:CK:4:ASP:HB2 | 8:CK:89:PRO:HG3 | 1.97 | 0.46 |
| 25:DA:239:U:C2' | 25:DA:240:G:H5' | 2.45 | 0.46 |
| 1:CA:192:U:H4' | 20:CW:103:GLY:HA3 | 1.98 | 0.46 |
| 28:DE:11:MET:HG3 | 28:DE:24:THR:HA | 1.96 | 0.46 |
| 27:BD:226:MET:O | 27:BD:234:GLY:HA2 | 2.15 | 0.46 |
| 19:CV:14:HIS:HD2 | 19:CV:15:LEU:N | 2.12 | 0.46 |
| 4:AG:28:SER:HB3 | 4:AG:29:PRO:CD | 2.45 | 0.46 |
| 25:DA:957:A:N6 | 25:DA:959:A:C2 | 2.84 | 0.46 |
| 43:DT:57:LEU:H | 43:DT:57:LEU:HD23 | 1.77 | 0.46 |
| 46:D3:56:ASP:CG | 46:D3:58:THR:HG1 | 2.17 | 0.46 |
| 46:D3:53:MET:HG3 | 46:D3:59:LEU:HD23 | 1.98 | 0.46 |
| 3:CF:70:VAL:O | 3:CF:106:VAL:HG23 | 2.14 | 0.46 |
| 1:AA:486:U:H2' | 1:AA:487:A:H8 | 1.78 | 0.46 |
| 1:AA:942:G:N3 | 1:AA:943:U:C6 | 2.84 | 0.46 |
| 25:DA:128:C:H2' | 25:DA:129:C:H6 | 1.79 | 0.46 |
| 25:BA:2820:A:C4 | 37:B0:4:LEU:HD21 | 2.50 | 0.46 |
| 43:BT:57:LEU:N | 43:BT:57:LEU:HD12 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 30:DG:108:ASN:HA | 50:D4:38:LYS:HG2 | 1.97 | 0.46 |
| 25:BA:2208:U:H4' | 27:BD:151:LYS:HG2 | 1.96 | 0.46 |
| 25:DA:234:C:H2' | 25:DA:235:U:C6 | 2.47 | 0.46 |
| 33:DM:17:ASP:O | 33:DM:18:ALA:HB3 | 2.15 | 0.46 |
| 33:DM:17:ASP:O | 33:DM:55:VAL:O | 2.34 | 0.46 |
| 1:CA:1047:G:C2' | 1:CA:1048:G:H5' | 2.45 | 0.46 |
| 14:CQ:4:LYS:HA | 14:CQ:7:ILE:HG12 | 1.97 | 0.46 |
| 1:AA:1389:C:H2' | 1:AA:1390:U:O4' | 2.15 | 0.46 |
| 3:AF:114:PRO:O | 3:AF:118:GLN:HG3 | 2.16 | 0.46 |
| 17:AT:18:THR:CG2 | 17:AT:69:LYS:HD2 | 2.44 | 0.46 |
| 1:AA:949:A:C4 | 1:AA:1233:G:N2 | 2.84 | 0.46 |
| 25:BA:1547:C:H2' | 25:BA:1548:C:C6 | 2.51 | 0.46 |
| 1:CA:692:U:O2' | 1:CA:694:A:N7 | 2.39 | 0.46 |
| 26:DB:65:C:N4 | 26:DB:108:C:C2 | 2.84 | 0.46 |
| 25:BA:1376:C:C2' | 25:BA:1377:G:O5' | 2.64 | 0.46 |
| 46:B3:36:ILE:CD1 | 46:B3:39:ARG:HG2 | 2.46 | 0.46 |
| 4:CG:196:LEU:HB3 | 4:CG:197:PRO:HD2 | 1.97 | 0.46 |
| 25:BA:1935:G:H1' | 25:BA:1964:G:N2 | 2.30 | 0.46 |
| 15:AR:63:ARG:O | 15:AR:67:LEU:HD12 | 2.16 | 0.46 |
| 25:BA:2321:G:H5'' | 25:BA:2322:A:OP2 | 2.15 | 0.46 |
| 1:AA:408:A:H2' | 1:AA:409:G:O4' | 2.16 | 0.46 |
| 25:DA:921:G:H4' | 25:DA:2269:A:C5 | 2.51 | 0.46 |
| 29:BF:23:ASP:CG | 29:BF:24:LEU:H | 2.18 | 0.46 |
| 6:AI:21:LEU:HA | 6:AI:21:LEU:HD13 | 1.78 | 0.46 |
| 13:CP:36:LYS:HB3 | 13:CP:36:LYS:HE2 | 1.72 | 0.46 |
| 53:B7:36:GLN:HG2 | 53:B7:36:GLN:O | 2.15 | 0.46 |
| 10:AM:89:ASP:HB3 | 10:AM:91:PRO:HD3 | 1.97 | 0.46 |
| 25:BA:332:A:C2 | 25:BA:335:C:C5 | 3.04 | 0.46 |
| 25:BA:2461:C:H2' | 25:BA:2462:U:C6 | 2.50 | 0.46 |
| 20:AW:30:LYS:NZ | 20:AW:80:ARG:NH1 | 2.64 | 0.46 |
| 25:BA:1077:A:OP1 | 25:BA:1077:A:H4' | 2.14 | 0.46 |
| 52:D6:26:ASN:OD1 | 52:D6:28:ARG:HB2 | 2.15 | 0.46 |
| 35:DO:19:VAL:HG22 | 35:DO:20:GLY:N | 2.23 | 0.46 |
| 25:DA:2798:C:H5 | 25:DA:2799:A:H62 | 1.63 | 0.46 |
| 27:DD:35:LYS:CD | 27:DD:63:ARG:HB3 | 2.45 | 0.46 |
| 33:DM:33:LEU:CD1 | 33:DM:38:HIS:CD2 | 2.98 | 0.46 |
| 28:BE:6:GLY:CA | 28:BE:27:LEU:O | 2.64 | 0.46 |
| 28:BE:81:ILE:H | 28:BE:81:ILE:HD13 | 1.81 | 0.46 |
| 33:BM:36:GLY:O | 33:BM:42:TRP:HB2 | 2.15 | 0.46 |
| 28:DE:36:ARG:CG | 28:DE:36:ARG:NH1 | 2.77 | 0.46 |
| 23:CC:19:G:N2 | 23:CC:58:A:H2' | 2.31 | 0.46 |
| 26:DB:73:A:H2' | 26:DB:73:A:N3 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 26:DB:73:A:H3' | 26:DB:74:U:H6 | 1.80 | 0.46 |
| 25:DA:1084:A:H3' | 25:DA:1085:A:C8 | 2.50 | 0.46 |
| 25:DA:1084:A:H5'' | 25:DA:1085:A:OP2 | 2.16 | 0.46 |
| 25:DA:1022:G:N2 | 25:DA:1142(A):A:C2 | 2.74 | 0.46 |
| 9:AL:114:TYR:HD2 | 9:AL:114:TYR:H | 1.62 | 0.46 |
| 1:CA:1305:G:O2' | 1:CA:1306:A:O5' | 2.33 | 0.46 |
| 23:CD:15:G:C2' | 23:CD:60:A:C2 | 2.91 | 0.46 |
| 43:BT:87:GLN:HE21 | 43:BT:87:GLN:HB2 | 1.62 | 0.46 |
| 2:CE:89:GLY:O | 2:CE:154:LEU:HD11 | 2.15 | 0.46 |
| 9:CL:99:LEU:HB3 | 9:CL:101:PHE:HE1 | 1.80 | 0.46 |
| 25:BA:2117:A:H62 | 25:BA:2172:U:H3 | 1.60 | 0.46 |
| 1:CA:1434:A:H2' | 1:CA:1435:G:O4' | 2.15 | 0.46 |
| 45:DV:108:PRO:HA | 45:DV:143:GLY:CA | 2.45 | 0.46 |
| 45:DV:150:LEU:CD2 | 45:DV:154:ASP:HB2 | 2.46 | 0.46 |
| 1:CA:624:C:O3' | 16:CS:10:GLY:HA2 | 2.16 | 0.46 |
| 1:CA:625:G:H2' | 1:CA:626:U:H6 | 1.81 | 0.46 |
| 2:CE:163:PHE:HA | 2:CE:185:ILE:O | 2.15 | 0.46 |
| 31:BH:152:ARG:HB3 | 31:BH:153:LYS:HD2 | 1.98 | 0.46 |
| 17:CT:59:ILE:CG2 | 17:CT:71:PHE:CD1 | 2.99 | 0.46 |
| 13:AP:80:ARG:NH1 | 19:AV:65:ASN:O | 2.49 | 0.46 |
| 25:BA:1169:G:H1 | 25:BA:1180:C:H42 | 1.63 | 0.46 |
| 25:BA:958:U:OP2 | 36:BP:14:ARG:NH1 | 2.48 | 0.46 |
| 25:BA:1639:U:H4' | 25:BA:2699:C:H4' | 1.97 | 0.46 |
| 9:AL:4:TYR:CZ | 9:AL:88:TYR:HD2 | 2.33 | 0.46 |
| 29:BF:127:GLU:OE1 | 29:BF:128:ALA:N | 2.49 | 0.46 |
| 23:AD:49:C:P | 23:AD:49:C:H6 | 2.39 | 0.46 |
| 25:DA:1235:G:C6 | 25:DA:1236:G:N1 | 2.83 | 0.46 |
| 1:AA:1256:A:C2 | 1:AA:1277:C:C5 | 3.03 | 0.46 |
| 25:DA:977:G:C6 | 25:DA:987:G:C6 | 3.04 | 0.46 |
| 1:CA:1086:U:H6 | 1:CA:1086:U:OP2 | 1.99 | 0.46 |
| 25:DA:565:C:H2' | 25:DA:566:U:O4' | 2.16 | 0.46 |
| 3:CF:157:ILE:CD1 | 3:CF:166:GLU:HB2 | 2.45 | 0.46 |
| 28:BE:167:VAL:HG22 | 28:BE:170:LEU:HD12 | 1.98 | 0.46 |
| 4:CG:105:VAL:HG13 | 4:CG:110:PHE:HB2 | 1.98 | 0.46 |
| 42:BS:1:MET:C | 42:BS:64:MET:HE1 | 2.36 | 0.46 |
| 25:BA:645:C:C2' | 25:BA:646:A:OP1 | 2.64 | 0.46 |
| 25:DA:274:G:OP1 | 25:DA:274:G:O4' | 2.34 | 0.46 |
| 39:DR:29:ARG:HH11 | 39:DR:29:ARG:CG | 2.28 | 0.46 |
| 26:BB:79:C:H2' | 26:BB:80:U:O4' | 2.16 | 0.46 |
| 1:CA:177:C:H2' | 1:CA:178:C:H6 | 1.80 | 0.46 |
| 25:DA:1509:C:OP2 | 25:DA:1509:C:H4' | 2.15 | 0.46 |
| 34:DN:7:TYR:HE1 | 34:DN:20:MET:HG3 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:851:U:H5' | 49:BX:46:ASN:HD21 | 1.81 | 0.46 |
| 47:BZ:45:ASN:O | 47:BZ:47:GLN:HG2 | 2.16 | 0.46 |
| 25:BA:1718:G:C2 | 25:BA:1725:G:C8 | 3.03 | 0.46 |
| 25:BA:2675:A:H5' | 34:BN:29:ASN:O | 2.15 | 0.46 |
| 47:BZ:72:GLU:O | 47:BZ:76:ARG:HD2 | 2.15 | 0.46 |
| 7:AJ:77:SER:OG | 23:AD:33:C:H4' | 2.15 | 0.46 |
| 8:AK:121:ASP:HB2 | 8:AK:125:ARG:NH2 | 2.31 | 0.46 |
| 32:BK:63:ALA:HA | 32:BK:66:GLU:CD | 2.35 | 0.46 |
| 25:BA:46:C:OP2 | 25:BA:215:G:H2' | 2.16 | 0.46 |
| 1:AA:925:G:N2 | 1:AA:1503:A:OP1 | 2.47 | 0.46 |
| 28:DE:16:ARG:O | 28:DE:16:ARG:HD2 | 2.16 | 0.46 |
| 26:DB:91:C:H6 | 26:DB:91:C:O5' | 1.99 | 0.46 |
| 1:CA:218:C:O2' | 1:CA:219:C:H5' | 2.15 | 0.46 |
| 25:BA:1060:U:C5 | 25:BA:1062:G:H4' | 2.51 | 0.46 |
| 25:BA:1083:U:H3' | 25:BA:1084:A:H5'' | 1.98 | 0.46 |
| 25:BA:2393:A:H4' | 35:BO:62:LEU:N | 2.30 | 0.46 |
| 25:BA:2394:C:OP1 | 35:BO:63:PRO:CD | 2.45 | 0.46 |
| 38:DQ:44:LYS:O | 38:DQ:46:VAL:HG23 | 2.14 | 0.46 |
| 33:BM:38:HIS:HE1 | 33:BM:50:ASP:OD2 | 1.98 | 0.46 |
| 28:DE:37:ARG:CD | 28:DE:44:TYR:CE2 | 2.93 | 0.46 |
| 30:BG:64:THR:HG23 | 30:BG:66:GLN:N | 2.29 | 0.46 |
| 47:DZ:87:PRO:O | 47:DZ:88:LYS:C | 2.53 | 0.46 |
| 31:BH:159:GLU:HG2 | 31:BH:170:ARG:HH11 | 1.74 | 0.46 |
| 31:BH:169:VAL:HG12 | 31:BH:170:ARG:N | 2.31 | 0.46 |
| 1:AA:1033:G:H2' | 1:AA:1034:G:H5' | 1.97 | 0.46 |
| 25:DA:1062:G:H2' | 25:DA:1063:G:H8 | 1.80 | 0.46 |
| 34:BN:107:ARG:NH1 | 39:BR:36:GLU:OE2 | 2.48 | 0.46 |
| 29:DF:117:ARG:HH12 | 35:DO:1:MET:H2 | 1.62 | 0.46 |
| 1:AA:1368:G:OP1 | 10:AM:62:HIS:HE1 | 1.98 | 0.46 |
| 44:DU:72:VAL:O | 44:DU:73:ARG:HG3 | 2.15 | 0.46 |
| 25:DA:1111:A:O2' | 25:DA:1112:G:H4' | 2.16 | 0.46 |
| 36:DP:78:PRO:O | 36:DP:79:LEU:O | 2.34 | 0.46 |
| 25:BA:2555:U:H2' | 25:BA:2556:C:H5' | 1.97 | 0.46 |
| 5:CH:93:PRO:HG2 | 8:CK:105:ARG:NE | 2.31 | 0.46 |
| 31:DH:102:ALA:CA | 31:DH:117:PRO:HD3 | 2.45 | 0.46 |
| 25:DA:2562:U:O2' | 34:DN:23:ARG:HD3 | 2.16 | 0.46 |
| 2:CE:237:ALA:H | 2:CE:239:VAL:HB | 1.80 | 0.46 |
| 1:CA:686:U:H2' | 1:CA:687:A:C8 | 2.51 | 0.46 |
| 17:CT:44:ALA:HA | 17:CT:71:PHE:O | 2.16 | 0.46 |
| 41:D2:44:LYS:HG3 | 41:D2:45:THR:OG1 | 2.15 | 0.46 |
| 49:DX:29:ARG:N | 49:DX:33:GLN:HE22 | 2.04 | 0.46 |
| 7:CJ:13:GLN:HG2 | 7:CJ:14:PRO:HD2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:CA:1095:U:OP1 | 1:CA:1108:G:N1 | 2.48 | 0.46 |
| 34:BN:71:ARG:NH1 | 34:BN:71:ARG:HG3 | 2.20 | 0.46 |
| 45:DV:30:ASN:OD1 | 45:DV:90:VAL:HB | 2.15 | 0.46 |
| 41:B2:35:LEU:HB2 | 41:B2:37:VAL:HG23 | 1.97 | 0.46 |
| 25:BA:565:C:H2' | 25:BA:566:U:O4' | 2.16 | 0.46 |
| 1:AA:218:C:C2' | 1:AA:219:C:H5' | 2.46 | 0.46 |
| 1:CA:1504:G:H4' | 1:CA:1505:G:O5' | 2.16 | 0.46 |
| 4:AG:81:GLU:CD | 4:AG:139:ARG:HH22 | 2.19 | 0.46 |
| 36:DP:20:ALA:O | 36:DP:21:THR:HB | 2.15 | 0.46 |
| 25:BA:2315:G:H2' | 25:BA:2316:C:C6 | 2.51 | 0.46 |
| 25:BA:2563:U:O2 | 25:BA:2565:A:H8 | 1.97 | 0.46 |
| 25:BA:2566:A:H4' | 25:BA:2567:G:O5' | 2.15 | 0.46 |
| 31:BH:94:TYR:CE2 | 31:BH:160:LYS:HD3 | 2.51 | 0.46 |
| 31:DH:26:VAL:HG13 | 31:DH:27:LYS:N | 2.31 | 0.46 |
| 3:CF:70:VAL:HG11 | 3:CF:76:VAL:CG1 | 2.46 | 0.46 |
| 33:DM:68:GLU:HG2 | 33:DM:88:GLU:OE1 | 2.15 | 0.46 |
| 1:AA:1190:G:C5' | 3:AF:176:HIS:CE1 | 2.99 | 0.46 |
| 28:DE:120:TRP:CD1 | 28:DE:155:LYS:HB3 | 2.51 | 0.46 |
| 15:AR:18:PHE:CZ | 15:AR:21:ASP:HB2 | 2.51 | 0.46 |
| 30:DG:97:ASP:H | 30:DG:100:TRP:HD1 | 1.64 | 0.46 |
| 47:DZ:7:ILE:CD1 | 47:DZ:70:VAL:HG22 | 2.45 | 0.46 |
| 25:BA:2766:G:H5'' | 25:BA:2767:C:OP2 | 2.16 | 0.46 |
| 25:DA:1686:C:H2' | 25:DA:1687:G:H5' | 1.98 | 0.46 |
| 1:CA:194:C:C2' | 1:CA:195:A:H5'' | 2.46 | 0.46 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:C6 | 2.51 | 0.46 |
| 3:CF:188:LEU:HD12 | 3:CF:195:VAL:CG1 | 2.45 | 0.46 |
| 2:AE:130:ARG:HE | 2:AE:138:LEU:HD11 | 1.80 | 0.46 |
| 1:CA:1171:G:H2' | 1:CA:1172:C:C6 | 2.51 | 0.46 |
| 1:AA:1014:A:H2 | 1:AA:1219:U:O2 | 1.98 | 0.46 |
| 25:DA:1215:G:C2' | 25:DA:1216:G:H5' | 2.46 | 0.46 |
| 25:DA:85:G:H5' | 44:DU:32:PRO:HD3 | 1.97 | 0.46 |
| 1:CA:683:G:C6 | 1:CA:684:A:C6 | 3.04 | 0.46 |
| 25:BA:1655:A:H3' | 25:BA:1656:C:H6 | 1.80 | 0.46 |
| 36:BP:136:ALA:HB2 | 45:BV:52:SER:HB2 | 1.98 | 0.46 |
| 42:BS:37:ARG:HG2 | 42:BS:38:TYR:CE2 | 2.51 | 0.46 |
| 7:AJ:51:GLN:OE1 | 7:AJ:51:GLN:HA | 2.16 | 0.46 |
| 25:DA:1347:G:C2' | 25:DA:1348:G:H5' | 2.46 | 0.46 |
| 47:DZ:20:ARG:HB3 | 47:DZ:32:LYS:HE2 | 1.98 | 0.46 |
| 25:BA:86:C:H4' | 25:BA:104:U:H1' | 1.97 | 0.46 |
| 25:BA:2141:G:H2' | 25:BA:2142:C:C6 | 2.50 | 0.46 |
| 25:BA:1948:G:O2' | 25:BA:1949:G:H5' | 2.16 | 0.46 |
| 39:BR:99:LEU:HB3 | 39:BR:101:PHE:CE1 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 9:AL:121:ARG:NH1 | 9:AL:122:ALA:O | 2.39 | 0.46 |
| 1:CA:870:U:H6 | 1:CA:870:U:H5' | 1.81 | 0.46 |
| 25:BA:954:G:N3 | 25:BA:2274:A:C2 | 2.84 | 0.46 |
| 1:AA:329:A:C2 | 1:AA:332:G:C4 | 3.04 | 0.46 |
| 27:BD:218:ARG:HB3 | 27:BD:219:PRO:HD2 | 1.95 | 0.46 |
| 16:AS:14:ASN:OD1 | 16:AS:14:ASN:O | 2.34 | 0.46 |
| 25:BA:1069:A:H5'' | 25:BA:1070:A:OP1 | 2.16 | 0.46 |
| 25:BA:1101:U:O2' | 25:BA:1102:C:H5' | 2.15 | 0.46 |
| 38:BQ:106:ARG:HB3 | 38:BQ:110:LEU:HD21 | 1.98 | 0.46 |
| 27:BD:33:LEU:HD13 | 27:BD:34:VAL:N | 2.31 | 0.46 |
| 16:AS:19:ILE:HD12 | 16:AS:19:ILE:HA | 1.68 | 0.46 |
| 28:BE:49:LEU:HD12 | 28:BE:49:LEU:HA | 1.82 | 0.46 |
| 1:CA:979:C:C5 | 1:CA:980:C:C5 | 3.04 | 0.46 |
| 1:CA:511:C:C2 | 1:CA:512:U:C5 | 3.04 | 0.46 |
| 25:BA:885:C:H2' | 25:BA:890:A:N6 | 2.27 | 0.46 |
| 1:CA:1175:G:C2 | 1:CA:1176:A:C5 | 3.04 | 0.46 |
| 25:DA:953:A:OP2 | 36:DP:16:ARG:HD3 | 2.16 | 0.46 |
| 13:CP:60:VAL:HG13 | 13:CP:64:TRP:HE1 | 1.80 | 0.46 |
| 23:CD:13:C:C2' | 23:CD:14:A:OP1 | 2.64 | 0.46 |
| 30:BG:131:TYR:HE2 | 30:BG:133:LEU:HD13 | 1.81 | 0.46 |
| 40:B1:92:ARG:O | 40:B1:93:LYS:C | 2.54 | 0.46 |
| 39:BR:54:ARG:HA | 39:BR:59:THR:HB | 1.98 | 0.46 |
| 25:BA:2156:G:H5'' | 25:BA:2157:G:P | 2.56 | 0.46 |
| 38:DQ:3:ARG:HD2 | 38:DQ:4:LEU:H | 1.81 | 0.46 |
| 35:DO:39:LYS:HB2 | 35:DO:45:LEU:HD21 | 1.96 | 0.46 |
| 25:BA:2666:C:H42 | 31:BH:109:PHE:HA | 1.81 | 0.46 |
| 6:CI:61:LEU:HB3 | 6:CI:63:TYR:CE2 | 2.50 | 0.46 |
| 25:BA:1473:G:O2' | 25:BA:1474:C:H5' | 2.15 | 0.46 |
| 1:AA:406:G:C5' | 4:AG:5:ILE:HD13 | 2.46 | 0.46 |
| 28:DE:70:ALA:C | 28:DE:72:VAL:H | 2.16 | 0.46 |
| 52:D6:52:VAL:HG22 | 52:D6:53:LYS:N | 2.25 | 0.46 |
| 51:B5:51:TYR:O | 51:B5:56:LYS:HE3 | 2.15 | 0.46 |
| 48:DW:53:LEU:O | 48:DW:56:GLN:HB2 | 2.16 | 0.46 |
| 7:CJ:78:ARG:NH1 | 7:CJ:80:VAL:HB | 2.30 | 0.46 |
| 5:CH:101:ILE:HD11 | 5:CH:119:LEU:CD2 | 2.43 | 0.46 |
| 25:DA:205:G:C1' | 25:DA:206:U:OP2 | 2.60 | 0.46 |
| 47:DZ:78:LYS:CD | 47:DZ:78:LYS:O | 2.61 | 0.46 |
| 39:BR:58:ASN:H | 39:BR:58:ASN:HD22 | 1.62 | 0.46 |
| 1:AA:353:A:C8 | 1:AA:353:A:H5' | 2.44 | 0.46 |
| 26:BB:70:C:N3 | 26:BB:71:C:C5 | 2.83 | 0.46 |
| 25:BA:588:U:H1' | 29:BF:90:PHE:CD1 | 2.51 | 0.46 |
| 1:AA:429:U:H1' | 1:AA:430:A:H5'' | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:938:A:C2 | 1:CA:1376:U:H1' | 2.51 | 0.46 |
| 19:CV:43:GLU:H | 19:CV:45:VAL:HG22 | 1.80 | 0.46 |
| 25:BA:232:G:OP2 | 25:BA:232:G:C8 | 2.67 | 0.46 |
| 25:DA:2584:U:C5' | 25:DA:2585:U:OP2 | 2.64 | 0.46 |
| 1:AA:763:G:H2' | 1:AA:764:C:C6 | 2.50 | 0.46 |
| 25:DA:912:C:N3 | 25:DA:913:U:C5 | 2.83 | 0.46 |
| 37:B0:97:VAL:HG22 | 37:B0:114:VAL:HG22 | 1.98 | 0.46 |
| 25:DA:709:U:H2' | 25:DA:710:G:C8 | 2.50 | 0.46 |
| 25:DA:1809:A:N6 | 25:DA:1810:A:N1 | 2.63 | 0.46 |
| 25:BA:650:C:H2' | 25:BA:651:G:O5' | 2.16 | 0.46 |
| 45:BV:48:PHE:CZ | 45:BV:74:VAL:HG21 | 2.51 | 0.46 |
| 38:BQ:67:ARG:HH11 | 38:BQ:67:ARG:CB | 2.28 | 0.46 |
| 3:CF:196:LEU:HD23 | 3:CF:196:LEU:N | 2.31 | 0.46 |
| 1:CA:195:A:C6 | 1:CA:196:A:N1 | 2.84 | 0.46 |
| 25:BA:2301:C:C6 | 25:BA:2301:C:H3' | 2.51 | 0.46 |
| 1:CA:31:G:H2' | 1:CA:48:C:N4 | 2.31 | 0.46 |
| 1:AA:264:U:O2' | 17:AT:64:PRO:HD2 | 2.16 | 0.46 |
| 25:BA:539:G:N3 | 25:BA:539:G:H2' | 2.30 | 0.46 |
| 49:DX:6:VAL:HG22 | 49:DX:35:ARG:O | 2.16 | 0.46 |
| 25:DA:717:G:H2' | 25:DA:718:A:O4' | 2.15 | 0.46 |
| 25:DA:633:A:H8 | 25:DA:633:A:O5' | 1.98 | 0.46 |
| 28:DE:91:VAL:HG23 | 28:DE:95:ILE:HD11 | 1.98 | 0.46 |
| 47:DZ:67:ILE:N | 47:DZ:68:PRO:HD2 | 2.31 | 0.46 |
| 25:BA:1754:C:OP1 | 39:BR:96:ARG:NH1 | 2.48 | 0.46 |
| 10:CM:31:GLY:O | 10:CM:32:ALA:HB2 | 2.16 | 0.46 |
| 1:CA:300:A:H8 | 1:CA:300:A:O5' | 1.99 | 0.46 |
| 31:DH:85:LYS:HD2 | 31:DH:85:LYS:HA | 1.73 | 0.46 |
| 41:B2:99:ILE:HD13 | 41:B2:99:ILE:N | 2.30 | 0.46 |
| 3:AF:26:LYS:H | 3:AF:26:LYS:HD3 | 1.80 | 0.46 |
| 25:BA:887:A:H5' | 25:BA:888:C:OP1 | 2.15 | 0.46 |
| 37:B0:56:LYS:NZ | 37:B0:90:ARG:O | 2.47 | 0.46 |
| 1:CA:313:A:H2' | 1:CA:314:C:C6 | 2.51 | 0.46 |
| 4:CG:172:PRO:HD2 | 4:CG:173:TRP:CZ3 | 2.51 | 0.46 |
| 1:AA:22:G:C5 | 1:AA:23:C:C4 | 3.03 | 0.46 |
| 25:BA:1069:A:H5'' | 25:BA:1070:A:P | 2.55 | 0.46 |
| 25:BA:2481:G:C2' | 25:BA:2482:G:OP2 | 2.64 | 0.46 |
| 35:BO:61:ARG:HG3 | 54:B8:27:THR:HG22 | 1.97 | 0.46 |
| 25:DA:2896:C:H5' | 25:DA:2897:U:OP2 | 2.16 | 0.46 |
| 25:BA:2785:C:O2' | 28:BE:64:LYS:HD3 | 2.16 | 0.46 |
| 23:AC:21:U:C3' | 23:AC:22:A:H5' | 2.46 | 0.46 |
| 35:BO:15:ARG:CB | 35:BO:15:ARG:NH1 | 2.75 | 0.46 |
| 28:DE:25:VAL:O | 28:DE:26:ILE:HG13 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:AD:69:C:H2' | 23:AD:70:C:O4' | 2.16 | 0.46 |
| 54:D8:47:LYS:C | 54:D8:48:PHE:CD1 | 2.89 | 0.46 |
| 25:BA:2287:A:C2 | 25:BA:2346:A:C2 | 3.04 | 0.46 |
| 36:BP:85:LYS:HG2 | 36:BP:86:GLY:N | 2.31 | 0.46 |
| 25:DA:1097:U:H6 | 25:DA:1097:U:OP2 | 1.98 | 0.46 |
| 43:DT:50:LYS:O | 43:DT:51:VAL:HB | 2.15 | 0.46 |
| 25:DA:2271:G:C5 | 25:DA:2272:U:C5 | 3.04 | 0.46 |
| 9:AL:114:TYR:HD1 | 10:AM:60:ARG:HB2 | 1.80 | 0.46 |
| 25:DA:1536:A:C8 | 25:DA:1537:C:H1' | 2.51 | 0.46 |
| 25:DA:547:A:H2' | 25:DA:548:A:C8 | 2.51 | 0.46 |
| 25:DA:1434:A:N6 | 25:DA:1558:A:N6 | 2.57 | 0.46 |
| 1:AA:827:U:H5 | 1:AA:872:A:C6 | 2.33 | 0.46 |
| 35:BO:50:ARG:NH2 | 35:BO:50:ARG:HG3 | 2.24 | 0.46 |
| 1:AA:686:U:H2' | 1:AA:687:A:C8 | 2.51 | 0.46 |
| 25:BA:2161:C:H2' | 25:BA:2162:G:H5' | 1.98 | 0.46 |
| 25:BA:2134:A:N7 | 25:BA:2158:A:H2 | 2.13 | 0.46 |
| 25:DA:2876:G:O5' | 39:DR:3:ARG:HA | 2.16 | 0.46 |
| 11:AN:121:PRO:CG | 11:AN:126:ARG:HG3 | 2.38 | 0.46 |
| 13:CP:3:ARG:NH1 | 30:DG:113:ARG:HH21 | 2.09 | 0.46 |
| 7:AJ:26:PHE:HE2 | 7:AJ:30:ILE:HD11 | 1.78 | 0.46 |
| 25:BA:774:A:H2 | 25:BA:787:U:C2' | 2.29 | 0.46 |
| 25:DA:2410:G:H2' | 25:DA:2411:A:O4' | 2.16 | 0.46 |
| 40:B1:112:ARG:NH1 | 40:B1:112:ARG:HG3 | 2.27 | 0.46 |
| 51:B5:40:LYS:CE | 51:B5:46:CYS:HB3 | 2.45 | 0.46 |
| 25:BA:2701:C:H2' | 25:BA:2702:U:OP1 | 2.15 | 0.46 |
| 22:AB:18:G:OP2 | 22:AB:18:G:C8 | 2.69 | 0.46 |
| 25:BA:806:C:OP2 | 35:BO:41:ARG:HD3 | 2.16 | 0.46 |
| 27:DD:68:LYS:HB2 | 27:DD:70:TRP:CZ3 | 2.51 | 0.46 |
| 23:AD:18:C:OP1 | 25:BA:2180:U:O3' | 2.34 | 0.46 |
| 31:DH:169:VAL:HG22 | 31:DH:170:ARG:N | 2.30 | 0.46 |
| 30:BG:91:ARG:C | 30:BG:91:ARG:HD2 | 2.36 | 0.46 |
| 1:CA:242:C:H2' | 1:CA:243:A:H5' | 1.98 | 0.46 |
| 1:CA:943:U:H1' | 9:CL:124:GLN:HE22 | 1.81 | 0.46 |
| 25:BA:2592:G:C6 | 25:BA:2593:U:C4 | 3.04 | 0.46 |
| 25:BA:128:C:H4' | 53:B7:49:ARG:HH21 | 1.81 | 0.46 |
| 1:CA:16:A:H2 | 1:CA:1080:A:N3 | 2.13 | 0.46 |
| 1:CA:1348:U:H3 | 1:CA:1374:A:H2 | 1.64 | 0.46 |
| 25:DA:362:U:H3' | 25:DA:362:U:C6 | 2.50 | 0.46 |
| 18:AU:29:PHE:CE1 | 18:AU:31:LEU:HB3 | 2.51 | 0.46 |
| 1:CA:577:G:H2' | 1:CA:578:C:H6 | 1.81 | 0.46 |
| 25:DA:1396:U:H2' | 25:DA:1396:U:O2 | 2.14 | 0.46 |
| 1:CA:608:A:H2' | 1:CA:609:A:O4' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 8:AK:109:ILE:HD11 | 8:AK:120:THR:CG2 | 2.46 | 0.46 |
| 25:DA:492:A:H2' | 25:DA:493:G:H5' | 1.97 | 0.46 |
| 4:AG:61:LYS:HA | 4:AG:203:VAL:HG22 | 1.98 | 0.46 |
| 25:BA:911:A:H2' | 36:BP:9:TYR:OH | 2.15 | 0.46 |
| 25:DA:2815:C:O2' | 51:D5:43:HIS:HD2 | 1.99 | 0.46 |
| 30:DG:6:ALA:O | 30:DG:9:ARG:N | 2.49 | 0.46 |
| 20:CW:96:GLY:O | 20:CW:97:ALA:HB3 | 2.16 | 0.46 |
| 1:CA:644:G:C2' | 1:CA:645:C:H5' | 2.46 | 0.46 |
| 25:BA:1750:G:C2 | 25:BA:1751:C:C6 | 3.04 | 0.46 |
| 1:CA:1468:A:H2' | 1:CA:1469:G:O4' | 2.16 | 0.46 |
| 25:BA:478:A:C6 | 25:BA:480:A:C6 | 3.04 | 0.46 |
| 6:CI:8:ILE:HD11 | 6:CI:79:LEU:HD13 | 1.97 | 0.46 |
| 3:AF:23:TYR:CD2 | 3:AF:24:ALA:N | 2.84 | 0.46 |
| 25:DA:922:U:H2' | 25:DA:923:C:C6 | 2.50 | 0.46 |
| 10:AM:42:THR:HG23 | 10:AM:68:HIS:HA | 1.98 | 0.46 |
| 25:BA:654(H):G:N3 | 25:BA:654(H):G:H2' | 2.31 | 0.46 |
| 8:CK:120:THR:H | 8:CK:123:GLU:HG3 | 1.81 | 0.46 |
| 29:DF:93:LYS:HE2 | 29:DF:93:LYS:HB3 | 1.57 | 0.46 |
| 36:BP:10:ARG:HG2 | 36:BP:10:ARG:H | 1.45 | 0.46 |
| 25:DA:68:G:H2' | 25:DA:69:C:O4' | 2.15 | 0.46 |
| 25:DA:1264:G:H5' | 51:D5:11:THR:OG1 | 2.16 | 0.46 |
| 52:D6:15:GLU:OE2 | 52:D6:41:PRO:CB | 2.63 | 0.46 |
| 30:BG:93:THR:O | 30:BG:93:THR:HG22 | 2.15 | 0.46 |
| 10:CM:56:HIS:O | 10:CM:57:LYS:C | 2.53 | 0.46 |
| 25:DA:270(H):C:H2' | 25:DA:270(I):G:C8 | 2.51 | 0.46 |
| 25:DA:1058:U:H3 | 25:DA:1080:A:N6 | 2.11 | 0.46 |
| 23:AC:77:A:O2' | 25:BA:2602:A:N7 | 2.46 | 0.46 |
| 25:BA:442:G:O4' | 29:BF:46:ARG:HD3 | 2.15 | 0.46 |
| 25:DA:1012:U:N3 | 25:DA:1143:A:C6 | 2.82 | 0.46 |
| 44:DU:97:ARG:N | 44:DU:97:ARG:HD3 | 2.29 | 0.46 |
| 25:BA:481:G:H4' | 25:BA:482:A:O5' | 2.16 | 0.46 |
| 41:B2:5:VAL:O | 41:B2:11:GLN:HA | 2.15 | 0.46 |
| 25:DA:2115:G:H2' | 25:DA:2116:G:N7 | 2.30 | 0.46 |
| 25:DA:2129:C:N4 | 25:DA:2130:U:O4 | 2.49 | 0.46 |
| 34:DN:22:ILE:HD13 | 34:DN:22:ILE:HA | 1.41 | 0.46 |
| 25:BA:2789:C:O2' | 25:BA:2892:A:C2 | 2.68 | 0.46 |
| 19:CV:9:VAL:HB | 19:CV:11:VAL:HG12 | 1.98 | 0.46 |
| 2:AE:80:ILE:CG2 | 2:AE:212:GLN:HA | 2.40 | 0.46 |
| 41:D2:46:VAL:O | 41:D2:46:VAL:HG22 | 2.16 | 0.46 |
| 25:DA:2411:A:H2' | 25:DA:2411:A:N3 | 2.30 | 0.46 |
| 25:DA:2261:C:C2' | 25:DA:2262:U:H5' | 2.46 | 0.46 |
| 39:BR:16:ARG:HG2 | 39:BR:18:ASP:OD1 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:1091:U:O2 | 1:CA:1093:A:C8 | 2.67 | 0.46 |
| 1:CA:409:G:OP1 | 4:CG:24:GLU:HG2 | 2.16 | 0.46 |
| 1:AA:380:G:N2 | 1:AA:384:G:C4 | 2.84 | 0.46 |
| 1:CA:1392:G:C2' | 1:CA:1393:U:H5' | 2.46 | 0.46 |
| 1:AA:166:G:H2' | 1:AA:167:G:C8 | 2.50 | 0.46 |
| 25:BA:1203:G:H5' | 35:BO:3:LEU:CD1 | 2.46 | 0.46 |
| 25:DA:1416:G:H1 | 25:DA:1582:C:H42 | 1.62 | 0.46 |
| 14:CQ:53:LEU:HA | 14:CQ:54:PRO:HD3 | 1.84 | 0.46 |
| 1:AA:1258:G:O2' | 1:AA:1259:C:H5' | 2.15 | 0.46 |
| 21:CX:9:ARG:HG3 | 21:CX:10:ARG:N | 2.31 | 0.46 |
| 1:CA:1055:A:C8 | 1:CA:1206:G:C2 | 3.04 | 0.46 |
| 1:CA:922:G:N3 | 1:CA:1398:A:H2 | 2.14 | 0.46 |
| 27:DD:268:ARG:HG2 | 27:DD:268:ARG:NH1 | 2.31 | 0.46 |
| 25:BA:2283:C:C2 | 25:BA:2389:G:C2 | 3.04 | 0.46 |
| 25:DA:154:G:H3' | 25:DA:155:C:C6 | 2.51 | 0.46 |
| 1:AA:663:A:H5'' | 18:AU:61:LYS:HE3 | 1.97 | 0.46 |
| 1:CA:1151:A:C6 | 1:CA:1152:A:C6 | 3.04 | 0.46 |
| 1:CA:1153:C:C4 | 1:CA:1154:G:N7 | 2.84 | 0.46 |
| 30:DG:45:GLU:H | 30:DG:45:GLU:HG2 | 1.35 | 0.46 |
| 25:BA:1845:G:O2' | 25:BA:1846:G:H5' | 2.15 | 0.46 |
| 26:BB:116:G:C5' | 38:BQ:55:ALA:HB2 | 2.46 | 0.46 |
| 38:DQ:38:GLN:HG3 | 38:DQ:47:THR:CG2 | 2.46 | 0.46 |
| 39:DR:136:GLN:HB3 | 39:DR:136:GLN:HE21 | 1.53 | 0.46 |
| 24:A1:20:U:H2' | 24:A1:21:U:C6 | 2.51 | 0.46 |
| 52:B6:52:VAL:HG22 | 52:B6:53:LYS:N | 2.31 | 0.46 |
| 25:BA:2760:C:O2' | 25:BA:2761:G:H5' | 2.16 | 0.46 |
| 25:BA:2788:C:O2' | 25:BA:2809:A:N3 | 2.46 | 0.46 |
| 1:AA:578:C:H2' | 1:AA:579:G:O5' | 2.16 | 0.46 |
| 1:AA:491:G:H2' | 1:AA:492:G:O4' | 2.16 | 0.46 |
| 42:BS:7:ALA:HB2 | 42:BS:50:VAL:HG22 | 1.97 | 0.46 |
| 4:CG:119:GLN:O | 4:CG:123:HIS:CD2 | 2.69 | 0.46 |
| 1:AA:864:A:C2 | 1:AA:917:G:N3 | 2.84 | 0.46 |
| 7:CJ:40:ALA:O | 7:CJ:44:TYR:CD1 | 2.69 | 0.46 |
| 25:BA:2881:C:C4 | 25:BA:2882:A:N7 | 2.84 | 0.46 |
| 25:DA:1439:A:C2 | 25:DA:1553:A:C4 | 3.04 | 0.46 |
| 25:DA:1922:G:H2' | 25:DA:1923:U:O4' | 2.16 | 0.46 |
| 28:BE:107:THR:O | 28:BE:107:THR:HG22 | 2.15 | 0.46 |
| 11:CN:54:ARG:HB3 | 11:CN:54:ARG:CZ | 2.46 | 0.46 |
| 18:CU:32:ARG:HA | 18:CU:69:THR:HG21 | 1.98 | 0.46 |
| 25:BA:1701:A:C3' | 25:BA:1702:G:H5' | 2.46 | 0.46 |
| 1:AA:729:A:O2' | 1:AA:730:G:H5' | 2.16 | 0.46 |
| 38:BQ:78:LEU:HD12 | 38:BQ:107:GLU:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 36:DP:64:ILE:H | 36:DP:64:ILE:HD13 | 1.77 | 0.45 |
| 36:DP:64:ILE:HG22 | 36:DP:65:PHE:H | 1.81 | 0.45 |
| 52:D6:39:TYR:CD1 | 52:D6:40:CYS:N | 2.84 | 0.45 |
| 33:BM:112:LEU:O | 33:BM:116:LEU:HG | 2.17 | 0.45 |
| 13:CP:102:ARG:HG2 | 13:CP:103:THR:N | 2.31 | 0.45 |
| 21:AX:2:GLY:O | 21:AX:4:GLY:N | 2.49 | 0.45 |
| 1:CA:974:A:P | 14:CQ:41:ARG:HH12 | 2.39 | 0.45 |
| 1:AA:1002:G:C2' | 1:AA:1003:G:H5' | 2.46 | 0.45 |
| 25:DA:1005:C:O4' | 25:DA:1143:A:C2 | 2.68 | 0.45 |
| 29:DF:18:ARG:HG2 | 29:DF:19:GLU:H | 1.80 | 0.45 |
| 45:BV:5:LEU:HD22 | 45:BV:47:VAL:HG21 | 1.98 | 0.45 |
| 25:BA:1022:G:H4' | 25:BA:1023:U:O5' | 2.16 | 0.45 |
| 1:CA:1132:C:C2' | 1:CA:1133:G:H5' | 2.46 | 0.45 |
| 25:DA:2304:G:C2' | 25:DA:2305:A:O5' | 2.64 | 0.45 |
| 25:DA:2315:G:H2' | 25:DA:2316:C:C6 | 2.51 | 0.45 |
| 32:BK:102:SER:HB3 | 32:BK:103:ARG:HE | 1.81 | 0.45 |
| 25:DA:2168:G:C6 | 25:DA:2171:A:N1 | 2.84 | 0.45 |
| 31:DH:102:ALA:HB1 | 31:DH:116:GLU:HA | 1.98 | 0.45 |
| 25:DA:2032:G:H21 | 28:DE:146:THR:CG2 | 2.20 | 0.45 |
| 28:DE:55:ASN:C | 28:DE:57:LYS:H | 2.12 | 0.45 |
| 19:CV:31:ILE:HG23 | 19:CV:33:THR:HG22 | 1.98 | 0.45 |
| 25:BA:139:G:N2 | 25:BA:141:A:N1 | 2.63 | 0.45 |
| 3:CF:7:PRO:O | 3:CF:11:ARG:NH1 | 2.50 | 0.45 |
| 25:DA:322:A:H3' | 29:DF:169:ASN:HD21 | 1.78 | 0.45 |
| 31:BH:137:ASP:HB3 | 31:BH:140:LYS:HB3 | 1.98 | 0.45 |
| 48:DW:17:SER:HB3 | 48:DW:21:LEU:HG | 1.98 | 0.45 |
| 43:DT:11:PRO:CB | 43:DT:92:LEU:HD21 | 2.46 | 0.45 |
| 3:AF:92:ALA:HB2 | 3:AF:99:VAL:HG22 | 1.97 | 0.45 |
| 1:AA:102:G:C5 | 1:AA:103:C:C5 | 3.04 | 0.45 |
| 25:DA:753:C:H2' | 25:DA:754:C:C6 | 2.46 | 0.45 |
| 1:AA:428:G:C8 | 1:AA:430:A:C5 | 3.04 | 0.45 |
| 25:DA:1820:U:H4' | 25:DA:1821:A:OP2 | 2.16 | 0.45 |
| 25:BA:654(V):A:C2 | 25:BA:655:A:C2 | 2.99 | 0.45 |
| 25:DA:2364:C:H4' | 46:D3:56:ASP:OD2 | 2.16 | 0.45 |
| 25:BA:2224:G:H4' | 25:BA:2226:C:C2 | 2.51 | 0.45 |
| 45:DV:53:ILE:HG22 | 45:DV:71:VAL:HG13 | 1.97 | 0.45 |
| 23:CC:41:C:C2 | 23:CC:42:C:C5 | 3.04 | 0.45 |
| 26:DB:60:C:H2' | 26:DB:61:G:C8 | 2.51 | 0.45 |
| 1:AA:942:G:C2 | 1:AA:1342:C:C2 | 3.04 | 0.45 |
| 44:DU:50:ARG:CG | 44:DU:53:PRO:HG3 | 2.46 | 0.45 |
| 3:CF:75:VAL:O | 3:CF:75:VAL:HG12 | 2.16 | 0.45 |
| 10:AM:16:LEU:HD12 | 10:AM:70:ARG:HE | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:1829:A:H2' | 25:BA:1830:C:H5' | 1.99 | 0.45 |
| 25:BA:547:A:C3' | 25:BA:548:A:C8 | 2.99 | 0.45 |
| 1:CA:1107:C:OP1 | 3:CF:172:ARG:HB3 | 2.16 | 0.45 |
| 39:DR:29:ARG:HB3 | 39:DR:29:ARG:HH11 | 1.80 | 0.45 |
| 3:CF:120:VAL:HA | 3:CF:123:GLN:HE21 | 1.81 | 0.45 |
| 25:DA:606:U:H4' | 25:DA:658:C:H4' | 1.97 | 0.45 |
| 25:DA:1540:G:H2' | 25:DA:1541:U:O4' | 2.15 | 0.45 |
| 25:BA:250:G:H2' | 25:BA:251:A:C8 | 2.51 | 0.45 |
| 1:CA:600:C:O2' | 1:CA:601:C:H5' | 2.16 | 0.45 |
| 1:AA:297:G:H4' | 1:AA:557:G:H4' | 1.98 | 0.45 |
| 25:DA:1999:C:H5'' | 25:DA:2723:C:O2' | 2.16 | 0.45 |
| 25:DA:349:G:H2' | 25:DA:350:U:O4' | 2.16 | 0.45 |
| 1:AA:1308:U:H5'' | 13:AP:98:VAL:CG2 | 2.46 | 0.45 |
| 25:DA:2017:U:H5'' | 25:DA:2018:G:P | 2.56 | 0.45 |
| 25:BA:2235:G:H2' | 25:BA:2236:C:C6 | 2.51 | 0.45 |
| 16:CS:52:ASP:OD1 | 16:CS:55:ARG:HG3 | 2.16 | 0.45 |
| 3:AF:35:GLU:O | 3:AF:39:ILE:N | 2.43 | 0.45 |
| 1:CA:488:C:O2' | 1:CA:489:C:H5' | 2.16 | 0.45 |
| 1:CA:393:A:C6 | 1:CA:394:G:N7 | 2.84 | 0.45 |
| 25:DA:1292:U:H2' | 25:DA:1293:C:C6 | 2.50 | 0.45 |
| 23:AC:6:G:C2' | 23:AC:6:G:N3 | 2.78 | 0.45 |
| 11:CN:38:ASN:H | 11:CN:38:ASN:HD22 | 1.63 | 0.45 |
| 25:DA:847:U:C5 | 25:DA:933:A:H61 | 1.65 | 0.45 |
| 1:AA:1159:U:N3 | 1:AA:1182:G:N1 | 2.64 | 0.45 |
| 25:DA:2801:A:H2' | 25:DA:2802:G:O4' | 2.16 | 0.45 |
| 41:D2:85:LYS:CD | 41:D2:86:GLY:H | 2.28 | 0.45 |
| 28:DE:26:ILE:HG22 | 28:DE:28:ALA:N | 2.32 | 0.45 |
| 1:CA:1321:C:C5 | 1:CA:1322:C:C5 | 3.04 | 0.45 |
| 25:BA:2344:U:OP1 | 52:B6:38:LYS:HE3 | 2.16 | 0.45 |
| 1:CA:485:G:C2' | 1:CA:486:U:OP2 | 2.64 | 0.45 |
| 25:DA:1069:A:H4' | 25:DA:1070:A:H5'' | 1.98 | 0.45 |
| 28:DE:134:ILE:HD12 | 28:DE:134:ILE:C | 2.31 | 0.45 |
| 54:B8:26:LYS:HE2 | 54:B8:47:LYS:HG2 | 1.98 | 0.45 |
| 25:BA:1728:G:H2' | 25:BA:1731:G:O6 | 2.16 | 0.45 |
| 25:DA:273(D):C:N4 | 25:DA:363(B):G:H1 | 2.09 | 0.45 |
| 25:DA:2713:A:C3' | 25:DA:2714:G:C5' | 2.94 | 0.45 |
| 25:DA:529:A:H8 | 25:DA:530:G:N1 | 2.13 | 0.45 |
| 25:DA:2304:G:C2 | 25:DA:2313:C:N3 | 2.84 | 0.45 |
| 30:DG:102:PHE:HE2 | 30:DG:141:PHE:CZ | 2.34 | 0.45 |
| 38:BQ:25:ARG:HD2 | 38:BQ:88:ASP:OD2 | 2.16 | 0.45 |
| 40:B1:61:TRP:CE2 | 40:B1:94:ASN:HA | 2.51 | 0.45 |
| 1:AA:687:A:C4' | 1:AA:688:G:O5' | 2.59 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 11:AN:41:THR:HG23 | 11:AN:42:TRP:N | 2.31 | 0.45 |
| 7:CJ:115:ARG:O | 7:CJ:118:VAL:HG13 | 2.16 | 0.45 |
| 25:BA:2113:U:C5' | 25:BA:2114:A:C8 | 2.94 | 0.45 |
| 16:CS:9:PHE:HB2 | 16:CS:16:HIS:O | 2.17 | 0.45 |
| 33:BM:55:VAL:HG12 | 33:BM:127:ASP:O | 2.16 | 0.45 |
| 25:BA:2131:G:C1' | 25:BA:2158:A:H62 | 2.29 | 0.45 |
| 1:AA:1286:A:H2' | 1:AA:1287:A:H4' | 1.97 | 0.45 |
| 27:DD:24:ILE:HD11 | 27:DD:91:ARG:CD | 2.37 | 0.45 |
| 1:AA:1078:U:C5 | 1:AA:1079:G:C5 | 3.04 | 0.45 |
| 1:AA:1079:G:H2' | 1:AA:1080:A:C8 | 2.52 | 0.45 |
| 25:BA:2472:G:H2' | 25:BA:2475:C:H42 | 1.81 | 0.45 |
| 29:BF:32:LEU:HD21 | 29:BF:108:LYS:HB3 | 1.97 | 0.45 |
| 25:BA:1181:C:O2' | 25:BA:1182:A:H5' | 2.16 | 0.45 |
| 2:AE:72:GLY:HA3 | 2:AE:165:VAL:HG22 | 1.98 | 0.45 |
| 22:AB:19:G:C4' | 22:AB:20:U:OP2 | 2.65 | 0.45 |
| 50:B4:37:SER:HB3 | 50:B4:42:PHE:CB | 2.42 | 0.45 |
| 35:BO:113:LYS:HA | 35:BO:129:ALA:O | 2.16 | 0.45 |
| 29:DF:178:PRO:HB2 | 29:DF:201:VAL:CG1 | 2.40 | 0.45 |
| 25:DA:2657:A:C2 | 25:DA:2665:A:C8 | 3.04 | 0.45 |
| 23:AD:49:C:C2 | 23:AD:60:A:O4' | 2.70 | 0.45 |
| 23:CD:31:G:H2' | 23:CD:32:G:C8 | 2.50 | 0.45 |
| 1:AA:660:G:C2 | 1:AA:746:A:C2 | 3.05 | 0.45 |
| 25:BA:1014:U:C2' | 25:BA:1015:G:H5'' | 2.42 | 0.45 |
| 20:AW:73:HIS:O | 20:AW:76:ALA:HB3 | 2.16 | 0.45 |
| 39:BR:108:ARG:O | 39:BR:111:ARG:HB2 | 2.16 | 0.45 |
| 1:AA:1489:G:H2' | 1:AA:1490:C:O4' | 2.15 | 0.45 |
| 25:DA:634:C:H2' | 25:DA:635:C:H6 | 1.82 | 0.45 |
| 41:B2:64:HIS:CG | 41:B2:92:THR:HG22 | 2.52 | 0.45 |
| 28:BE:167:VAL:HG22 | 28:BE:170:LEU:CD1 | 2.45 | 0.45 |
| 25:BA:988:A:H4' | 25:BA:1155:A:N1 | 2.31 | 0.45 |
| 1:AA:1118:C:P | 9:AL:104:ARG:HH11 | 2.39 | 0.45 |
| 1:AA:90:C:C5 | 1:AA:91:C:H5 | 2.33 | 0.45 |
| 25:BA:1278:A:OP1 | 37:B0:36:THR:CG2 | 2.64 | 0.45 |
| 23:CD:24:C:H2' | 23:CD:25:U:C6 | 2.52 | 0.45 |
| 11:CN:95:ILE:HG21 | 11:CN:108:ILE:HD13 | 1.97 | 0.45 |
| 25:DA:708:C:H5' | 25:DA:709:U:OP2 | 2.16 | 0.45 |
| 33:BM:30:ILE:HG23 | 33:BM:52:VAL:HG11 | 1.97 | 0.45 |
| 5:CH:100:VAL:O | 5:CH:100:VAL:CG1 | 2.65 | 0.45 |
| 53:B7:5:TRP:CD1 | 53:B7:7:PRO:HG3 | 2.50 | 0.45 |
| 25:DA:534:U:O2' | 40:D1:49:HIS:CD2 | 2.69 | 0.45 |
| 16:AS:51:VAL:HG11 | 16:AS:74:LEU:CD2 | 2.45 | 0.45 |
| 40:D1:68:ALA:O | 40:D1:71:GLN:HB2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:2520:C:C6 | 25:DA:2567:G:H1' | 2.51 | 0.45 |
| 1:AA:22:G:H4' | 1:AA:885:G:C8 | 2.51 | 0.45 |
| 1:AA:1248:A:C5 | 1:AA:1249:C:C5 | 3.04 | 0.45 |
| 3:AF:138:VAL:HG12 | 3:AF:139:GLN:N | 2.31 | 0.45 |
| 25:BA:2102:U:H3 | 25:BA:2187:G:H1 | 1.64 | 0.45 |
| 25:BA:2753:A:O2' | 25:BA:2754:U:H5' | 2.17 | 0.45 |
| 28:BE:174:ASP:OD2 | 28:BE:175:VAL:N | 2.49 | 0.45 |
| 35:BO:114:ILE:HG12 | 35:BO:130:PHE:CD1 | 2.52 | 0.45 |
| 45:BV:14:LYS:HA | 45:BV:15:PRO:HD3 | 1.83 | 0.45 |
| 20:CW:14:LYS:HB2 | 20:CW:17:ARG:NH2 | 2.32 | 0.45 |
| 1:CA:201:C:H4' | 1:CA:208:U:OP1 | 2.14 | 0.45 |
| 52:B6:9:LEU:O | 52:B6:9:LEU:HD13 | 2.16 | 0.45 |
| 25:BA:1244:G:OP1 | 35:BO:7:ARG:HD3 | 2.16 | 0.45 |
| 30:BG:82:LEU:C | 30:BG:82:LEU:HD22 | 2.37 | 0.45 |
| 54:D8:30:ARG:O | 54:D8:30:ARG:HG3 | 2.16 | 0.45 |
| 25:DA:2286:A:H5' | 52:D6:28:ARG:HE | 1.80 | 0.45 |
| 38:DQ:83:LYS:HB3 | 38:DQ:83:LYS:HE3 | 1.74 | 0.45 |
| 25:DA:1009:A:C4' | 40:D1:59:ARG:HG3 | 2.46 | 0.45 |
| 28:BE:33:VAL:HG23 | 28:BE:35:GLN:O | 2.16 | 0.45 |
| 44:BU:78:ALA:HB3 | 44:BU:81:LYS:CE | 2.46 | 0.45 |
| 1:CA:1235:U:H2' | 1:CA:1236:A:O4' | 2.17 | 0.45 |
| 54:B8:36:LYS:CD | 54:B8:40:GLU:CG | 2.93 | 0.45 |
| 1:CA:1124:G:O2' | 1:CA:1125:U:OP2 | 2.34 | 0.45 |
| 1:CA:1141:C:H2' | 1:CA:1142:G:H8 | 1.81 | 0.45 |
| 25:DA:330:A:O2' | 25:DA:331:A:H8 | 1.99 | 0.45 |
| 32:BK:106:GLY:O | 32:BK:107:VAL:CG2 | 2.50 | 0.45 |
| 9:CL:4:TYR:HA | 9:CL:88:TYR:HE1 | 1.80 | 0.45 |
| 1:AA:689:C:C4 | 1:AA:690:G:C2 | 3.04 | 0.45 |
| 25:BA:2168:G:P | 25:BA:2168:G:O4' | 2.74 | 0.45 |
| 25:DA:2687:U:H2' | 25:DA:2688:U:O4' | 2.17 | 0.45 |
| 22:AB:60:A:H2' | 22:AB:60:A:N3 | 2.30 | 0.45 |
| 25:DA:2875:C:HO2' | 39:DR:3:ARG:HG3 | 1.81 | 0.45 |
| 35:DO:50:ARG:HB2 | 54:D8:59:LYS:HD3 | 1.98 | 0.45 |
| 35:DO:47:ASP:C | 35:DO:49:ARG:N | 2.70 | 0.45 |
| 25:DA:2298:A:H61 | 25:DA:2318:G:H1' | 1.82 | 0.45 |
| 3:AF:70:VAL:CG1 | 3:AF:72:LYS:H | 2.27 | 0.45 |
| 25:BA:973:A:O4' | 25:BA:1188:U:C6 | 2.69 | 0.45 |
| 4:AG:138:TYR:CE2 | 4:AG:139:ARG:O | 2.70 | 0.45 |
| 25:DA:11:G:C2' | 25:DA:12:U:H5' | 2.45 | 0.45 |
| 22:AB:50:A:H3' | 22:AB:51:A:H5'' | 1.98 | 0.45 |
| 48:DW:17:SER:HB2 | 48:DW:18:PRO:O | 2.15 | 0.45 |
| 3:CF:18:TRP:HB3 | 3:CF:20:SER:H | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:1211:U:H1' | 1:AA:1213:A:C2 | 2.51 | 0.45 |
| 46:B3:72:ARG:HB3 | 46:B3:75:LEU:HB2 | 1.97 | 0.45 |
| 1:CA:941:G:H2' | 1:CA:942:G:O5' | 2.16 | 0.45 |
| 25:BA:2035:G:C4' | 25:BA:2036:C:OP2 | 2.64 | 0.45 |
| 31:DH:32:GLU:O | 31:DH:33:LEU:HD23 | 2.17 | 0.45 |
| 51:B5:16:ARG:HD2 | 51:B5:20:ARG:NH1 | 2.31 | 0.45 |
| 1:AA:725:G:O2' | 1:AA:726:C:H5' | 2.16 | 0.45 |
| 1:AA:195:A:C5 | 1:AA:196:A:C2 | 3.04 | 0.45 |
| 1:AA:1263:C:H2' | 1:AA:1264:C:C6 | 2.46 | 0.45 |
| 26:DB:60:C:H2' | 26:DB:61:G:H8 | 1.82 | 0.45 |
| 2:CE:28:PHE:CE2 | 2:CE:31:TYR:HD1 | 2.35 | 0.45 |
| 1:AA:73:G:C2 | 1:AA:74:C:H5 | 2.33 | 0.45 |
| 25:BA:2259:G:C2 | 25:BA:2282:G:C6 | 3.05 | 0.45 |
| 44:DU:47:LYS:CA | 44:DU:60:PHE:HB3 | 2.46 | 0.45 |
| 1:CA:843:U:OP1 | 1:CA:843:U:H6 | 1.98 | 0.45 |
| 25:BA:2159:G:O2' | 25:BA:2160:G:H5' | 2.17 | 0.45 |
| 46:D3:82:ARG:HA | 46:D3:83:PRO:HD2 | 1.82 | 0.45 |
| 23:CD:9:G:O6 | 23:CD:23:G:N7 | 2.50 | 0.45 |
| 32:BK:81:VAL:HG21 | 32:BK:88:ILE:HD13 | 1.98 | 0.45 |
| 1:AA:948:C:O2' | 1:AA:949:A:H5' | 2.16 | 0.45 |
| 18:AU:53:ARG:HE | 18:AU:59:SER:C | 2.20 | 0.45 |
| 1:AA:130:A:C8 | 17:AT:63:ARG:HD3 | 2.51 | 0.45 |
| 29:BF:7:TYR:HA | 29:BF:22:ALA:H | 1.81 | 0.45 |
| 37:B0:60:LEU:O | 37:B0:64:ARG:HG3 | 2.16 | 0.45 |
| 4:CG:119:GLN:O | 4:CG:123:HIS:HD2 | 1.99 | 0.45 |
| 11:CN:38:ASN:HA | 11:CN:39:PRO:HD3 | 1.86 | 0.45 |
| 25:DA:2258:C:H4' | 25:DA:2259:G:OP2 | 2.15 | 0.45 |
| 25:DA:2443:C:O2' | 25:DA:2444:G:H5' | 2.16 | 0.45 |
| 1:AA:1009:G:C2 | 1:AA:1010:G:C8 | 3.04 | 0.45 |
| 25:DA:271(B):G:N7 | 25:DA:421:U:H2' | 2.31 | 0.45 |
| 25:BA:760:G:H2' | 25:BA:761:A:O4' | 2.17 | 0.45 |
| 27:DD:244:ARG:HB2 | 27:DD:245:PRO:CD | 2.45 | 0.45 |
| 27:DD:244:ARG:HB2 | 27:DD:245:PRO:HD2 | 1.98 | 0.45 |
| 25:BA:2704:C:H2' | 25:BA:2705:A:C8 | 2.51 | 0.45 |
| 45:BV:80:ARG:HG2 | 45:BV:80:ARG:H | 1.60 | 0.45 |
| 28:BE:169:ASN:O | 28:BE:169:ASN:ND2 | 2.49 | 0.45 |
| 1:CA:1057:G:O2' | 1:CA:1058:G:H5' | 2.16 | 0.45 |
| 30:BG:86:MET:O | 30:BG:87:PRO:C | 2.54 | 0.45 |
| 25:DA:225:A:N6 | 25:DA:226:G:N1 | 2.64 | 0.45 |
| 25:BA:1794:U:H1' | 25:BA:1900:A:N3 | 2.31 | 0.45 |
| 22:CB:21:A:C4 | 22:CB:22:G:H4' | 2.51 | 0.45 |
| 1:AA:1035:A:N6 | 1:AA:1036:G:C8 | 2.84 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 29:DF:24:LEU:HB3 | 29:DF:25:PRO:HD2 | 1.97 | 0.45 |
| 25:DA:329:G:O6 | 44:DU:19:LYS:CG | 2.61 | 0.45 |
| 26:DB:9:G:N2 | 26:DB:112:G:C4 | 2.85 | 0.45 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:H5' | 1.97 | 0.45 |
| 1:CA:1298:C:P | 7:CJ:114:ARG:HH22 | 2.39 | 0.45 |
| 25:BA:2115:G:O6 | 25:BA:2118:U:OP2 | 2.34 | 0.45 |
| 25:BA:2168:G:H2' | 25:BA:2169:A:OP1 | 2.16 | 0.45 |
| 1:CA:626:U:C2 | 1:CA:627:G:C8 | 3.05 | 0.45 |
| 48:DW:38:GLN:O | 48:DW:41:ILE:HG12 | 2.17 | 0.45 |
| 33:DM:127:ASP:O | 33:DM:128:HIS:HB3 | 2.16 | 0.45 |
| 38:DQ:66:ALA:HA | 38:DQ:69:VAL:HG12 | 1.98 | 0.45 |
| 25:DA:654(B):C:C2 | 25:DA:654(T):A:C2 | 3.05 | 0.45 |
| 25:BA:1385:G:O2' | 25:BA:1396:U:H6 | 1.99 | 0.45 |
| 3:CF:150:LYS:CG | 3:CF:169:ALA:HB2 | 2.40 | 0.45 |
| 7:AJ:78:ARG:NH2 | 7:AJ:156:TRP:HB3 | 2.30 | 0.45 |
| 29:DF:177:ALA:HB1 | 29:DF:178:PRO:HD2 | 1.99 | 0.45 |
| 1:AA:165:C:O2' | 1:AA:166:G:H5' | 2.15 | 0.45 |
| 25:BA:1677:A:H2' | 25:BA:1678:G:C8 | 2.50 | 0.45 |
| 29:BF:34:TRP:HB2 | 35:BO:6:LEU:HG | 1.98 | 0.45 |
| 1:CA:994:A:C2 | 1:CA:995:C:C5 | 3.04 | 0.45 |
| 53:D7:16:HIS:HB2 | 53:D7:44:PRO:HG2 | 1.98 | 0.45 |
| 1:AA:291:C:O2 | 1:AA:310:G:C2 | 2.70 | 0.45 |
| 1:CA:940:C:O2' | 1:CA:941:G:H5' | 2.17 | 0.45 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:C6 | 2.52 | 0.45 |
| 25:BA:1465:G:C4 | 25:BA:1466:G:C8 | 3.04 | 0.45 |
| 38:BQ:93:LYS:CG | 38:BQ:94:TYR:N | 2.80 | 0.45 |
| 1:AA:723:U:C2' | 1:AA:723:U:O2 | 2.64 | 0.45 |
| 1:AA:451:A:H4' | 1:AA:452:A:O4' | 2.17 | 0.45 |
| 25:BA:756:C:C2' | 25:BA:757:U:O5' | 2.63 | 0.45 |
| 22:CB:33:U:C4 | 22:CB:34:U:C4 | 3.04 | 0.45 |
| 1:CA:777:A:C2 | 11:CN:119:CYS:HB3 | 2.50 | 0.45 |
| 25:BA:637:A:H4' | 25:BA:638:G:O5' | 2.16 | 0.45 |
| 43:DT:18:TYR:CD1 | 43:DT:21:PHE:CE2 | 3.05 | 0.45 |
| 44:DU:43:ASN:HD22 | 44:DU:43:ASN:H | 1.64 | 0.45 |
| 44:DU:43:ASN:N | 44:DU:43:ASN:ND2 | 2.64 | 0.45 |
| 25:BA:340:A:H2' | 25:BA:341:G:H5' | 1.97 | 0.45 |
| 25:BA:850:C:O2' | 49:BX:46:ASN:ND2 | 2.49 | 0.45 |
| 3:CF:100:ALA:O | 3:CF:101:LEU:HB2 | 2.16 | 0.45 |
| 17:AT:27:PHE:CZ | 17:AT:36:ILE:HD11 | 2.52 | 0.45 |
| 25:DA:2695:C:H2' | 25:DA:2696:U:C6 | 2.51 | 0.45 |
| 29:DF:57:VAL:HG13 | 29:DF:58:ALA:N | 2.32 | 0.45 |
| 17:CT:18:THR:OG1 | 17:CT:69:LYS:NZ | 2.45 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 30:DG:59:GLU:CD | 30:DG:153:ARG:HH21 | 2.19 | 0.45 |
| 25:DA:30:G:H2' | 25:DA:31:C:C6 | 2.51 | 0.45 |
| 18:CU:21:LYS:HE2 | 18:CU:54:ARG:O | 2.17 | 0.45 |
| 35:BO:24:GLY:C | 35:BO:26:GLY:H | 2.20 | 0.45 |
| 32:DK:44:LEU:HD23 | 32:DK:44:LEU:HA | 1.75 | 0.45 |
| 25:DA:1585:C:O2 | 25:DA:1585:C:H2' | 2.15 | 0.45 |
| 11:AN:113:PRO:C | 11:AN:114:VAL:HG12 | 2.37 | 0.45 |
| 50:B4:47:GLN:O | 50:B4:48:ARG:CB | 2.64 | 0.45 |
| 48:BW:32:LEU:HG | 48:BW:53:LEU:HD13 | 1.96 | 0.45 |
| 1:CA:799:G:O6 | 1:CA:800:G:C2 | 2.70 | 0.45 |
| 25:BA:1063:G:C2 | 25:BA:1064:C:C2 | 3.04 | 0.45 |
| 28:BE:49:LEU:HB3 | 28:BE:50:GLY:H | 1.47 | 0.45 |
| 23:AC:20:G:C2 | 23:AC:58:A:C2 | 3.04 | 0.45 |
| 23:CC:17:C:OP1 | 23:CC:62:C:H5' | 2.16 | 0.45 |
| 1:CA:1323:G:H4' | 1:CA:1362(A):C:C2 | 2.52 | 0.45 |
| 52:B6:15:GLU:OE2 | 52:B6:44:ARG:CZ | 2.64 | 0.45 |
| 36:DP:31:ASP:N | 36:DP:107:ALA:HB2 | 2.30 | 0.45 |
| 25:BA:1885:A:H2' | 25:BA:1886:C:O4' | 2.17 | 0.45 |
| 25:DA:2749:A:H5' | 31:DH:62:LYS:O | 2.16 | 0.45 |
| 25:DA:882:G:H2' | 25:DA:883:G:O4' | 2.17 | 0.45 |
| 54:B8:26:LYS:CB | 54:B8:44:LYS:HG3 | 2.44 | 0.45 |
| 54:B8:29:LYS:HB2 | 54:B8:44:LYS:HG2 | 1.98 | 0.45 |
| 33:DM:94:HIS:O | 33:DM:97:ARG:HB2 | 2.16 | 0.45 |
| 23:CD:62:C:C5 | 23:CD:63:C:N4 | 2.85 | 0.45 |
| 25:DA:2777:G:OP2 | 25:DA:2781:A:O2' | 2.28 | 0.45 |
| 25:DA:547:A:C5 | 25:DA:548:A:C6 | 3.04 | 0.45 |
| 32:BK:101:LEU:HD23 | 32:BK:107:VAL:HB | 1.98 | 0.45 |
| 1:AA:1299:A:H2' | 1:AA:1301:U:C1' | 2.47 | 0.45 |
| 25:DA:2168:G:N2 | 25:DA:2170:A:O5' | 2.48 | 0.45 |
| 25:BA:2169:A:N3 | 25:BA:2169:A:OP1 | 2.49 | 0.45 |
| 31:DH:102:ALA:HB2 | 31:DH:117:PRO:HD3 | 1.97 | 0.45 |
| 25:DA:856:C:C2' | 25:DA:857:C:O5' | 2.65 | 0.45 |
| 25:DA:2320:A:H1' | 25:DA:2321:G:C6 | 2.51 | 0.45 |
| 25:BA:1332:G:N2 | 25:BA:1609:A:C2' | 2.80 | 0.45 |
| 25:BA:1536:A:H2' | 25:BA:1537:C:OP1 | 2.17 | 0.45 |
| 1:AA:1288:A:O2' | 1:AA:1289:A:H5' | 2.15 | 0.45 |
| 25:DA:660:G:H5' | 29:DF:99:TYR:CE2 | 2.51 | 0.45 |
| 47:BZ:78:LYS:O | 47:BZ:80:LEU:HD13 | 2.16 | 0.45 |
| 25:BA:848:G:H2' | 25:BA:849:A:C8 | 2.51 | 0.45 |
| 25:BA:627:A:N1 | 25:BA:636:G:O2' | 2.48 | 0.45 |
| 51:D5:6:VAL:CG1 | 51:D5:7:PRO:N | 2.75 | 0.45 |
| 2:CE:7:VAL:HG13 | 2:CE:8:LYS:HG3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 22:CB:26:C:N4 | 22:CB:27:G:C2 | 2.85 | 0.45 |
| 9:CL:79:LEU:CD1 | 9:CL:83:ARG:HD2 | 2.44 | 0.45 |
| 36:DP:3:MET:H | 36:DP:70:PRO:HG2 | 1.81 | 0.45 |
| 23:AD:8:U:OP2 | 23:AD:13:C:H5 | 1.99 | 0.45 |
| 38:DQ:59:LYS:HD2 | 38:DQ:60:GLY:H | 1.82 | 0.45 |
| 1:CA:1270:C:H2' | 1:CA:1271:G:H8 | 1.81 | 0.45 |
| 25:DA:2838:G:C6 | 25:DA:2839:G:C5 | 3.05 | 0.45 |
| 32:DK:7:GLU:O | 32:DK:9:LEU:HD23 | 2.16 | 0.45 |
| 5:CH:50:GLU:OE2 | 5:CH:50:GLU:HA | 2.15 | 0.45 |
| 1:CA:987:G:N2 | 1:CA:1219:U:N3 | 2.65 | 0.45 |
| 25:BA:613:U:H5' | 25:BA:616:A:N6 | 2.31 | 0.45 |
| 26:BB:13:A:O2' | 26:BB:14:U:H3' | 2.16 | 0.45 |
| 1:AA:1211:U:C5' | 1:AA:1212:U:OP1 | 2.64 | 0.45 |
| 1:AA:1333:A:C2' | 1:AA:1334:G:O5' | 2.64 | 0.45 |
| 32:BK:21:VAL:HG21 | 32:BK:25:TYR:HD1 | 1.82 | 0.45 |
| 1:CA:719:C:O2' | 18:CU:49:LYS:HB3 | 2.15 | 0.45 |
| 25:DA:2188:C:H2' | 25:DA:2189:U:O4' | 2.17 | 0.45 |
| 1:CA:1028(B):C:H3' | 1:CA:1029:G:C5' | 2.47 | 0.45 |
| 23:CD:20:G:H1' | 23:CD:58:A:N1 | 2.31 | 0.45 |
| 32:BK:112:LYS:HB3 | 32:BK:112:LYS:HE2 | 1.85 | 0.45 |
| 22:CB:30:A:C6 | 22:CB:31:C:N3 | 2.85 | 0.45 |
| 25:BA:1336:A:H2' | 25:BA:1337:G:H8 | 1.81 | 0.45 |
| 25:BA:288:C:H2' | 25:BA:289:A:H8 | 1.81 | 0.45 |
| 2:CE:5:ILE:CG2 | 2:CE:5:ILE:O | 2.64 | 0.45 |
| 1:AA:342:C:C2 | 1:AA:348:G:N2 | 2.84 | 0.45 |
| 25:BA:320:A:H2' | 29:BF:136:THR:CG2 | 2.46 | 0.45 |
| 25:DA:1542:G:O6 | 25:DA:1543:A:N6 | 2.49 | 0.45 |
| 25:DA:269:U:C5 | 25:DA:270(Z):U:C5 | 3.04 | 0.45 |
| 3:AF:141:VAL:CG1 | 3:AF:202:ILE:HG23 | 2.46 | 0.45 |
| 29:BF:129:PHE:HA | 29:BF:142:TRP:NE1 | 2.31 | 0.45 |
| 25:BA:2544:G:O5' | 25:BA:2544:G:H8 | 1.99 | 0.45 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:C5 | 3.05 | 0.45 |
| 26:BB:116:G:H2' | 26:BB:117:G:O4' | 2.16 | 0.45 |
| 26:BB:80:U:H2' | 26:BB:81:G:H21 | 1.81 | 0.45 |
| 35:DO:124:LYS:HE3 | 35:DO:145:PRO:HD3 | 1.97 | 0.45 |
| 25:BA:2615:U:H2' | 25:BA:2616:C:C6 | 2.51 | 0.45 |
| 25:BA:2183:C:H2' | 25:BA:2184:G:O4' | 2.17 | 0.45 |
| 27:DD:14:ARG:HD3 | 27:DD:15:PHE:CZ | 2.52 | 0.45 |
| 49:BX:21:ALA:O | 49:BX:24:LYS:HB3 | 2.17 | 0.45 |
| 42:DS:76:VAL:O | 42:DS:76:VAL:HG22 | 2.17 | 0.45 |
| 14:AQ:13:THR:N | 14:AQ:14:PRO:CD | 2.80 | 0.45 |
| 19:CV:74:PHE:HD2 | 19:CV:74:PHE:N | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:AC:6:G:H2' | 23:AC:6:G:N3 | 2.31 | 0.45 |
| 11:AN:85:ARG:HD3 | 11:AN:113:PRO:HD3 | 1.99 | 0.45 |
| 45:BV:68:PRO:HB2 | 45:BV:91:LEU:HD23 | 1.98 | 0.45 |
| 25:DA:414:C:O2' | 25:DA:415:A:H5' | 2.16 | 0.45 |
| 25:BA:2660:A:C2 | 25:BA:2661:G:H1' | 2.52 | 0.45 |
| 25:DA:1705:G:C2' | 25:DA:1706:U:H5' | 2.47 | 0.45 |
| 1:AA:684:A:N6 | 1:AA:685:G:C6 | 2.85 | 0.45 |
| 9:CL:27:THR:HG23 | 9:CL:31:GLN:O | 2.16 | 0.45 |
| 1:CA:333:G:H4' | 20:CW:16:HIS:CE1 | 2.51 | 0.45 |
| 25:DA:1214:A:O5' | 25:DA:1214:A:H8 | 1.99 | 0.45 |
| 22:AB:1:G:N3 | 22:AB:1:G:H2' | 2.31 | 0.45 |
| 13:CP:117:VAL:O | 13:CP:117:VAL:HG12 | 2.17 | 0.45 |
| 25:DA:654(J):A:H2' | 25:DA:654(J):A:N3 | 2.31 | 0.45 |
| 1:CA:131:C:H2' | 1:CA:132:C:C6 | 2.52 | 0.45 |
| 25:BA:338:G:N2 | 25:BA:339:U:H1' | 2.32 | 0.45 |
| 5:AH:48:ALA:HB1 | 5:AH:49:PRO:CD | 2.47 | 0.45 |
| 25:BA:2468:G:H5'' | 36:BP:120:ILE:HD12 | 1.98 | 0.45 |
| 54:D8:22:VAL:HB | 54:D8:50:LEU:HD13 | 1.97 | 0.45 |
| 36:DP:27:VAL:HG11 | 36:DP:134:ARG:HB2 | 1.99 | 0.45 |
| 40:D1:50:ARG:CB | 40:D1:50:ARG:HH21 | 2.30 | 0.45 |
| 40:D1:76:TYR:CZ | 40:D1:80:ILE:HG13 | 2.52 | 0.45 |
| 25:DA:999:U:C5 | 25:DA:1154:G:C5 | 3.05 | 0.45 |
| 27:BD:35:LYS:HE2 | 27:BD:65:ILE:HG22 | 1.99 | 0.45 |
| 31:DH:154:PRO:O | 31:DH:155:SER:CB | 2.61 | 0.45 |
| 1:CA:1320:C:C2 | 1:CA:1321:C:C5 | 3.04 | 0.45 |
| 25:DA:2849:U:OP2 | 39:DR:95:ARG:NH1 | 2.47 | 0.45 |
| 45:BV:61:LEU:HD21 | 45:BV:67:LEU:HD12 | 1.99 | 0.45 |
| 1:AA:268:C:C4 | 1:AA:269:C:C5 | 3.05 | 0.45 |
| 10:CM:81:THR:C | 10:CM:83:GLU:N | 2.69 | 0.45 |
| 25:DA:259:G:N2 | 25:DA:621:A:C8 | 2.73 | 0.45 |
| 1:AA:857:C:C5 | 1:AA:858:G:N7 | 2.84 | 0.45 |
| 25:BA:483:A:O4' | 44:BU:47:LYS:HB3 | 2.17 | 0.45 |
| 41:B2:9:GLY:O | 41:B2:10:LYS:HG3 | 2.17 | 0.45 |
| 2:CE:112:VAL:O | 2:CE:115:LEU:HB3 | 2.15 | 0.45 |
| 45:DV:120:ILE:HG21 | 45:DV:170:THR:HG23 | 1.98 | 0.45 |
| 1:CA:619:U:C2 | 4:CG:135:LEU:HD22 | 2.51 | 0.45 |
| 25:BA:2667:C:H2' | 25:BA:2668:G:O4' | 2.15 | 0.45 |
| 1:CA:171:A:C6 | 1:CA:172:A:C6 | 3.05 | 0.45 |
| 5:AH:31:LEU:HD23 | 5:AH:31:LEU:HA | 1.82 | 0.45 |
| 26:BB:45:A:O4' | 30:BG:95:ARG:NH1 | 2.50 | 0.45 |
| 41:B2:76:LYS:HG3 | 41:B2:81:TYR:HD1 | 1.81 | 0.45 |
| 22:AB:15:A:N1 | 22:AB:70:G:C5 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:1187:G:H2' | 1:CA:1187:G:N3 | 2.32 | 0.45 |
| 54:D8:39:LYS:C | 54:D8:41:ILE:H | 2.19 | 0.45 |
| 1:CA:1372:U:H2' | 1:CA:1373:G:O4' | 2.16 | 0.45 |
| 1:AA:464:G:H21 | 1:AA:468:A:H62 | 1.65 | 0.45 |
| 1:CA:498:A:C4' | 1:CA:500:G:OP1 | 2.63 | 0.45 |
| 25:DA:333:G:H5'' | 25:DA:334:C:OP2 | 2.17 | 0.45 |
| 31:BH:137:ASP:O | 31:BH:138:LYS:HB3 | 2.16 | 0.45 |
| 3:CF:29:TYR:CD1 | 14:CQ:36:PHE:CE1 | 3.05 | 0.45 |
| 25:BA:1545:A:C6 | 25:BA:1545(A):A:C2 | 3.05 | 0.45 |
| 1:AA:814:A:C8 | 1:AA:816:A:C8 | 3.05 | 0.45 |
| 1:CA:691:G:H1' | 1:CA:696:A:N6 | 2.31 | 0.45 |
| 1:AA:173:U:C6 | 1:AA:197:A:C2 | 3.05 | 0.45 |
| 25:DA:1784:A:H4' | 25:DA:1785:A:O5' | 2.16 | 0.45 |
| 2:CE:28:PHE:CE2 | 2:CE:189:ASP:O | 2.70 | 0.45 |
| 32:BK:112:LYS:H | 32:BK:112:LYS:HG2 | 1.57 | 0.45 |
| 25:BA:2259:G:C2 | 25:BA:2282:G:N1 | 2.85 | 0.45 |
| 22:AB:27:G:H3' | 22:AB:28:C:C6 | 2.51 | 0.45 |
| 34:BN:7:TYR:OH | 34:BN:44:LYS:HG3 | 2.17 | 0.45 |
| 1:CA:45:U:H2' | 1:CA:46:G:H8 | 1.80 | 0.45 |
| 25:BA:989:G:N7 | 49:BX:13:ILE:HD12 | 2.31 | 0.45 |
| 1:AA:90:C:N4 | 1:AA:91:C:H41 | 2.14 | 0.45 |
| 37:B0:41:ALA:HB1 | 37:B0:114:VAL:CG2 | 2.47 | 0.45 |
| 1:CA:1047:G:H5'' | 14:CQ:4:LYS:HE3 | 1.98 | 0.45 |
| 1:AA:1083:U:C5 | 1:AA:1084:G:C6 | 3.04 | 0.45 |
| 1:CA:677:U:H1' | 11:CN:119:CYS:SG | 2.57 | 0.45 |
| 25:DA:2564:A:C2 | 25:DA:2647:U:H4' | 2.52 | 0.45 |
| 25:DA:1467:C:C5 | 25:DA:1546:C:H2' | 2.52 | 0.45 |
| 28:DE:27:LEU:CD2 | 39:DR:1:MET:HE2 | 2.46 | 0.45 |
| 16:CS:70:ALA:O | 16:CS:74:LEU:HB2 | 2.16 | 0.45 |
| 30:DG:31:VAL:HA | 30:DG:32:PRO:HD3 | 1.83 | 0.45 |
| 1:CA:1170:A:H2' | 1:CA:1171:G:O4' | 2.17 | 0.45 |
| 1:CA:671:G:C5 | 1:CA:672:U:C5 | 3.05 | 0.45 |
| 1:CA:146:G:N2 | 1:CA:177:C:C2 | 2.85 | 0.45 |
| 25:BA:835:A:C2' | 25:BA:836:G:O5' | 2.65 | 0.45 |
| 46:B3:36:ILE:HD13 | 46:B3:39:ARG:HG2 | 1.98 | 0.45 |
| 25:BA:712:G:H2' | 25:BA:713:G:O5' | 2.16 | 0.45 |
| 18:CU:87:ARG:O | 18:CU:88:LYS:HG3 | 2.16 | 0.45 |
| 25:BA:28:A:C5 | 25:BA:29:U:C5 | 3.04 | 0.45 |
| 25:BA:2395:C:H2' | 25:BA:2396:G:O4' | 2.17 | 0.45 |
| 30:DG:181:ARG:O | 30:DG:182:LYS:HB2 | 2.16 | 0.45 |
| 20:AW:16:HIS:O | 20:AW:19:SER:HB2 | 2.17 | 0.45 |
| 1:CA:1361:G:C2' | 1:CA:1362:C:H5' | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 15:AR:29:VAL:HB | 15:AR:81:LEU:HD21 | 1.98 | 0.45 |
| 1:CA:1100:C:HO2' | 1:CA:1102:A:P | 2.40 | 0.45 |
| 4:AG:176:LEU:HD12 | 4:AG:182:LYS:O | 2.16 | 0.45 |
| 20:AW:87:LYS:HD2 | 20:AW:87:LYS:HA | 1.73 | 0.45 |
| 25:BA:1975:G:C2 | 25:BA:1976:U:C2 | 3.05 | 0.45 |
| 37:B0:18:LEU:HD23 | 37:B0:18:LEU:HA | 1.74 | 0.45 |
| 15:CR:48:LYS:HA | 15:CR:48:LYS:HD3 | 1.50 | 0.45 |
| 1:AA:621:A:O2' | 1:AA:622:A:H5' | 2.16 | 0.45 |
| 2:CE:36:ARG:HB3 | 2:CE:41:ILE:HD11 | 1.97 | 0.45 |
| 25:BA:77:C:OP1 | 48:BW:59:ARG:HD3 | 2.17 | 0.45 |
| 25:BA:1705:G:C2' | 25:BA:1706:U:H5' | 2.46 | 0.45 |
| 20:AW:10:LEU:HD22 | 20:AW:12:ALA:HB3 | 1.78 | 0.45 |
| 27:DD:33:LEU:CD2 | 27:DD:34:VAL:H | 2.30 | 0.45 |
| 36:DP:38:GLU:HB2 | 36:DP:127:ILE:CG2 | 2.46 | 0.45 |
| 25:DA:2378:A:H5'' | 38:DQ:23:ARG:NH1 | 2.31 | 0.45 |
| 40:D1:50:ARG:HH12 | 41:D2:72:VAL:HG22 | 1.81 | 0.45 |
| 41:D2:75:PHE:CE2 | 41:D2:81:TYR:CE1 | 3.04 | 0.45 |
| 25:BA:1794:U:O2' | 25:BA:1795:C:H5' | 2.17 | 0.45 |
| 1:AA:1128:C:H5' | 9:AL:16:ARG:HH12 | 1.80 | 0.45 |
| 28:DE:5:LEU:N | 28:DE:5:LEU:HD23 | 2.31 | 0.45 |
| 27:DD:28:GLU:O | 27:DD:29:PRO:C | 2.55 | 0.45 |
| 25:BA:2285:C:P | 52:B6:28:ARG:HD3 | 2.56 | 0.45 |
| 4:CG:11:LEU:C | 4:CG:13:ARG:N | 2.67 | 0.45 |
| 25:DA:951:C:C2' | 25:DA:952:G:H5' | 2.47 | 0.45 |
| 1:AA:975:A:C5' | 1:AA:976:G:H5'' | 2.47 | 0.45 |
| 23:CD:63:C:H3' | 23:CD:63:C:H6 | 1.82 | 0.45 |
| 25:DA:1043:C:H2' | 25:DA:1044:G:H5' | 1.99 | 0.45 |
| 25:BA:1796:U:H2' | 25:BA:1797:C:H6 | 1.77 | 0.45 |
| 50:D4:25:TYR:O | 50:D4:26:SER:OG | 2.31 | 0.45 |
| 44:DU:17:SER:HB3 | 44:DU:71:LYS:HB3 | 1.97 | 0.45 |
| 40:B1:92:ARG:NH2 | 41:B2:11:GLN:H | 2.13 | 0.45 |
| 25:DA:858:U:O2 | 25:DA:2268:A:N3 | 2.50 | 0.45 |
| 42:DS:59:VAL:O | 42:DS:63:ASP:HA | 2.16 | 0.45 |
| 1:AA:1288:A:H1' | 1:AA:1352:C:O2' | 2.16 | 0.45 |
| 37:B0:2:ARG:CG | 37:B0:5:LYS:HZ3 | 2.29 | 0.45 |
| 27:DD:186:HIS:HD2 | 27:DD:187:GLY:N | 2.13 | 0.45 |
| 25:BA:1385:G:H1' | 25:BA:1386:C:C6 | 2.52 | 0.45 |
| 25:DA:2336:A:H61 | 46:D3:43:THR:HB | 1.82 | 0.45 |
| 1:AA:1393:U:O4' | 1:AA:1502:A:H5' | 2.17 | 0.45 |
| 1:AA:1091:U:O2 | 1:AA:1093:A:H8 | 2.00 | 0.45 |
| 45:DV:30:ASN:HA | 45:DV:89:PHE:HE2 | 1.82 | 0.45 |
| 25:BA:654(B):C:C2 | 25:BA:654(T):A:C2 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 22:CB:55:G:C6 | 22:CB:56:G:C6 | 3.05 | 0.45 |
| 45:BV:155:LEU:HD23 | 45:BV:155:LEU:HA | 1.75 | 0.45 |
| 25:BA:2109:U:O2 | 25:BA:2181:G:C2 | 2.70 | 0.45 |
| 25:BA:1903:G:P | 27:BD:241:PRO:HB2 | 2.57 | 0.45 |
| 1:AA:1171:G:C2' | 1:AA:1172:C:H5' | 2.47 | 0.45 |
| 2:AE:87:ARG:NH2 | 2:AE:233:SER:OG | 2.45 | 0.45 |
| 1:CA:922:G:C6 | 1:CA:923:A:C6 | 3.05 | 0.45 |
| 37:B0:9:LYS:H | 37:B0:9:LYS:HG2 | 1.61 | 0.45 |
| 1:AA:1102:A:C2' | 1:AA:1103:C:H5' | 2.47 | 0.45 |
| 1:AA:373:A:H2' | 1:AA:374:A:O4' | 2.17 | 0.45 |
| 25:BA:856:C:C3' | 25:BA:856:C:C6 | 3.00 | 0.45 |
| 45:BV:142:SER:H | 45:BV:143:GLY:HA2 | 1.80 | 0.45 |
| 10:CM:24:VAL:HG21 | 10:CM:37:PRO:HG3 | 1.98 | 0.45 |
| 25:DA:2861:G:C2' | 25:DA:2862:G:H5' | 2.46 | 0.45 |
| 30:DG:99:MET:HG3 | 30:DG:100:TRP:N | 2.31 | 0.45 |
| 4:CG:60:GLU:HG2 | 4:CG:202:LEU:HB2 | 1.99 | 0.45 |
| 42:BS:84:ARG:HB2 | 42:BS:96:ILE:HD13 | 1.99 | 0.45 |
| 1:AA:1076:C:C2 | 1:AA:1082:G:C2 | 3.04 | 0.45 |
| 25:DA:2593:U:H2' | 25:DA:2594:C:H6 | 1.81 | 0.45 |
| 25:BA:960:A:C8 | 25:BA:962:G:C8 | 3.04 | 0.45 |
| 34:DN:2:ILE:HD12 | 34:DN:6:THR:HG21 | 1.99 | 0.45 |
| 1:AA:601:C:H2' | 1:AA:602:A:H8 | 1.82 | 0.45 |
| 1:CA:393:A:C2 | 1:CA:394:G:C8 | 3.05 | 0.45 |
| 1:AA:621:A:C2' | 1:AA:622:A:H5' | 2.47 | 0.45 |
| 1:AA:370:C:H2' | 1:AA:371:G:O4' | 2.16 | 0.45 |
| 25:BA:571:A:C8 | 25:BA:2030:A:N6 | 2.85 | 0.45 |
| 9:AL:47:LEU:O | 9:AL:50:LEU:HB2 | 2.16 | 0.45 |
| 27:DD:141:VAL:HG23 | 27:DD:162:SER:HB2 | 1.99 | 0.45 |
| 25:DA:2607:G:H2' | 25:DA:2608:G:O4' | 2.17 | 0.45 |
| 1:CA:1231:G:C2' | 1:CA:1232:U:H5' | 2.47 | 0.45 |
| 25:BA:1998:G:O2' | 25:BA:1999:C:H5' | 2.17 | 0.45 |
| 35:DO:19:VAL:HG21 | 35:DO:32:THR:HG23 | 1.99 | 0.45 |
| 25:DA:998:C:H2' | 25:DA:999:U:O5' | 2.17 | 0.45 |
| 25:BA:1568:G:H5'' | 27:BD:61:LEU:CD2 | 2.46 | 0.45 |
| 52:D6:15:GLU:OE2 | 52:D6:41:PRO:HB3 | 2.17 | 0.45 |
| 28:BE:61:ARG:N | 28:BE:62:PRO:HD2 | 2.30 | 0.45 |
| 28:BE:81:ILE:O | 28:BE:82:ARG:O | 2.35 | 0.45 |
| 23:AC:19:G:N3 | 23:AC:59:A:C2 | 2.85 | 0.45 |
| 23:AC:59:A:C8 | 23:AC:62:C:N4 | 2.85 | 0.45 |
| 25:BA:2415:G:C3' | 35:BO:66:GLY:HA3 | 2.47 | 0.45 |
| 40:B1:60:LEU:HD21 | 40:B1:64:ARG:NH2 | 2.32 | 0.45 |
| 33:BM:115:ARG:N | 33:BM:118:LYS:HE3 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:1200:C:H5' | 1:CA:1201:A:H5' | 1.99 | 0.45 |
| 1:AA:1305:G:N2 | 1:AA:1331:G:C2' | 2.73 | 0.45 |
| 25:BA:1026:U:C1' | 25:BA:1027:A:P | 3.05 | 0.45 |
| 1:CA:963:G:N2 | 10:CM:55:LYS:HG2 | 2.32 | 0.45 |
| 25:BA:1885:A:C8 | 25:BA:1885:A:H5' | 2.42 | 0.45 |
| 1:CA:1156:G:H5'' | 1:CA:1157:A:OP2 | 2.17 | 0.45 |
| 45:BV:7:ALA:O | 45:BV:8:TYR:CG | 2.70 | 0.45 |
| 1:AA:1358:U:H2' | 1:AA:1359:C:O4' | 2.17 | 0.45 |
| 9:AL:114:TYR:HD1 | 10:AM:60:ARG:CB | 2.29 | 0.45 |
| 44:DU:75:ILE:HA | 44:DU:80:GLY:HA2 | 1.98 | 0.45 |
| 23:CD:54:G:H2' | 23:CD:55:U:C5 | 2.51 | 0.45 |
| 25:BA:1006:C:C2 | 25:BA:1138:G:N2 | 2.85 | 0.45 |
| 17:AT:68:ARG:H | 17:AT:70:ARG:NH1 | 2.14 | 0.45 |
| 50:D4:11:PRO:HA | 50:D4:25:TYR:N | 2.30 | 0.45 |
| 25:BA:1478:G:N2 | 25:BA:1516:U:C2 | 2.84 | 0.45 |
| 25:DA:259:G:C2' | 25:DA:621:A:O2' | 2.64 | 0.45 |
| 29:DF:102:PRO:HB2 | 29:DF:105:VAL:HG23 | 1.98 | 0.45 |
| 32:BK:77:LEU:HD23 | 32:BK:101:LEU:HA | 1.99 | 0.45 |
| 2:CE:42:ILE:HD13 | 2:CE:203:GLY:N | 2.32 | 0.45 |
| 1:CA:561:U:O2' | 1:CA:562:C:P | 2.75 | 0.45 |
| 38:BQ:34:HIS:CB | 38:BQ:36:TYR:CE1 | 2.96 | 0.45 |
| 27:BD:270:ILE:CG2 | 27:BD:271:ILE:H | 2.30 | 0.45 |
| 19:CV:68:GLY:HA3 | 50:D4:59:PHE:CE1 | 2.49 | 0.45 |
| 25:DA:137(A):G:H2' | 25:DA:139:G:N7 | 2.31 | 0.45 |
| 33:BM:22:THR:CG2 | 33:BM:23:LEU:N | 2.69 | 0.45 |
| 33:BM:59:LYS:NZ | 33:BM:61:ARG:HH22 | 2.15 | 0.45 |
| 50:D4:16:CYS:HB3 | 50:D4:20:ASN:N | 2.31 | 0.45 |
| 29:DF:134:GLY:CA | 29:DF:166:ALA:HB2 | 2.38 | 0.45 |
| 33:DM:30:ILE:HG21 | 33:DM:120:LEU:HD12 | 1.99 | 0.45 |
| 35:BO:82:GLY:HA2 | 35:BO:113:LYS:O | 2.16 | 0.45 |
| 1:AA:1090:U:O2' | 1:AA:1091:U:H5' | 2.16 | 0.45 |
| 51:D5:6:VAL:HG22 | 51:D5:7:PRO:HD2 | 1.98 | 0.45 |
| 23:CC:43:G:O2' | 23:CC:44:A:H5' | 2.17 | 0.45 |
| 3:CF:66:VAL:HG12 | 3:CF:66:VAL:O | 2.17 | 0.45 |
| 28:BE:2:LYS:HB3 | 28:BE:95:ILE:HG21 | 1.99 | 0.45 |
| 1:CA:273:A:H1' | 17:CT:16:GLN:OE1 | 2.17 | 0.45 |
| 2:AE:58:ILE:HD11 | 2:AE:185:ILE:CD1 | 2.46 | 0.45 |
| 14:CQ:40:CYS:SG | 14:CQ:43:CYS:HB2 | 2.57 | 0.45 |
| 1:AA:181:G:N2 | 1:AA:195:A:C4 | 2.85 | 0.45 |
| 1:AA:149:A:C2 | 1:AA:150:C:C4 | 3.05 | 0.45 |
| 1:AA:1065:U:C2' | 1:AA:1066:C:OP2 | 2.64 | 0.45 |
| 33:DM:99:LEU:HD22 | 33:DM:99:LEU:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:BB:89:G:C6 | 26:BB:89(A):A:C6 | 3.04 | 0.45 |
| 25:DA:1666:G:H2' | 25:DA:1667:G:H5' | 1.98 | 0.45 |
| 13:CP:108:ARG:NH1 | 13:CP:108:ARG:HG3 | 2.31 | 0.45 |
| 7:AJ:27:ILE:HD12 | 7:AJ:40:ALA:HB2 | 1.99 | 0.45 |
| 25:DA:2494:G:C4 | 25:DA:2495:G:C8 | 3.05 | 0.45 |
| 27:BD:108:PRO:HG3 | 27:BD:143:HIS:CE1 | 2.51 | 0.45 |
| 37:B0:10:LEU:O | 37:B0:11:ASN:C | 2.55 | 0.45 |
| 12:AO:75:HIS:HD2 | 12:AO:77:LEU:N | 2.14 | 0.45 |
| 31:DH:41:MET:HE2 | 31:DH:64:LEU:HB2 | 1.99 | 0.45 |
| 1:CA:439:A:C2' | 1:CA:440:A:O5' | 2.65 | 0.45 |
| 11:AN:124:LYS:HD2 | 11:AN:125:PHE:CZ | 2.52 | 0.45 |
| 25:BA:250:G:C6 | 25:BA:251:A:C6 | 3.05 | 0.45 |
| 41:D2:21:ARG:NH1 | 41:D2:21:ARG:HG3 | 2.32 | 0.45 |
| 25:DA:315:G:H2' | 25:DA:316:C:C6 | 2.52 | 0.45 |
| 1:AA:775:G:O2' | 1:AA:776:G:H5' | 2.17 | 0.45 |
| 1:AA:139:G:N2 | 1:AA:225:C:C2 | 2.85 | 0.45 |
| 1:AA:1414:U:H2' | 1:AA:1415:G:H8 | 1.82 | 0.45 |
| 23:AC:73:A:C6 | 23:AC:74:A:C6 | 3.05 | 0.45 |
| 25:BA:2619:C:H4' | 28:BE:151:TYR:O | 2.17 | 0.45 |
| 40:B1:5:LYS:H | 40:B1:5:LYS:HG3 | 1.55 | 0.45 |
| 1:CA:1314:C:H2' | 1:CA:1315:U:C6 | 2.52 | 0.45 |
| 5:CH:10:MET:HA | 5:CH:32:VAL:HG22 | 1.98 | 0.45 |
| 20:AW:82:SER:O | 20:AW:86:ARG:HB2 | 2.17 | 0.45 |
| 25:DA:848:G:C4 | 25:DA:933:A:C8 | 3.04 | 0.45 |
| 38:BQ:86:ALA:O | 38:BQ:87:PHE:CB | 2.64 | 0.45 |
| 41:D2:70:ILE:CB | 41:D2:86:GLY:O | 2.56 | 0.45 |
| 25:DA:2371:G:H4' | 52:D6:45:LYS:CD | 2.47 | 0.45 |
| 26:BB:66:A:C6 | 26:BB:108:C:C6 | 3.04 | 0.45 |
| 39:DR:56:GLY:O | 39:DR:57:PHE:C | 2.56 | 0.45 |
| 1:CA:1321:C:H4' | 13:CP:87:TYR:CZ | 2.52 | 0.45 |
| 1:CA:1321:C:C3' | 1:CA:1322:C:H5'' | 2.46 | 0.45 |
| 19:CV:80:TYR:C | 19:CV:82:GLY:H | 2.20 | 0.45 |
| 35:DO:15:ARG:NH1 | 35:DO:15:ARG:CB | 2.75 | 0.45 |
| 1:CA:485:G:O2' | 1:CA:486:U:O5' | 2.34 | 0.45 |
| 25:DA:2582:G:C2 | 25:DA:2583:G:C8 | 3.05 | 0.45 |
| 1:CA:803:G:C6 | 1:CA:804:U:N3 | 2.85 | 0.45 |
| 25:BA:997:G:C2' | 25:BA:998:C:H5' | 2.47 | 0.45 |
| 9:CL:48:GLU:HB3 | 9:CL:101:PHE:HE2 | 1.81 | 0.45 |
| 16:CS:15:PRO:O | 16:CS:16:HIS:ND1 | 2.50 | 0.45 |
| 35:DO:47:ASP:CG | 35:DO:49:ARG:HE | 2.19 | 0.45 |
| 25:DA:2296:U:H4' | 25:DA:2297:C:OP1 | 2.17 | 0.45 |
| 50:D4:21:VAL:HG22 | 50:D4:22:ILE:N | 2.21 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 33:BM:12:ARG:HG2 | 33:BM:13:TRP:N | 2.31 | 0.45 |
| 1:CA:502:G:H2' | 1:CA:503:C:O4' | 2.17 | 0.45 |
| 9:CL:95:LYS:HE2 | 9:CL:95:LYS:HB2 | 1.56 | 0.45 |
| 25:DA:1869:G:N2 | 25:DA:1872:A:C8 | 2.85 | 0.45 |
| 35:DO:111:ARG:HG3 | 35:DO:128:HIS:CD2 | 2.51 | 0.45 |
| 1:AA:1079:G:C6 | 1:AA:1080:A:N6 | 2.85 | 0.45 |
| 1:CA:957:U:H2' | 1:CA:959:A:OP2 | 2.16 | 0.45 |
| 20:AW:104:LEU:HD12 | 20:AW:105:SER:N | 2.32 | 0.45 |
| 4:AG:103:ASN:OD1 | 4:AG:114:ARG:NH2 | 2.39 | 0.45 |
| 30:BG:112:PRO:HB3 | 50:B4:37:SER:H | 1.80 | 0.45 |
| 1:CA:411:A:H62 | 1:CA:413:G:N2 | 2.13 | 0.45 |
| 4:CG:23:GLY:O | 4:CG:27:TYR:CD1 | 2.70 | 0.45 |
| 1:AA:187:C:O2 | 1:AA:191(A):G:C2 | 2.70 | 0.45 |
| 25:DA:2057:A:H2' | 25:DA:2058:A:O4' | 2.17 | 0.45 |
| 1:AA:281:G:H8 | 1:AA:281:G:OP2 | 2.00 | 0.45 |
| 1:AA:164:U:H2' | 1:AA:165:C:C6 | 2.51 | 0.45 |
| 45:DV:158:PRO:HB2 | 45:DV:159:PRO:CD | 2.46 | 0.45 |
| 29:DF:34:TRP:CH2 | 35:DO:8:PRO:HB3 | 2.51 | 0.45 |
| 3:CF:64:VAL:HG22 | 3:CF:66:VAL:HG23 | 1.99 | 0.45 |
| 25:BA:1113:U:H2' | 25:BA:1114:G:C8 | 2.51 | 0.45 |
| 1:AA:658:G:C4 | 1:AA:659:U:C6 | 3.05 | 0.45 |
| 25:BA:2312:U:O2' | 25:BA:2313:C:H5' | 2.16 | 0.45 |
| 25:DA:372:G:O2' | 25:DA:373:U:P | 2.74 | 0.45 |
| 25:DA:1011:G:H1 | 25:DA:1150:C:N4 | 2.15 | 0.45 |
| 25:BA:2591:C:H2' | 25:BA:2592:G:C8 | 2.52 | 0.45 |
| 27:BD:228:PRO:HD3 | 27:BD:235:GLY:CA | 2.47 | 0.45 |
| 20:AW:69:GLY:O | 20:AW:73:HIS:CE1 | 2.70 | 0.45 |
| 1:CA:1055:A:C8 | 1:CA:1206:G:N2 | 2.85 | 0.45 |
| 25:DA:444:C:C4' | 29:DF:49:ALA:HB2 | 2.47 | 0.45 |
| 25:DA:987:G:O2' | 25:DA:1000:A:N3 | 2.46 | 0.45 |
| 25:BA:164:U:H5'' | 25:BA:165:U:O2 | 2.16 | 0.45 |
| 27:BD:70:TRP:CZ3 | 27:BD:150:LYS:HA | 2.52 | 0.45 |
| 25:DA:817:C:HO2' | 25:DA:818:G:H5' | 1.82 | 0.45 |
| 30:DG:73:ALA:HB2 | 30:DG:82:LEU:HD21 | 1.99 | 0.45 |
| 1:CA:791:G:C5 | 1:CA:792:A:N7 | 2.84 | 0.45 |
| 48:BW:24:LEU:HD22 | 48:BW:24:LEU:O | 2.17 | 0.45 |
| 6:CI:11:ASN:OD1 | 6:CI:12:PRO:HD2 | 2.17 | 0.45 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:C8 | 2.51 | 0.45 |
| 40:D1:25:TRP:CD1 | 40:D1:26:GLY:N | 2.85 | 0.45 |
| 45:BV:169:GLU:CD | 45:BV:170:THR:H | 2.19 | 0.45 |
| 8:CK:38:ILE:HD12 | 8:CK:118:VAL:HG12 | 1.98 | 0.45 |
| 23:CC:12:G:C6 | 23:CC:13:C:C4 | 3.05 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:1058:G:H2' | 1:CA:1059:C:O4' | 2.17 | 0.45 |
| 1:CA:433:C:O2' | 1:CA:434:U:H5' | 2.17 | 0.45 |
| 38:BQ:58:LEU:N | 38:BQ:58:LEU:HD23 | 2.31 | 0.45 |
| 17:AT:48:GLU:HB2 | 17:AT:50:LYS:HG2 | 1.99 | 0.45 |
| 25:BA:2716:U:O2' | 25:BA:2717:G:H5' | 2.16 | 0.45 |
| 25:DA:1726:G:C6 | 25:DA:1727:U:C4 | 3.05 | 0.45 |
| 31:DH:69:ARG:NH1 | 31:DH:73:ALA:HB2 | 2.31 | 0.45 |
| 20:CW:11:SER:HA | 20:CW:13:LEU:H | 1.82 | 0.45 |
| 40:B1:89:GLU:O | 40:B1:89:GLU:HG3 | 2.15 | 0.45 |
| 2:CE:102:LEU:N | 2:CE:102:LEU:HD12 | 2.31 | 0.45 |
| 1:CA:536:C:H2' | 1:CA:536:C:O2 | 2.16 | 0.45 |
| 25:BA:2631:G:C6 | 25:BA:2632:A:N7 | 2.85 | 0.45 |
| 25:BA:162:U:HO2' | 25:BA:163:U:H5 | 1.65 | 0.45 |
| 25:BA:2481:G:H2' | 25:BA:2482:G:OP2 | 2.17 | 0.45 |
| 25:DA:2420:C:O5' | 25:DA:2420:C:H6 | 2.00 | 0.45 |
| 36:DP:35:VAL:CG2 | 36:DP:130:LYS:HE2 | 2.47 | 0.45 |
| 25:BA:2309:A:C3' | 25:BA:2310:A:C5' | 2.95 | 0.45 |
| 33:DM:35:ARG:HB2 | 33:DM:42:TRP:CZ3 | 2.52 | 0.45 |
| 35:DO:65:ARG:HE | 54:D8:15:LYS:HB2 | 1.82 | 0.45 |
| 25:DA:1080:A:H2' | 25:DA:1081:U:C6 | 2.52 | 0.45 |
| 1:AA:791:G:C2' | 1:AA:792:A:C5' | 2.92 | 0.45 |
| 23:CD:49:C:H5'' | 23:CD:50:G:H5'' | 1.99 | 0.45 |
| 1:CA:1149:C:O2' | 1:CA:1280:A:C2 | 2.67 | 0.45 |
| 30:DG:86:MET:O | 30:DG:88:ILE:N | 2.50 | 0.45 |
| 10:CM:78:ASN:HB2 | 10:CM:81:THR:HG23 | 1.98 | 0.45 |
| 2:AE:59:GLU:HB2 | 2:AE:221:LEU:HD11 | 1.98 | 0.45 |
| 25:BA:2125:G:H1 | 25:BA:2172:U:P | 2.40 | 0.45 |
| 25:BA:2168:G:H21 | 25:BA:2169:A:H3' | 1.82 | 0.45 |
| 2:CE:237:ALA:O | 2:CE:238:LEU:HD23 | 2.17 | 0.45 |
| 25:DA:858:U:O2 | 25:DA:2268:A:H2' | 2.17 | 0.45 |
| 25:BA:2392:A:H8 | 35:BO:60:MET:HB3 | 1.77 | 0.45 |
| 33:DM:15:LEU:HD13 | 33:DM:16:ILE:N | 2.32 | 0.45 |
| 35:DO:110:TYR:HB3 | 35:DO:111:ARG:H | 1.66 | 0.45 |
| 32:BK:11:ASN:O | 32:BK:12:LEU:HD22 | 2.17 | 0.45 |
| 43:DT:53:LYS:NZ | 43:DT:55:ASN:HD21 | 2.15 | 0.45 |
| 54:B8:57:ARG:O | 54:B8:61:LEU:HG | 2.17 | 0.45 |
| 50:D4:53:GLU:OE2 | 50:D4:58:ARG:HB2 | 2.16 | 0.45 |
| 48:DW:28:LYS:HE3 | 48:DW:56:GLN:OE1 | 2.17 | 0.45 |
| 37:D0:37:THR:HB | 37:D0:40:LYS:HE3 | 1.98 | 0.45 |
| 1:AA:1392:G:H21 | 1:AA:1502:A:H8 | 1.65 | 0.45 |
| 30:BG:114:ILE:HG22 | 30:BG:115:ARG:O | 2.17 | 0.45 |
| 25:DA:2211:G:H2' | 25:DA:2211:G:N3 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 22:CB:47:C:C2 | 22:CB:56:G:N2 | 2.85 | 0.45 |
| 5:CH:147:ASP:HA | 5:CH:150:ARG:CB | 2.47 | 0.45 |
| 25:DA:1416:G:H2' | 25:DA:1417:C:C6 | 2.52 | 0.45 |
| 6:CI:100:ASN:HB2 | 18:CU:23:LYS:CD | 2.47 | 0.45 |
| 1:AA:1195:C:H5'' | 1:AA:1196:U:O5' | 2.17 | 0.45 |
| 42:BS:80:PRO:O | 42:BS:100:THR:HB | 2.17 | 0.45 |
| 1:AA:1320:C:H42 | 19:AV:36:ARG:HG3 | 1.82 | 0.45 |
| 4:CG:162:LEU:HD23 | 4:CG:162:LEU:HA | 1.65 | 0.45 |
| 31:DH:9:ILE:HB | 31:DH:49:VAL:HB | 1.99 | 0.45 |
| 25:BA:1638:C:H4' | 25:BA:2710:C:O2 | 2.17 | 0.45 |
| 25:BA:2266:A:H4' | 25:BA:2267:A:N3 | 2.32 | 0.45 |
| 17:CT:9:VAL:HG21 | 17:CT:84:LEU:HD13 | 1.98 | 0.45 |
| 25:DA:389:G:H22 | 35:DO:72:PRO:HD3 | 1.82 | 0.45 |
| 25:BA:1095:A:N3 | 25:BA:1095:A:C2' | 2.79 | 0.45 |
| 25:DA:1392:A:N6 | 25:DA:1393:A:H61 | 2.14 | 0.45 |
| 25:DA:1925:C:O2' | 25:DA:1926:U:H5' | 2.17 | 0.45 |
| 1:AA:1364:U:O5' | 1:AA:1364:U:H6 | 2.00 | 0.45 |
| 25:DA:571:A:C5 | 25:DA:575:A:C8 | 3.04 | 0.45 |
| 47:BZ:11:ARG:HB2 | 47:BZ:12:PRO:HD2 | 1.99 | 0.45 |
| 1:AA:1164:G:H2' | 1:AA:1165:C:H6 | 1.81 | 0.45 |
| 25:BA:1578:U:C2' | 25:BA:1579:A:H5' | 2.47 | 0.45 |
| 19:CV:51:VAL:HG23 | 19:CV:60:VAL:CG1 | 2.47 | 0.45 |
| 27:DD:145:VAL:HG13 | 27:DD:191:ALA:HB2 | 1.99 | 0.45 |
| 25:BA:850:C:O3' | 49:BX:49:LYS:HE2 | 2.17 | 0.45 |
| 28:BE:96:PHE:O | 28:BE:175:VAL:HG11 | 2.17 | 0.45 |
| 38:BQ:56:LEU:HB2 | 38:BQ:58:LEU:HD21 | 1.99 | 0.45 |
| 7:AJ:50:ILE:HB | 7:AJ:58:PRO:HG3 | 1.99 | 0.45 |
| 2:AE:160:ASP:O | 2:AE:183:PRO:HD2 | 2.17 | 0.45 |
| 13:AP:90:LEU:HA | 13:AP:93:ARG:HG3 | 1.98 | 0.45 |
| 32:DK:31:LEU:N | 32:DK:32:PRO:HD2 | 2.30 | 0.45 |
| 25:BA:1064:C:O2 | 25:BA:1075:C:C2 | 2.70 | 0.44 |
| 27:DD:43:ARG:NH1 | 27:DD:44:ASN:HD22 | 2.00 | 0.44 |
| 40:D1:92:ARG:NH1 | 41:D2:11:GLN:H | 2.15 | 0.44 |
| 28:BE:57:LYS:O | 28:BE:57:LYS:HD3 | 2.17 | 0.44 |
| 28:DE:50:GLY:CA | 28:DE:74:PRO:HG3 | 2.47 | 0.44 |
| 44:BU:96:ILE:N | 44:BU:99:CYS:O | 2.50 | 0.44 |
| 25:BA:2371:G:H4' | 52:B6:45:LYS:HG3 | 1.98 | 0.44 |
| 10:CM:56:HIS:O | 10:CM:58:ASP:N | 2.50 | 0.44 |
| 47:DZ:88:LYS:HE2 | 47:DZ:88:LYS:HB3 | 1.68 | 0.44 |
| 2:CE:166:ASP:OD1 | 2:CE:205:ASP:OD2 | 2.35 | 0.44 |
| 1:CA:1158:C:C2 | 1:CA:1160:G:N7 | 2.85 | 0.44 |
| 45:BV:62:PRO:C | 45:BV:64:GLY:N | 2.69 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 35:BO:50:ARG:NH2 | 35:BO:50:ARG:CG | 2.71 | 0.44 |
| 25:BA:1161:C:H4' | 41:B2:8:GLY:HA2 | 1.99 | 0.44 |
| 26:BB:29:A:C2 | 26:BB:30:C:C2 | 3.05 | 0.44 |
| 33:BM:95:PRO:O | 33:BM:96:GLU:O | 2.34 | 0.44 |
| 25:DA:676:A:H2 | 25:DA:802:A:H61 | 1.63 | 0.44 |
| 2:CE:237:ALA:O | 2:CE:238:LEU:CB | 2.65 | 0.44 |
| 29:DF:31:HIS:NE2 | 29:DF:35:GLU:OE1 | 2.48 | 0.44 |
| 37:B0:2:ARG:HG3 | 37:B0:5:LYS:HZ3 | 1.81 | 0.44 |
| 25:DA:660:G:H21 | 35:DO:12:ALA:CA | 2.22 | 0.44 |
| 25:DA:2523:G:C2' | 25:DA:2524:G:H5' | 2.47 | 0.44 |
| 34:BN:71:ARG:HD3 | 34:BN:105:GLU:OE2 | 2.17 | 0.44 |
| 3:AF:70:VAL:CG1 | 3:AF:71:ALA:N | 2.79 | 0.44 |
| 25:BA:1299:G:H5'' | 25:BA:1300:U:P | 2.57 | 0.44 |
| 1:AA:968:A:H4' | 1:AA:969:A:OP2 | 2.17 | 0.44 |
| 23:AC:1:C:H3' | 23:AC:1:C:H6 | 1.83 | 0.44 |
| 25:DA:1483:G:C2 | 25:DA:1484:G:C8 | 3.05 | 0.44 |
| 23:AD:53:G:N3 | 23:AD:64:G:N2 | 2.65 | 0.44 |
| 45:DV:10:ARG:NH2 | 45:DV:26:GLY:H | 2.14 | 0.44 |
| 45:DV:4:ARG:HA | 45:DV:58:VAL:HB | 1.99 | 0.44 |
| 1:AA:1371:G:C6 | 1:AA:1372:U:C4 | 3.05 | 0.44 |
| 1:CA:412:A:O2' | 1:CA:413:G:OP2 | 2.23 | 0.44 |
| 17:AT:65:ILE:HD12 | 17:AT:65:ILE:H | 1.82 | 0.44 |
| 50:B4:14:ILE:C | 50:B4:15:ILE:HG12 | 2.38 | 0.44 |
| 39:BR:107:ASP:N | 39:BR:107:ASP:OD1 | 2.51 | 0.44 |
| 35:DO:58:THR:CG2 | 35:DO:58:THR:O | 2.62 | 0.44 |
| 25:DA:962:G:O2' | 25:DA:963:U:H5' | 2.16 | 0.44 |
| 1:CA:1288:A:H1' | 1:CA:1352:C:O2' | 2.16 | 0.44 |
| 31:DH:12:PRO:HB3 | 31:DH:17:VAL:HG21 | 1.99 | 0.44 |
| 1:AA:626:U:N3 | 1:AA:627:G:N7 | 2.65 | 0.44 |
| 25:BA:649:G:C6 | 25:BA:650:C:N3 | 2.85 | 0.44 |
| 25:DA:445:C:OP1 | 40:D1:2:PRO:HA | 2.17 | 0.44 |
| 34:BN:35:VAL:HG11 | 34:BN:103:ALA:HB2 | 1.98 | 0.44 |
| 33:BM:54:VAL:HB | 33:BM:122:VAL:HG22 | 1.99 | 0.44 |
| 38:BQ:67:ARG:CB | 38:BQ:67:ARG:NH1 | 2.79 | 0.44 |
| 37:D0:78:LYS:O | 37:D0:82:GLU:HB2 | 2.17 | 0.44 |
| 25:DA:250:G:C6 | 25:DA:251:A:C6 | 3.05 | 0.44 |
| 42:BS:4:LYS:HB2 | 42:BS:106:ILE:HG22 | 1.99 | 0.44 |
| 48:BW:41:ILE:HD11 | 48:BW:44:LEU:HD12 | 1.99 | 0.44 |
| 40:D1:17:ILE:HD12 | 40:D1:32:PHE:CE2 | 2.52 | 0.44 |
| 25:BA:558:G:P | 33:BM:111:PRO:HG2 | 2.58 | 0.44 |
| 25:BA:2355:C:H1' | 46:B3:39:ARG:HH21 | 1.82 | 0.44 |
| 18:CU:50:ILE:HG22 | 18:CU:51:LEU:N | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 48:BW:53:LEU:O | 48:BW:57:ILE:HG13 | 2.18 | 0.44 |
| 26:DB:80:U:O2' | 26:DB:81:G:H5'' | 2.18 | 0.44 |
| 1:AA:648:A:C6 | 1:AA:649:G:C5 | 3.05 | 0.44 |
| 1:AA:386:C:C2' | 1:AA:387:U:H5' | 2.47 | 0.44 |
| 25:DA:1336:A:H2' | 25:DA:1337:G:C8 | 2.53 | 0.44 |
| 3:CF:60:ALA:HA | 10:CM:93:GLY:HA2 | 2.00 | 0.44 |
| 2:CE:87:ARG:NH1 | 2:CE:220:ASP:OD1 | 2.40 | 0.44 |
| 1:CA:723:U:C2' | 1:CA:724:G:OP1 | 2.64 | 0.44 |
| 16:AS:75:ARG:NH2 | 16:AS:80:PHE:CD2 | 2.85 | 0.44 |
| 25:BA:1489:U:HO2' | 25:BA:1490:A:H8 | 1.65 | 0.44 |
| 1:AA:1280:A:C8 | 10:AM:41:PRO:HD3 | 2.51 | 0.44 |
| 5:CH:141:GLN:HB2 | 5:CH:141:GLN:HE21 | 1.66 | 0.44 |
| 1:AA:901:A:C5 | 1:AA:902:G:H1' | 2.52 | 0.44 |
| 1:AA:909:A:H2' | 1:AA:910:C:O4' | 2.18 | 0.44 |
| 51:D5:4:HIS:CB | 51:D5:5:PRO:HD2 | 2.35 | 0.44 |
| 27:BD:33:LEU:CD1 | 27:BD:34:VAL:H | 2.30 | 0.44 |
| 33:DM:46:VAL:O | 33:DM:47:ALA:HB3 | 2.17 | 0.44 |
| 28:BE:84:PHE:CZ | 28:BE:86:PRO:HB3 | 2.52 | 0.44 |
| 1:AA:1055:A:C8 | 1:AA:1206:G:N2 | 2.85 | 0.44 |
| 1:CA:978:A:H8 | 1:CA:978:A:OP1 | 2.00 | 0.44 |
| 52:B6:14:THR:HG21 | 52:B6:19:ARG:HH21 | 1.83 | 0.44 |
| 1:AA:1037:C:H2' | 1:AA:1038:C:C5 | 2.52 | 0.44 |
| 25:DA:1021:A:C2 | 25:DA:1023:U:C2 | 3.06 | 0.44 |
| 39:DR:90:GLN:NE2 | 39:DR:121:ILE:HD11 | 2.33 | 0.44 |
| 25:BA:890:A:H2' | 25:BA:892:G:O4' | 2.17 | 0.44 |
| 48:DW:15:LYS:HE2 | 48:DW:67:LYS:CE | 2.47 | 0.44 |
| 25:DA:2271:G:C6 | 25:DA:2272:U:C4 | 3.05 | 0.44 |
| 44:DU:83:THR:HG23 | 44:DU:94:LYS:HG2 | 1.99 | 0.44 |
| 23:CD:6:G:O2' | 23:CD:7:G:H5' | 2.18 | 0.44 |
| 25:DA:1110:G:O2' | 25:DA:1111:A:O4' | 2.35 | 0.44 |
| 31:DH:4:ILE:CG1 | 31:DH:6:ARG:HG2 | 2.45 | 0.44 |
| 26:DB:44:G:OP1 | 30:DG:98:ARG:NH2 | 2.42 | 0.44 |
| 43:BT:84:ALA:HB1 | 43:BT:85:PRO:CD | 2.38 | 0.44 |
| 1:AA:210:U:O2' | 1:AA:216:G:C8 | 2.64 | 0.44 |
| 4:AG:173:TRP:CD2 | 4:AG:189:PRO:HB3 | 2.52 | 0.44 |
| 26:DB:8:U:O2' | 38:DQ:40:ILE:HD13 | 2.18 | 0.44 |
| 25:BA:782:A:H5' | 25:BA:783:A:C2 | 2.52 | 0.44 |
| 33:BM:94:HIS:C | 33:BM:95:PRO:O | 2.52 | 0.44 |
| 35:DO:41:ARG:N | 35:DO:41:ARG:HD2 | 2.32 | 0.44 |
| 46:D3:36:ILE:CD1 | 46:D3:36:ILE:H | 2.30 | 0.44 |
| 30:DG:111:LEU:HD13 | 30:DG:120:LEU:HD21 | 1.99 | 0.44 |
| 25:BA:1784:A:H4' | 25:BA:1785:A:O5' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 28:DE:55:ASN:C | 28:DE:57:LYS:N | 2.69 | 0.44 |
| 2:AE:165:VAL:O | 2:AE:187:LEU:O | 2.35 | 0.44 |
| 2:CE:85:ALA:HB3 | 2:CE:92:TYR:CD1 | 2.51 | 0.44 |
| 29:DF:123:LEU:O | 29:DF:124:LEU:C | 2.56 | 0.44 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:N1 | 2.13 | 0.44 |
| 40:B1:66:ASN:CB | 40:B1:76:TYR:HB2 | 2.42 | 0.44 |
| 3:CF:15:THR:HG21 | 3:CF:181:ASN:HA | 1.99 | 0.44 |
| 25:BA:1049:C:C2' | 25:BA:1050:A:H5' | 2.40 | 0.44 |
| 25:BA:2732:G:H3' | 25:BA:2733:A:O4' | 2.17 | 0.44 |
| 45:BV:140:ASP:OD1 | 45:BV:156:LYS:NZ | 2.50 | 0.44 |
| 23:AD:8:U:C2 | 23:AD:15:G:O6 | 2.70 | 0.44 |
| 1:CA:585:G:C6 | 1:CA:586:C:C4 | 3.06 | 0.44 |
| 35:BO:3:LEU:HA | 35:BO:3:LEU:HD23 | 1.74 | 0.44 |
| 8:AK:49:GLU:O | 8:AK:51:VAL:HG13 | 2.17 | 0.44 |
| 13:CP:92:HIS:CE1 | 13:CP:98:VAL:HG21 | 2.52 | 0.44 |
| 25:DA:1771:C:H1' | 25:DA:1786:A:H8 | 1.72 | 0.44 |
| 36:DP:135:ASP:OD1 | 36:DP:137:TYR:CD2 | 2.66 | 0.44 |
| 1:AA:428:G:H4' | 1:AA:429:U:O5' | 2.17 | 0.44 |
| 4:CG:162:LEU:HD22 | 4:CG:178:VAL:HG13 | 1.99 | 0.44 |
| 27:BD:221:VAL:HG22 | 27:BD:226:MET:CE | 2.47 | 0.44 |
| 2:AE:87:ARG:HE | 2:AE:233:SER:CB | 2.30 | 0.44 |
| 14:CQ:43:CYS:HA | 14:CQ:46:GLU:HB2 | 1.98 | 0.44 |
| 25:BA:1528:A:N1 | 25:BA:1543:A:C2 | 2.85 | 0.44 |
| 25:DA:566:U:H5'' | 35:DO:29:LYS:HE2 | 1.99 | 0.44 |
| 1:AA:68:G:C2 | 1:AA:69:G:C4 | 3.05 | 0.44 |
| 3:CF:164:ARG:HG2 | 3:CF:165:THR:N | 2.30 | 0.44 |
| 31:DH:149:ARG:CG | 31:DH:162:ILE:O | 2.64 | 0.44 |
| 1:AA:1179:A:C6 | 1:AA:1180:A:C2 | 3.05 | 0.44 |
| 25:DA:637:A:H5'' | 35:DO:117:GLU:HG3 | 1.98 | 0.44 |
| 1:CA:793:U:C6 | 1:CA:1516:G:O2' | 2.71 | 0.44 |
| 41:B2:22:VAL:CG1 | 41:B2:23:GLU:N | 2.80 | 0.44 |
| 40:B1:34:LYS:HA | 40:B1:34:LYS:HE3 | 1.99 | 0.44 |
| 25:BA:1043:C:H2' | 25:BA:1044:G:H5' | 1.98 | 0.44 |
| 25:BA:635:C:O2' | 25:BA:639:U:OP1 | 2.30 | 0.44 |
| 5:AH:71:LEU:HD11 | 5:AH:114:GLY:HA3 | 1.98 | 0.44 |
| 27:BD:10:THR:OG1 | 27:BD:13:ARG:HB2 | 2.17 | 0.44 |
| 1:CA:718:G:O6 | 18:CU:74:ARG:NH1 | 2.50 | 0.44 |
| 32:BK:4:ILE:HD11 | 32:BK:44:LEU:HD12 | 1.99 | 0.44 |
| 3:CF:52:LEU:H | 3:CF:52:LEU:HD23 | 1.82 | 0.44 |
| 1:CA:134:A:H61 | 16:CS:25:ARG:NH1 | 2.15 | 0.44 |
| 1:CA:649:G:O2' | 1:CA:650:G:H5' | 2.16 | 0.44 |
| 1:CA:1204:A:P | 14:CQ:3:ARG:HH12 | 2.40 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:616:G:C2 | 1:CA:617:G:C8 | 3.04 | 0.44 |
| 47:BZ:7:ILE:HD12 | 47:BZ:62:VAL:HG11 | 1.98 | 0.44 |
| 16:AS:53:VAL:HG12 | 16:AS:79:VAL:HG22 | 1.99 | 0.44 |
| 11:CN:17:GLY:O | 11:CN:80:VAL:HA | 2.17 | 0.44 |
| 44:DU:24:VAL:HG12 | 44:DU:25:GLY:N | 2.32 | 0.44 |
| 25:DA:2505:G:O2' | 25:DA:2506:U:C6 | 2.65 | 0.44 |
| 33:BM:107:LEU:HD12 | 33:BM:117:PHE:HB2 | 1.99 | 0.44 |
| 40:D1:102:GLU:O | 40:D1:105:VAL:HG23 | 2.16 | 0.44 |
| 41:D2:72:VAL:HG12 | 41:D2:72:VAL:O | 2.16 | 0.44 |
| 27:BD:85:ASP:HB2 | 27:BD:92:ILE:HD13 | 2.00 | 0.44 |
| 16:AS:26:ARG:HD2 | 16:AS:31:LYS:O | 2.17 | 0.44 |
| 52:D6:41:PRO:HD3 | 52:D6:47:THR:HG22 | 1.99 | 0.44 |
| 26:BB:43:C:P | 30:BG:67:LYS:NZ | 2.90 | 0.44 |
| 27:DD:27:THR:HG23 | 27:DD:28:GLU:N | 2.32 | 0.44 |
| 25:DA:1075:C:H2' | 25:DA:1076:C:H6 | 1.81 | 0.44 |
| 20:AW:33:ILE:CG2 | 20:AW:63:ILE:HG12 | 2.47 | 0.44 |
| 25:BA:1510:A:H2' | 25:BA:1510:A:N3 | 2.33 | 0.44 |
| 25:BA:1558:A:H1' | 25:BA:1559:G:OP2 | 2.17 | 0.44 |
| 25:DA:1652:A:H2' | 25:DA:1653:G:H5' | 1.98 | 0.44 |
| 1:AA:686:U:O2' | 1:AA:687:A:C5' | 2.65 | 0.44 |
| 25:BA:2168:G:C2 | 25:BA:2170:A:OP2 | 2.70 | 0.44 |
| 45:DV:150:LEU:O | 45:DV:170:THR:O | 2.35 | 0.44 |
| 25:BA:2156:G:C2 | 25:BA:2157:G:N2 | 2.86 | 0.44 |
| 27:BD:28:GLU:O | 27:BD:29:PRO:O | 2.35 | 0.44 |
| 25:DA:1864:U:C3' | 25:DA:1869:G:H5'' | 2.46 | 0.44 |
| 28:BE:26:ILE:HD11 | 28:BE:198:VAL:CG2 | 2.38 | 0.44 |
| 28:DE:68:ALA:C | 28:DE:70:ALA:H | 2.19 | 0.44 |
| 51:B5:56:LYS:N | 51:B5:56:LYS:HD2 | 2.25 | 0.44 |
| 52:B6:24:GLU:HG3 | 52:B6:25:LYS:N | 2.31 | 0.44 |
| 25:BA:1299:G:H3' | 25:BA:1639:U:O4 | 2.18 | 0.44 |
| 1:AA:926:G:H5'' | 1:AA:927:G:O5' | 2.18 | 0.44 |
| 1:CA:411:A:C2 | 1:CA:431:A:N6 | 2.85 | 0.44 |
| 25:BA:1264:G:H5' | 51:B5:11:THR:HG23 | 1.96 | 0.44 |
| 1:AA:167:G:H2' | 1:AA:168:G:H5' | 1.99 | 0.44 |
| 25:DA:1416:G:C2' | 25:DA:1417:C:C6 | 3.01 | 0.44 |
| 18:CU:22:VAL:CG1 | 18:CU:56:THR:HA | 2.44 | 0.44 |
| 27:BD:147:LEU:HD13 | 27:BD:155:LEU:HD21 | 1.99 | 0.44 |
| 1:AA:310:G:OP2 | 16:AS:27:LYS:NZ | 2.42 | 0.44 |
| 39:DR:51:ARG:CG | 39:DR:98:LYS:HG3 | 2.47 | 0.44 |
| 25:BA:580:C:O2' | 25:BA:581:C:H5' | 2.18 | 0.44 |
| 25:DA:2198:A:C2 | 32:DK:29:TYR:HB2 | 2.53 | 0.44 |
| 25:BA:142:G:C1' | 43:BT:37:THR:HG21 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|---------------------|-------------|----------|
| 25:BA:2250:G:C5 | 36:BP:82:ARG:CD | 3.00 | 0.44 |
| 25:DA:1404:C:C2' | 25:DA:1404:C:O2 | 2.65 | 0.44 |
| 25:BA:1699:G:H4' | 25:BA:1700:A:OP2 | 2.17 | 0.44 |
| 1:CA:1153:C:N3 | 1:CA:1154:G:C8 | 2.85 | 0.44 |
| 45:BV:107:THR:HB | 45:BV:108:PRO:CD | 2.46 | 0.44 |
| 42:BS:1:MET:HG3 | 42:BS:64:MET:CE | 2.48 | 0.44 |
| 25:BA:991:C:C5 | 25:BA:1185:C:N4 | 2.85 | 0.44 |
| 25:BA:639:U:C2' | 25:BA:640:C:H5' | 2.47 | 0.44 |
| 46:B3:11:ARG:HH11 | 46:B3:11:ARG:HB2 | 1.83 | 0.44 |
| 25:DA:1443:G:H8 | 25:DA:1443:G:H5'' | 1.81 | 0.44 |
| 25:BA:445:C:C2' | 25:BA:446:G:H5' | 2.48 | 0.44 |
| 20:CW:80:ARG:O | 20:CW:84:LEU:HB2 | 2.18 | 0.44 |
| 1:CA:373:A:C4 | 1:CA:374:A:C8 | 3.06 | 0.44 |
| 1:AA:1260:C:O5' | 1:AA:1284:C:H4' | 2.17 | 0.44 |
| 25:DA:1797:C:H4' | 27:DD:257:LEU:O | 2.18 | 0.44 |
| 32:DK:85:GLU:O | 32:DK:85:GLU:HG2 | 2.18 | 0.44 |
| 1:AA:1218:C:H2' | 1:AA:1219:U:C6 | 2.53 | 0.44 |
| 11:AN:99:GLN:HG2 | 11:AN:105:VAL:CG2 | 2.48 | 0.44 |
| 14:AQ:12:ARG:C | 14:AQ:14:PRO:CD | 2.86 | 0.44 |
| 1:AA:864:A:H5'' | 1:AA:865:A:OP2 | 2.17 | 0.44 |
| 25:DA:1229:G:N2 | 25:DA:1229(A):G:H1' | 2.33 | 0.44 |
| 25:BA:2746:U:H2' | 25:BA:2747:G:H5' | 1.98 | 0.44 |
| 1:AA:760:G:O2' | 17:AT:98:LEU:HD23 | 2.16 | 0.44 |
| 12:CO:53:ARG:HH12 | 12:CO:92:ASP:HB3 | 1.81 | 0.44 |
| 36:DP:41:TRP:HZ3 | 36:DP:74:TYR:HE1 | 1.66 | 0.44 |
| 41:D2:20:LEU:O | 41:D2:93:GLU:HA | 2.17 | 0.44 |
| 25:DA:2107:C:H42 | 25:DA:2182:G:H1 | 1.65 | 0.44 |
| 20:AW:42:GLN:O | 20:AW:46:GLU:HG2 | 2.18 | 0.44 |
| 2:CE:167:PRO:HG2 | 2:CE:192:SER:OG | 2.17 | 0.44 |
| 25:BA:2086:U:H2' | 25:BA:2087:G:C8 | 2.52 | 0.44 |
| 48:DW:68:ARG:HG3 | 48:DW:68:ARG:HH11 | 1.83 | 0.44 |
| 8:AK:15:ASN:O | 8:AK:19:VAL:HG22 | 2.17 | 0.44 |
| 25:BA:2468:G:O2' | 25:BA:2469:A:OP2 | 2.30 | 0.44 |
| 25:BA:631:A:H2' | 25:BA:632:A:O4' | 2.17 | 0.44 |
| 1:AA:1160:G:C6 | 1:AA:1181:G:O6 | 2.69 | 0.44 |
| 40:D1:62:ILE:HG13 | 40:D1:76:TYR:CZ | 2.52 | 0.44 |
| 40:D1:50:ARG:NH1 | 41:D2:72:VAL:HG22 | 2.32 | 0.44 |
| 28:BE:3:GLY:O | 28:BE:4:ILE:HB | 2.17 | 0.44 |
| 28:BE:59:VAL:O | 28:BE:59:VAL:HG13 | 2.16 | 0.44 |
| 29:DF:64:ILE:HD11 | 29:DF:83:PHE:HZ | 1.82 | 0.44 |
| 53:D7:8:ASN:HD21 | 53:D7:11:LYS:H | 1.51 | 0.44 |
| 44:BU:81:LYS:HG2 | 44:BU:97:ARG:HD3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:448:A:C4 | 1:CA:487:A:C2 | 3.05 | 0.44 |
| 22:CB:22:G:H3' | 22:CB:22:G:C8 | 2.53 | 0.44 |
| 25:DA:1060:U:N3 | 25:DA:1088:A:C8 | 2.85 | 0.44 |
| 46:B3:23:VAL:HG13 | 46:B3:38:VAL:CG2 | 2.47 | 0.44 |
| 1:AA:1202:G:C2 | 14:AQ:42:ILE:HG21 | 2.52 | 0.44 |
| 44:DU:81:LYS:HD3 | 44:DU:97:ARG:NH2 | 2.31 | 0.44 |
| 25:DA:1109:C:C5 | 25:DA:1110:G:C6 | 3.06 | 0.44 |
| 1:CA:181:G:O2' | 1:CA:183:G:O6 | 2.29 | 0.44 |
| 25:BA:1021:A:C8 | 25:BA:1021:A:H3' | 2.53 | 0.44 |
| 1:CA:1130:A:O5' | 1:CA:1131:G:OP2 | 2.35 | 0.44 |
| 1:CA:1129:C:N4 | 1:CA:1139:G:N2 | 2.66 | 0.44 |
| 25:DA:1301:A:N3 | 25:DA:1301:A:H2' | 2.33 | 0.44 |
| 34:DN:23:ARG:HG3 | 34:DN:24:VAL:N | 2.32 | 0.44 |
| 16:AS:34:GLU:HG2 | 16:AS:35:LYS:N | 2.32 | 0.44 |
| 25:DA:1359:A:H2' | 25:DA:1360:A:H5' | 2.00 | 0.44 |
| 1:CA:812:C:HO2' | 1:CA:813:U:P | 2.40 | 0.44 |
| 25:BA:229:A:O2' | 25:BA:230:U:P | 2.75 | 0.44 |
| 2:CE:164:VAL:O | 2:CE:186:ALA:HB1 | 2.17 | 0.44 |
| 6:AI:99:ALA:C | 6:AI:101:ALA:H | 2.21 | 0.44 |
| 25:DA:84:A:P | 44:DU:8:LYS:HD3 | 2.58 | 0.44 |
| 10:AM:8:LEU:CD2 | 10:AM:96:ILE:HG22 | 2.47 | 0.44 |
| 29:DF:132:VAL:HG22 | 29:DF:133:ASN:N | 2.24 | 0.44 |
| 38:DQ:19:LYS:O | 38:DQ:20:ARG:HB3 | 2.17 | 0.44 |
| 1:AA:218:C:O2' | 1:AA:219:C:H5' | 2.17 | 0.44 |
| 13:CP:81:LEU:HD22 | 13:CP:88:ARG:NH1 | 2.33 | 0.44 |
| 1:CA:197:A:H8 | 1:CA:198:G:C1' | 2.30 | 0.44 |
| 25:DA:686:G:O6 | 53:D7:12:ARG:HG3 | 2.17 | 0.44 |
| 25:BA:2470:G:O5' | 25:BA:2470:G:H8 | 2.00 | 0.44 |
| 25:BA:1464:C:O2' | 25:BA:1528:A:C8 | 2.66 | 0.44 |
| 1:CA:719:C:N4 | 18:CU:71:LYS:HE2 | 2.32 | 0.44 |
| 10:CM:4:ILE:HB | 10:CM:74:ILE:HG13 | 1.99 | 0.44 |
| 3:CF:73:PRO:HA | 3:CF:76:VAL:HG22 | 1.99 | 0.44 |
| 19:AV:24:ALA:C | 19:AV:26:GLY:H | 2.21 | 0.44 |
| 1:CA:1028(B):C:N4 | 1:CA:1032(B):G:N1 | 2.65 | 0.44 |
| 1:AA:1098:C:C2 | 1:AA:1099:G:C8 | 3.05 | 0.44 |
| 3:AF:34:LEU:CD2 | 3:AF:38:ARG:HH11 | 2.29 | 0.44 |
| 25:DA:2548:G:H2' | 25:DA:2549:G:O5' | 2.18 | 0.44 |
| 25:DA:1542:G:H5'' | 25:DA:1543:A:O5' | 2.17 | 0.44 |
| 26:BB:94:C:O2' | 26:BB:95:U:H5' | 2.17 | 0.44 |
| 8:CK:49:GLU:O | 8:CK:51:VAL:HG13 | 2.18 | 0.44 |
| 27:DD:96:HIS:CE1 | 27:DD:102:LYS:HE2 | 2.53 | 0.44 |
| 25:DA:57:C:H2' | 25:DA:58:G:O5' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:775:G:H2' | 1:CA:776:G:O4' | 2.17 | 0.44 |
| 42:BS:45:TYR:CE2 | 42:BS:49:LYS:HD2 | 2.51 | 0.44 |
| 25:BA:1844:C:H5'' | 27:BD:258:LYS:HG3 | 1.98 | 0.44 |
| 25:BA:1564:C:O2' | 25:BA:1565:C:H5' | 2.17 | 0.44 |
| 42:BS:2:GLU:OE1 | 42:BS:72:LYS:NZ | 2.49 | 0.44 |
| 35:DO:125:VAL:HG22 | 35:DO:125:VAL:O | 2.17 | 0.44 |
| 18:CU:58:LEU:H | 18:CU:58:LEU:HD12 | 1.82 | 0.44 |
| 32:DK:54:GLN:HB2 | 32:DK:54:GLN:HE21 | 1.52 | 0.44 |
| 34:BN:106:LEU:HD23 | 34:BN:106:LEU:HA | 1.63 | 0.44 |
| 30:BG:45:GLU:H | 30:BG:45:GLU:HG2 | 1.50 | 0.44 |
| 10:AM:25:GLU:HG2 | 10:AM:25:GLU:H | 1.64 | 0.44 |
| 30:DG:137:GLU:HB3 | 30:DG:152:LEU:HD22 | 1.99 | 0.44 |
| 25:DA:2881:C:C4 | 25:DA:2882:A:N7 | 2.86 | 0.44 |
| 29:DF:162:LEU:N | 29:DF:162:LEU:HD12 | 2.33 | 0.44 |
| 5:CH:94:ALA:HB1 | 5:CH:98:THR:OG1 | 2.17 | 0.44 |
| 25:BA:1060:U:H3 | 25:BA:1088:A:H8 | 1.66 | 0.44 |
| 25:DA:2286:A:C8 | 25:DA:2287:A:N6 | 2.86 | 0.44 |
| 28:BE:197:ILE:HD11 | 28:BE:199:ARG:HE | 1.83 | 0.44 |
| 1:AA:1160:G:C2 | 1:AA:1177:G:N2 | 2.82 | 0.44 |
| 27:DD:33:LEU:HD23 | 27:DD:34:VAL:H | 1.83 | 0.44 |
| 25:DA:997:G:C2 | 25:DA:998:C:C6 | 3.05 | 0.44 |
| 27:BD:30:GLU:CG | 27:BD:63:ARG:HH21 | 2.30 | 0.44 |
| 23:AC:17:C:O2 | 23:AC:17:C:C2' | 2.64 | 0.44 |
| 1:CA:1023:G:C6 | 1:CA:1024:G:N7 | 2.86 | 0.44 |
| 33:BM:4:TYR:O | 40:B1:64:ARG:NH1 | 2.51 | 0.44 |
| 33:BM:35:ARG:HB3 | 33:BM:116:LEU:CD1 | 2.47 | 0.44 |
| 9:AL:16:ARG:NH2 | 9:AL:64:THR:HG21 | 2.33 | 0.44 |
| 1:AA:1331:G:OP2 | 13:AP:23:TYR:HD2 | 2.01 | 0.44 |
| 13:AP:8:GLU:OE1 | 13:AP:67:GLU:HG3 | 2.18 | 0.44 |
| 45:DV:72:ARG:HA | 45:DV:72:ARG:HD2 | 1.83 | 0.44 |
| 25:DA:1057:A:H61 | 25:DA:1080:A:N6 | 2.16 | 0.44 |
| 29:DF:18:ARG:C | 29:DF:19:GLU:HG2 | 2.38 | 0.44 |
| 13:CP:39:ILE:CD1 | 13:CP:56:LEU:HG | 2.47 | 0.44 |
| 54:B8:36:LYS:CB | 54:B8:40:GLU:CG | 2.88 | 0.44 |
| 1:CA:1129:C:N3 | 1:CA:1139:G:N1 | 2.66 | 0.44 |
| 43:BT:84:ALA:HB3 | 43:BT:87:GLN:HE22 | 1.80 | 0.44 |
| 1:AA:1301:U:C3' | 1:AA:1302:U:H5' | 2.46 | 0.44 |
| 1:CA:1238:A:C8 | 1:CA:1303:C:H1' | 2.52 | 0.44 |
| 39:BR:53:ARG:O | 39:BR:59:THR:CB | 2.66 | 0.44 |
| 48:DW:43:GLN:O | 48:DW:44:LEU:HD23 | 2.17 | 0.44 |
| 30:DG:117:PHE:HE1 | 30:DG:119:GLY:HA2 | 1.83 | 0.44 |
| 25:BA:657:U:H2' | 25:BA:658:C:C6 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:CO:60:LEU:HD12 | 12:CO:60:LEU:HA | 1.86 | 0.44 |
| 25:DA:2893:G:OP2 | 25:DA:2893:G:H8 | 2.00 | 0.44 |
| 25:BA:529:A:H8 | 25:BA:530:G:O6 | 2.00 | 0.44 |
| 9:AL:17:VAL:HG11 | 9:AL:81:ILE:HD13 | 2.00 | 0.44 |
| 1:CA:408:A:C2 | 1:CA:409:G:C4 | 3.05 | 0.44 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:N1 | 2.09 | 0.44 |
| 25:BA:2108:C:H2' | 25:BA:2109:U:O4' | 2.18 | 0.44 |
| 25:BA:1047:G:H2' | 25:BA:1110:G:H1 | 1.82 | 0.44 |
| 4:AG:111:ALA:HB2 | 4:AG:120:LEU:CD1 | 2.45 | 0.44 |
| 25:DA:1771:C:O2' | 25:DA:1786:A:H8 | 2.01 | 0.44 |
| 1:AA:659:U:O2' | 1:AA:660:G:H5' | 2.17 | 0.44 |
| 1:CA:505:G:C6 | 1:CA:535:A:C2 | 3.04 | 0.44 |
| 27:BD:228:PRO:HD3 | 27:BD:235:GLY:N | 2.31 | 0.44 |
| 25:BA:130:C:O3' | 25:BA:1349:A:H1' | 2.18 | 0.44 |
| 16:CS:40:ASP:O | 16:CS:48:TRP:HB2 | 2.18 | 0.44 |
| 1:AA:723:U:H5' | 1:AA:724:G:OP2 | 2.17 | 0.44 |
| 10:CM:99:LYS:CD | 10:CM:100:THR:H | 2.31 | 0.44 |
| 3:CF:71:ALA:HA | 3:CF:106:VAL:HB | 1.99 | 0.44 |
| 25:DA:872:A:C6 | 25:DA:906:G:C2 | 3.05 | 0.44 |
| 25:BA:2850:A:H5' | 25:BA:2868:A:H2 | 1.80 | 0.44 |
| 7:AJ:15:ASP:OD2 | 7:AJ:16:LEU:N | 2.51 | 0.44 |
| 25:DA:1171:G:C8 | 25:DA:1173:G:N3 | 2.86 | 0.44 |
| 1:CA:584:G:OP1 | 17:CT:91:ARG:NH1 | 2.50 | 0.44 |
| 25:BA:643:A:H2' | 25:BA:644:A:O5' | 2.16 | 0.44 |
| 1:AA:575:G:H4' | 1:AA:576:G:OP1 | 2.17 | 0.44 |
| 25:DA:1810:A:C2' | 25:DA:1811:G:H5' | 2.46 | 0.44 |
| 25:BA:2751:G:C6 | 31:BH:3:ARG:HB3 | 2.53 | 0.44 |
| 7:AJ:17:VAL:HG12 | 7:AJ:18:TYR:CD1 | 2.52 | 0.44 |
| 1:CA:1165:C:H42 | 1:CA:1171:G:H1 | 1.64 | 0.44 |
| 25:DA:1658:C:H2' | 25:DA:1659:U:C6 | 2.52 | 0.44 |
| 34:DN:66:LYS:HA | 34:DN:79:PHE:O | 2.17 | 0.44 |
| 1:CA:1480:G:C4 | 1:CA:1481:U:C6 | 3.06 | 0.44 |
| 1:CA:785:G:N2 | 1:CA:798:G:C4 | 2.86 | 0.44 |
| 25:BA:1847:A:H8 | 25:BA:1847:A:OP1 | 2.00 | 0.44 |
| 23:CD:77:A:C2 | 25:DA:2421:G:C6 | 3.06 | 0.44 |
| 1:CA:526:C:OP2 | 12:CO:91:LYS:HE2 | 2.17 | 0.44 |
| 25:DA:1432:C:H2' | 25:DA:1433:U:O4' | 2.18 | 0.44 |
| 36:DP:47:ILE:HG22 | 36:DP:48:GLU:N | 2.33 | 0.44 |
| 1:AA:1111:A:N1 | 3:AF:177:THR:HG23 | 2.32 | 0.44 |
| 42:BS:78:GLU:OE1 | 42:BS:99:ARG:HG2 | 2.17 | 0.44 |
| 46:B3:31:VAL:CG1 | 46:B3:67:VAL:HG23 | 2.47 | 0.44 |
| 29:DF:205:ARG:HB2 | 29:DF:205:ARG:NH1 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 47:BZ:94:LEU:HA | 47:BZ:94:LEU:HD23 | 1.78 | 0.44 |
| 42:DS:4:LYS:HE3 | 42:DS:6:ILE:HD11 | 2.00 | 0.44 |
| 25:BA:2194:G:H2' | 25:BA:2195:C:C6 | 2.53 | 0.44 |
| 36:DP:26:TYR:HD2 | 36:DP:26:TYR:C | 2.21 | 0.44 |
| 25:BA:1078:U:H6 | 25:BA:1078:U:H3' | 1.83 | 0.44 |
| 52:D6:31:PRO:O | 52:D6:32:ASN:CB | 2.65 | 0.44 |
| 25:DA:2287:A:C2 | 25:DA:2289:G:C8 | 3.05 | 0.44 |
| 38:BQ:106:ARG:CZ | 38:BQ:106:ARG:HB2 | 2.48 | 0.44 |
| 27:BD:77:ALA:CB | 27:BD:97:TYR:HA | 2.48 | 0.44 |
| 1:AA:1206:G:C5 | 1:AA:1207:G:N7 | 2.85 | 0.44 |
| 33:BM:42:TRP:CD1 | 40:B1:63:VAL:CG1 | 3.00 | 0.44 |
| 27:DD:28:GLU:OE2 | 27:DD:29:PRO:HD2 | 2.17 | 0.44 |
| 1:CA:448:A:H2' | 1:CA:449:C:O2 | 2.17 | 0.44 |
| 25:DA:1070:A:C8 | 25:DA:1096:A:O2' | 2.61 | 0.44 |
| 25:BA:2602:A:H4' | 25:BA:2603:G:C5' | 2.47 | 0.44 |
| 51:D5:46:CYS:HB3 | 51:D5:49:CYS:SG | 2.58 | 0.44 |
| 25:BA:892:G:H2' | 25:BA:893:C:C6 | 2.52 | 0.44 |
| 1:AA:819:A:C4' | 1:AA:820:U:OP2 | 2.60 | 0.44 |
| 9:AL:118:LYS:O | 9:AL:119:ALA:CB | 2.64 | 0.44 |
| 1:CA:1305:G:C8 | 1:CA:1305:G:OP2 | 2.71 | 0.44 |
| 26:DB:38:C:O4' | 38:DQ:95:HIS:CE1 | 2.71 | 0.44 |
| 30:BG:99:MET:HG3 | 30:BG:100:TRP:N | 2.31 | 0.44 |
| 40:B1:61:TRP:CD2 | 40:B1:94:ASN:HA | 2.53 | 0.44 |
| 1:AA:703:G:H4' | 1:AA:704:A:O5' | 2.16 | 0.44 |
| 31:DH:102:ALA:CB | 31:DH:116:GLU:HA | 2.47 | 0.44 |
| 20:AW:55:ILE:HA | 20:AW:55:ILE:HD13 | 1.89 | 0.44 |
| 1:CA:501:C:H2' | 1:CA:502:G:C8 | 2.51 | 0.44 |
| 49:BX:39:ASP:C | 49:BX:39:ASP:OD1 | 2.54 | 0.44 |
| 27:BD:166:GLN:CA | 27:BD:166:GLN:NE2 | 2.77 | 0.44 |
| 25:BA:1639:U:O2' | 25:BA:1640:C:H5'' | 2.18 | 0.44 |
| 46:B3:43:THR:O | 46:B3:43:THR:HG23 | 2.18 | 0.44 |
| 2:AE:178:ARG:CG | 2:AE:178:ARG:HH11 | 2.31 | 0.44 |
| 25:DA:1582:C:O2' | 25:DA:1586:A:H8 | 2.00 | 0.44 |
| 28:BE:11:MET:HG2 | 28:BE:24:THR:HA | 1.99 | 0.44 |
| 1:AA:104:G:C2 | 1:AA:105:G:C8 | 3.05 | 0.44 |
| 1:AA:658:G:O2' | 1:AA:659:U:H5' | 2.18 | 0.44 |
| 1:CA:197:A:C8 | 1:CA:198:G:H1' | 2.53 | 0.44 |
| 26:BB:71:C:C4 | 26:BB:72:G:N7 | 2.86 | 0.44 |
| 1:CA:1378:C:H5 | 1:CA:1379:G:C8 | 2.36 | 0.44 |
| 32:BK:130:TYR:CG | 32:BK:131:LYS:N | 2.86 | 0.44 |
| 1:CA:736:C:H2' | 1:CA:737:A:H8 | 1.81 | 0.44 |
| 7:AJ:16:LEU:HD11 | 9:AL:45:ALA:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:2847:U:C3' | 25:DA:2848:G:H5' | 2.47 | 0.44 |
| 44:DU:49:VAL:HG12 | 44:DU:50:ARG:H | 1.82 | 0.44 |
| 25:DA:1323:U:C2' | 25:DA:1324:G:H5' | 2.47 | 0.44 |
| 43:BT:57:LEU:O | 43:BT:57:LEU:HD13 | 2.18 | 0.44 |
| 25:BA:1337:G:H2' | 25:BA:1338:G:H8 | 1.81 | 0.44 |
| 30:DG:43:LEU:HD12 | 30:DG:45:GLU:CG | 2.48 | 0.44 |
| 1:CA:892:A:H2' | 1:CA:893:C:C6 | 2.53 | 0.44 |
| 25:DA:1475:G:C2 | 25:DA:1519:G:C2 | 3.06 | 0.44 |
| 25:DA:1466:G:H5' | 25:DA:1467:C:OP1 | 2.17 | 0.44 |
| 3:AF:84:ILE:HG13 | 3:AF:101:LEU:HD22 | 1.99 | 0.44 |
| 25:BA:1124:C:H2' | 25:BA:1125:G:O4' | 2.18 | 0.44 |
| 25:DA:2859:G:H8 | 25:DA:2859:G:H3' | 1.83 | 0.44 |
| 25:DA:65:C:O2' | 43:DT:69:TYR:CD2 | 2.69 | 0.44 |
| 13:CP:65:LYS:HB3 | 50:D4:49:PHE:HD1 | 1.82 | 0.44 |
| 1:CA:292:G:N7 | 1:CA:293:G:H1' | 2.33 | 0.44 |
| 32:BK:63:ALA:HA | 32:BK:66:GLU:HG2 | 1.98 | 0.44 |
| 6:AI:12:PRO:HG3 | 6:AI:57:GLN:O | 2.18 | 0.44 |
| 4:CG:39:PRO:O | 4:CG:44:GLY:HA3 | 2.17 | 0.44 |
| 25:BA:1443:G:C2 | 25:BA:1549:C:C2 | 3.06 | 0.44 |
| 16:AS:59:TRP:O | 16:AS:64:ALA:CB | 2.66 | 0.44 |
| 26:BB:35:U:H2' | 26:BB:36:C:C6 | 2.53 | 0.44 |
| 46:D3:69:PHE:CE2 | 46:D3:79:VAL:HG22 | 2.52 | 0.44 |
| 25:BA:453:C:H4' | 25:BA:472:A:N6 | 2.33 | 0.44 |
| 1:CA:287:U:O2' | 1:CA:288:A:H5' | 2.17 | 0.44 |
| 1:CA:29:G:O2' | 1:CA:295:C:H4' | 2.18 | 0.44 |
| 2:CE:108:ILE:HG22 | 2:CE:108:ILE:O | 2.18 | 0.44 |
| 25:DA:2300:G:N2 | 25:DA:2317:C:O2 | 2.51 | 0.44 |
| 25:BA:775:G:C4 | 25:BA:794:G:C8 | 3.06 | 0.44 |
| 41:B2:72:VAL:O | 41:B2:72:VAL:HG22 | 2.17 | 0.44 |
| 25:DA:405:U:O2 | 25:DA:405:U:H2' | 2.17 | 0.44 |
| 39:BR:88:ILE:HG13 | 39:BR:88:ILE:O | 2.18 | 0.44 |
| 30:DG:128:ARG:HA | 30:DG:128:ARG:HD3 | 1.84 | 0.44 |
| 1:CA:1203:C:H6 | 1:CA:1203:C:O5' | 2.01 | 0.44 |
| 30:DG:150:ASP:CG | 30:DG:151:ALA:H | 2.20 | 0.44 |
| 4:CG:18:LYS:HD2 | 4:CG:20:TYR:CZ | 2.53 | 0.44 |
| 25:BA:2468:G:H22 | 25:BA:2481:G:H2' | 1.83 | 0.44 |
| 1:AA:1176:A:N1 | 1:AA:1177:G:C2 | 2.86 | 0.44 |
| 27:DD:34:VAL:HG22 | 27:DD:35:LYS:HG3 | 1.99 | 0.44 |
| 38:DQ:110:LEU:HD22 | 38:DQ:112:PHE:H | 1.82 | 0.44 |
| 25:DA:1152:C:O2' | 25:DA:1153:C:H5' | 2.16 | 0.44 |
| 25:BA:2633:G:H5' | 25:BA:2811:G:O2' | 2.17 | 0.44 |
| 28:DE:25:VAL:CG1 | 28:DE:26:ILE:H | 2.23 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 28:DE:36:ARG:O | 28:DE:37:ARG:C | 2.56 | 0.44 |
| 1:CA:977:A:N3 | 1:CA:977:A:H2' | 2.31 | 0.44 |
| 1:CA:980:C:H3' | 1:CA:981:U:O4' | 2.18 | 0.44 |
| 1:CA:1061:G:C1' | 10:CM:56:HIS:CE1 | 3.00 | 0.44 |
| 2:CE:16:HIS:HB2 | 2:CE:210:SER:HB2 | 2.00 | 0.44 |
| 25:DA:1021:A:C6 | 25:DA:1023:U:C5 | 3.05 | 0.44 |
| 1:CA:1176:A:H2' | 1:CA:1177:G:O4' | 2.18 | 0.44 |
| 25:DA:2309:A:O5' | 25:DA:2310:A:OP2 | 2.36 | 0.44 |
| 1:AA:827:U:C4 | 1:AA:870:U:C4 | 3.06 | 0.44 |
| 1:AA:856:C:C2' | 1:AA:857:C:H5' | 2.47 | 0.44 |
| 44:BU:49:VAL:O | 44:BU:51:VAL:N | 2.51 | 0.44 |
| 29:BF:9:ILE:HD11 | 29:BF:125:LEU:CD1 | 2.48 | 0.44 |
| 9:CL:89:ASN:ND2 | 9:CL:89:ASN:N | 2.66 | 0.44 |
| 25:BA:2115:G:N1 | 25:BA:2117:A:C8 | 2.86 | 0.44 |
| 16:AS:21:VAL:O | 16:AS:33:ILE:N | 2.44 | 0.44 |
| 25:BA:2138:C:N3 | 25:BA:2154:G:N2 | 2.65 | 0.44 |
| 9:CL:92:TYR:HA | 9:CL:95:LYS:HG3 | 1.99 | 0.44 |
| 25:BA:2656:U:O2 | 25:BA:2656:U:H2' | 2.18 | 0.44 |
| 35:DO:128:HIS:O | 35:DO:147:LEU:HB3 | 2.16 | 0.44 |
| 51:B5:40:LYS:HB2 | 51:B5:46:CYS:SG | 2.57 | 0.44 |
| 7:CJ:23:VAL:HG13 | 7:CJ:43:PHE:CE2 | 2.52 | 0.44 |
| 1:CA:167:G:O2' | 1:CA:168:G:H5' | 2.18 | 0.44 |
| 25:DA:2864:G:C6 | 25:DA:2865:U:N3 | 2.86 | 0.44 |
| 1:AA:1092:A:C6 | 1:AA:1093:A:C6 | 3.05 | 0.44 |
| 25:DA:2530:A:C8 | 31:DH:157:TYR:OH | 2.71 | 0.44 |
| 23:AD:8:U:O5' | 23:AD:8:U:H6 | 2.01 | 0.44 |
| 25:DA:2219:G:H2' | 25:DA:2224:G:C5' | 2.46 | 0.44 |
| 25:DA:2149:G:C6 | 25:DA:2150:U:C4 | 3.06 | 0.44 |
| 6:AI:72:VAL:HG13 | 6:AI:73:ASN:N | 2.32 | 0.44 |
| 9:AL:83:ARG:CA | 9:AL:86:VAL:HG12 | 2.47 | 0.44 |
| 1:AA:724:G:C2' | 1:AA:725:G:H5' | 2.47 | 0.44 |
| 25:DA:2196:C:O2' | 25:DA:2197:U:H5' | 2.17 | 0.44 |
| 25:BA:2219:G:H2' | 25:BA:2224:G:H5' | 1.99 | 0.44 |
| 52:B6:33:LYS:HA | 52:B6:33:LYS:HD3 | 1.69 | 0.44 |
| 27:BD:149:PRO:O | 27:BD:150:LYS:HB2 | 2.18 | 0.44 |
| 23:AC:50:G:N2 | 23:AC:67:C:C2 | 2.86 | 0.44 |
| 45:BV:143:GLY:HA3 | 45:BV:144:LEU:CG | 2.48 | 0.44 |
| 1:CA:1489:G:H2' | 1:CA:1490:C:O4' | 2.17 | 0.44 |
| 2:CE:128:GLU:O | 2:CE:129:GLU:HB2 | 2.18 | 0.44 |
| 25:BA:1355:G:H8 | 25:BA:1355:G:O5' | 2.01 | 0.44 |
| 46:B3:12:ASN:HA | 46:B3:14:ARG:HH21 | 1.82 | 0.44 |
| 25:DA:1638:C:H2' | 25:DA:1639:U:O5' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 6:CI:14:LEU:HD23 | 6:CI:14:LEU:O | 2.16 | 0.44 |
| 12:AO:46:LYS:HG3 | 12:AO:47:LYS:H | 1.83 | 0.44 |
| 1:CA:587:G:N2 | 1:CA:754:C:OP2 | 2.50 | 0.44 |
| 1:AA:914:A:C6 | 1:AA:915:A:C5 | 3.06 | 0.44 |
| 25:BA:2348:U:O4 | 25:BA:2382:G:N1 | 2.51 | 0.44 |
| 26:DB:6:C:HO2' | 38:DQ:29:PHE:HE1 | 1.64 | 0.44 |
| 1:AA:1378:C:H1' | 7:AJ:76:ARG:HH12 | 1.83 | 0.44 |
| 25:DA:2386:C:H4' | 46:D3:55:ARG:O | 2.18 | 0.44 |
| 8:CK:61:VAL:HG12 | 8:CK:63:LEU:CD1 | 2.47 | 0.44 |
| 1:AA:64:G:H4' | 1:AA:65:U:H5' | 2.00 | 0.44 |
| 7:CJ:38:LEU:O | 7:CJ:42:ILE:HG13 | 2.18 | 0.44 |
| 1:AA:587:G:N2 | 1:AA:755:G:C5 | 2.86 | 0.44 |
| 1:CA:864:A:H2 | 1:CA:917:G:N3 | 2.16 | 0.44 |
| 25:BA:2323:G:H2' | 25:BA:2324:C:O4' | 2.18 | 0.44 |
| 25:DA:1832:C:N4 | 25:DA:1833:U:C4 | 2.86 | 0.44 |
| 33:BM:78:TYR:CD1 | 33:BM:78:TYR:N | 2.86 | 0.44 |
| 15:AR:47:LYS:HE2 | 15:AR:47:LYS:HB3 | 1.79 | 0.44 |
| 36:DP:26:TYR:C | 36:DP:26:TYR:CD2 | 2.91 | 0.44 |
| 25:BA:1063:G:C5 | 25:BA:1064:C:C5 | 3.06 | 0.44 |
| 25:BA:1069:A:C4' | 25:BA:1070:A:O5' | 2.66 | 0.44 |
| 28:BE:21:VAL:CG2 | 28:BE:21:VAL:O | 2.64 | 0.44 |
| 28:DE:6:GLY:HA2 | 28:DE:51:PHE:CZ | 2.53 | 0.44 |
| 1:CA:509:A:H5'' | 4:CG:55:ALA:HB2 | 1.99 | 0.44 |
| 1:AA:1026:G:O6 | 1:AA:1036:G:C2 | 2.71 | 0.44 |
| 39:DR:26:ASP:HB3 | 39:DR:91:ARG:HA | 1.97 | 0.44 |
| 25:BA:654(M):C:H3' | 25:BA:654(N):G:C8 | 2.53 | 0.44 |
| 25:BA:2210:G:H2' | 25:BA:2210:G:N3 | 2.33 | 0.44 |
| 27:BD:270:ILE:C | 27:BD:271:ILE:HG13 | 2.37 | 0.44 |
| 7:CJ:113:GLU:HB2 | 7:CJ:119:ARG:CG | 2.39 | 0.44 |
| 13:CP:84:ILE:HG22 | 13:CP:84:ILE:O | 2.18 | 0.44 |
| 19:CV:27:GLU:O | 19:CV:47:HIS:CE1 | 2.70 | 0.44 |
| 38:DQ:66:ALA:HA | 38:DQ:69:VAL:CG1 | 2.47 | 0.44 |
| 25:DA:2328:A:H2' | 25:DA:2329:G:O4' | 2.18 | 0.44 |
| 1:CA:1190:G:H3' | 3:CF:3:ASN:HD21 | 1.78 | 0.44 |
| 25:BA:1385:G:HO2' | 25:BA:1396:U:H6 | 1.58 | 0.44 |
| 2:AE:14:GLY:CA | 2:AE:209:ARG:HH21 | 2.27 | 0.44 |
| 33:DM:29:LYS:CA | 33:DM:29:LYS:HE2 | 2.45 | 0.44 |
| 45:DV:30:ASN:ND2 | 45:DV:32:HIS:H | 2.16 | 0.44 |
| 1:AA:380:G:N2 | 1:AA:384:G:C5 | 2.86 | 0.44 |
| 1:AA:383:A:H8 | 1:AA:383:A:O5' | 2.00 | 0.44 |
| 1:CA:421:U:C2' | 1:CA:421:U:O2 | 2.65 | 0.44 |
| 1:CA:197:A:H8 | 1:CA:198:G:N9 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:580:C:H2' | 25:BA:581:C:C6 | 2.52 | 0.44 |
| 1:AA:725:G:C2 | 1:AA:726:C:C6 | 3.05 | 0.44 |
| 1:AA:960:U:O2 | 1:AA:960:U:C2' | 2.66 | 0.44 |
| 4:CG:146:ILE:HD12 | 4:CG:146:ILE:H | 1.83 | 0.44 |
| 1:CA:843:U:H3' | 1:CA:848:C:O4' | 2.17 | 0.44 |
| 1:CA:513:C:N4 | 1:CA:538:G:H1 | 2.16 | 0.44 |
| 1:AA:741:G:H2' | 1:AA:742:G:O4' | 2.18 | 0.44 |
| 1:AA:90:C:C5 | 1:AA:91:C:C5 | 3.06 | 0.44 |
| 23:CD:23:G:N2 | 23:CD:24:C:O2 | 2.51 | 0.44 |
| 25:BA:646:A:H2' | 25:BA:647:G:O4' | 2.18 | 0.44 |
| 44:DU:90:LEU:CD2 | 44:DU:90:LEU:H | 2.30 | 0.44 |
| 1:AA:600:C:H2' | 1:AA:600:C:O2 | 2.17 | 0.44 |
| 1:AA:1245:A:C2 | 1:AA:1293:G:C2 | 3.06 | 0.44 |
| 25:DA:1436:G:O2' | 25:DA:1477:A:H4' | 2.17 | 0.44 |
| 25:BA:1111:A:O2' | 25:BA:1112:G:C4' | 2.66 | 0.44 |
| 25:BA:2767:C:H2' | 25:BA:2768:C:H6 | 1.82 | 0.44 |
| 16:CS:74:LEU:HA | 16:CS:74:LEU:HD22 | 1.82 | 0.44 |
| 5:AH:147:ASP:HA | 5:AH:150:ARG:NH1 | 2.32 | 0.44 |
| 34:DN:120:GLU:HG2 | 34:DN:122:LEU:HG | 1.99 | 0.44 |
| 25:BA:317:G:N2 | 25:BA:318:C:O2 | 2.51 | 0.44 |
| 25:DA:1921:G:O2' | 25:DA:1922:G:H5' | 2.17 | 0.44 |
| 1:CA:201:C:C4' | 1:CA:208:U:OP1 | 2.66 | 0.44 |
| 31:DH:69:ARG:HH12 | 31:DH:73:ALA:HB2 | 1.83 | 0.44 |
| 7:AJ:46:ALA:HA | 7:AJ:49:ILE:HG13 | 1.98 | 0.44 |
| 1:AA:1493:A:H5'' | 1:AA:1494:G:OP2 | 2.18 | 0.44 |
| 6:CI:6:VAL:HG22 | 6:CI:90:VAL:HG22 | 1.99 | 0.44 |
| 25:BA:1773:A:H2' | 25:BA:1774:C:H5' | 1.99 | 0.44 |
| 26:DB:35:U:O2' | 26:DB:36:C:H5' | 2.18 | 0.44 |
| 25:DA:740:U:H2' | 25:DA:741:G:C8 | 2.53 | 0.44 |
| 8:AK:37:ARG:HB3 | 8:AK:37:ARG:HE | 1.39 | 0.44 |
| 7:AJ:104:LEU:HA | 7:AJ:104:LEU:HD13 | 1.71 | 0.44 |
| 17:CT:31:LEU:HD12 | 17:CT:31:LEU:HA | 1.78 | 0.44 |
| 12:AO:71:PRO:O | 12:AO:102:ARG:HD3 | 2.17 | 0.44 |
| 12:AO:104:VAL:HG12 | 12:AO:105:TYR:CD1 | 2.53 | 0.44 |
| 42:DS:26:GLY:HA2 | 42:DS:71:VAL:O | 2.17 | 0.44 |
| 30:BG:82:LEU:HD22 | 30:BG:83:ARG:N | 2.33 | 0.44 |
| 25:BA:2361:A:O5' | 54:B8:27:THR:OG1 | 2.35 | 0.44 |
| 25:DA:2419:U:O4 | 54:D8:31:HIS:CD2 | 2.70 | 0.44 |
| 27:DD:35:LYS:HD3 | 27:DD:63:ARG:CB | 2.46 | 0.44 |
| 25:DA:1009:A:OP2 | 25:DA:1010:A:OP2 | 2.36 | 0.44 |
| 28:BE:51:PHE:N | 28:BE:76:ARG:O | 2.47 | 0.44 |
| 31:DH:151:ILE:C | 31:DH:152:ARG:CG | 2.64 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 30:BG:63:ILE:HD12 | 30:BG:141:PHE:CE2 | 2.53 | 0.44 |
| 47:DZ:95:LEU:C | 47:DZ:97:LEU:H | 2.22 | 0.44 |
| 25:DA:1341:U:OP2 | 25:DA:1394:U:O2' | 2.21 | 0.44 |
| 25:BA:70:G:H4' | 25:BA:71:A:OP1 | 2.16 | 0.44 |
| 2:AE:21:ARG:C | 2:AE:23:ARG:N | 2.72 | 0.44 |
| 1:AA:344:A:H5'' | 1:AA:345:C:P | 2.58 | 0.44 |
| 2:CE:72:GLY:HA3 | 2:CE:165:VAL:CG2 | 2.48 | 0.44 |
| 28:BE:101:ARG:HD2 | 28:BE:101:ARG:HA | 1.55 | 0.44 |
| 9:AL:111:ARG:NH2 | 10:AM:62:HIS:HE1 | 2.16 | 0.44 |
| 44:DU:75:ILE:HG13 | 44:DU:76:CYS:N | 2.32 | 0.44 |
| 26:DB:4:C:N3 | 26:DB:117:G:N2 | 2.66 | 0.44 |
| 1:CA:1127:G:C2 | 1:CA:1145:C:C2 | 3.06 | 0.44 |
| 1:CA:706:A:C4' | 11:CN:29:ILE:HD11 | 2.48 | 0.44 |
| 10:CM:81:THR:O | 10:CM:84:GLN:N | 2.51 | 0.44 |
| 44:DU:71:LYS:HG3 | 44:DU:71:LYS:HZ3 | 1.59 | 0.44 |
| 40:B1:90:VAL:O | 40:B1:91:ASP:C | 2.55 | 0.44 |
| 38:BQ:34:HIS:CB | 38:BQ:36:TYR:HE1 | 2.19 | 0.44 |
| 38:BQ:70:GLY:CA | 38:BQ:101:LEU:HD13 | 2.47 | 0.44 |
| 43:DT:49:VAL:HB | 43:DT:83:VAL:HG21 | 1.99 | 0.44 |
| 45:DV:131:ARG:HD2 | 45:DV:131:ARG:H | 1.82 | 0.44 |
| 2:CE:71:VAL:HG13 | 2:CE:93:VAL:HB | 1.99 | 0.44 |
| 33:BM:15:LEU:O | 33:BM:136:GLU:HA | 2.18 | 0.44 |
| 35:DO:147:LEU:CD2 | 35:DO:148:LEU:H | 2.31 | 0.44 |
| 1:CA:1191:A:OP1 | 3:CF:3:ASN:ND2 | 2.50 | 0.44 |
| 1:AA:1387:G:C6 | 1:AA:1388:C:N4 | 2.86 | 0.44 |
| 1:AA:474:G:C2 | 1:AA:475:G:C5 | 3.06 | 0.44 |
| 30:BG:115:ARG:HB3 | 30:BG:115:ARG:HH11 | 1.82 | 0.44 |
| 25:BA:101:G:H3' | 25:BA:102:G:H5' | 2.00 | 0.44 |
| 25:DA:1027:A:C2 | 25:DA:2488:A:H5' | 2.53 | 0.44 |
| 1:AA:200:G:H1 | 1:AA:217:C:N4 | 2.13 | 0.44 |
| 25:BA:270(L):U:C2 | 32:BK:50:ARG:HD2 | 2.53 | 0.44 |
| 25:BA:1800:C:OP1 | 27:BD:266:SER:OG | 2.33 | 0.44 |
| 25:BA:1799:G:C5' | 25:BA:1819:A:H61 | 2.29 | 0.44 |
| 3:AF:64:VAL:HG21 | 3:AF:99:VAL:HG12 | 1.98 | 0.44 |
| 25:BA:2688:U:H1' | 25:BA:2721:A:N6 | 2.33 | 0.44 |
| 42:BS:70:TYR:N | 42:BS:70:TYR:CD2 | 2.83 | 0.44 |
| 20:CW:53:LEU:CB | 20:CW:102:GLY:HA3 | 2.48 | 0.44 |
| 25:BA:2590:A:H2' | 25:BA:2591:C:H6 | 1.83 | 0.44 |
| 25:BA:602:G:H3' | 25:BA:654(V):A:H61 | 1.83 | 0.44 |
| 1:CA:1288:A:H2' | 1:CA:1289:A:H8 | 1.82 | 0.44 |
| 27:BD:123:ALA:HB1 | 27:BD:131:LEU:HG | 2.00 | 0.44 |
| 25:DA:2516:G:C6 | 25:DA:2517:C:N4 | 2.86 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:538:G:OP2 | 12:CO:115:LYS:HB2 | 2.18 | 0.44 |
| 25:BA:1668:A:OP1 | 34:BN:5:GLN:HG3 | 2.18 | 0.44 |
| 25:DA:2351:G:H1' | 25:DA:2366:A:H61 | 1.83 | 0.44 |
| 25:DA:2351:G:H8 | 25:DA:2351:G:O5' | 2.01 | 0.44 |
| 1:AA:929:G:C2 | 1:AA:1389:C:C2 | 3.05 | 0.44 |
| 1:CA:888:G:O2' | 1:CA:1488:G:O2' | 2.34 | 0.44 |
| 7:CJ:69:VAL:HG22 | 7:CJ:135:VAL:CG2 | 2.48 | 0.44 |
| 7:CJ:72:ARG:HB2 | 7:CJ:142:GLU:OE2 | 2.18 | 0.44 |
| 25:DA:653:A:H5'' | 25:DA:654:A:P | 2.57 | 0.44 |
| 25:DA:2064:C:H2' | 25:DA:2065:C:C6 | 2.53 | 0.44 |
| 25:DA:729:G:C5 | 27:DD:208:LYS:HB2 | 2.53 | 0.44 |
| 32:DK:47:LEU:HA | 32:DK:50:ARG:HG2 | 1.99 | 0.44 |
| 1:CA:358:U:C5 | 1:CA:359:U:C5 | 3.05 | 0.44 |
| 25:DA:1585:C:O2 | 25:DA:1585:C:C2' | 2.66 | 0.44 |
| 50:B4:48:ARG:HA | 50:B4:48:ARG:HD2 | 1.73 | 0.44 |
| 9:AL:50:LEU:HD22 | 9:AL:55:ALA:HB3 | 1.99 | 0.44 |
| 9:AL:23:ASN:OD1 | 9:AL:25:LYS:HB3 | 2.18 | 0.44 |
| 25:DA:981:A:N1 | 25:DA:2027:G:O2' | 2.48 | 0.44 |
| 1:CA:742:G:OP1 | 15:CR:35:ARG:NH2 | 2.51 | 0.44 |
| 25:DA:1349:A:H5' | 25:DA:1350:C:C5' | 2.47 | 0.44 |
| 25:BA:1000:A:C6 | 25:BA:1001:A:C6 | 3.06 | 0.44 |
| 25:DA:1716:U:H2' | 25:DA:1717:G:H8 | 1.83 | 0.44 |
| 33:BM:108:PRO:O | 33:BM:113:GLY:HA3 | 2.18 | 0.44 |
| 26:DB:14:U:O3' | 26:DB:107:U:O2' | 2.32 | 0.44 |
| 20:CW:20:LEU:HA | 20:CW:20:LEU:HD23 | 1.81 | 0.44 |
| 7:AJ:69:VAL:O | 7:AJ:69:VAL:CG1 | 2.66 | 0.44 |
| 25:DA:2612:C:C5 | 25:DA:2613:U:H5 | 2.35 | 0.44 |
| 25:BA:1063:G:C4 | 25:BA:1064:C:C6 | 3.06 | 0.43 |
| 27:BD:181:GLU:CA | 27:BD:272:ALA:HB2 | 2.39 | 0.43 |
| 1:AA:1162:C:O5' | 1:AA:1162:C:H6 | 2.00 | 0.43 |
| 27:DD:43:ARG:HG2 | 27:DD:54:ARG:O | 2.18 | 0.43 |
| 25:DA:1152:C:H4' | 40:D1:77:SER:HA | 1.99 | 0.43 |
| 33:BM:43:THR:HG23 | 40:B1:64:ARG:HH22 | 1.82 | 0.43 |
| 28:DE:188:VAL:HG23 | 28:DE:189:PRO:HD2 | 1.99 | 0.43 |
| 28:DE:48:GLN:HG2 | 28:DE:78:LEU:HB2 | 1.93 | 0.43 |
| 41:D2:77:ALA:O | 41:D2:79:VAL:HG22 | 2.18 | 0.43 |
| 26:BB:43:C:H5' | 30:BG:66:GLN:NE2 | 2.32 | 0.43 |
| 1:CA:510:A:H5'' | 1:CA:511:C:OP2 | 2.18 | 0.43 |
| 36:BP:88:GLY:O | 36:BP:90:VAL:N | 2.51 | 0.43 |
| 25:DA:1069:A:H5' | 25:DA:1070:A:C8 | 2.53 | 0.43 |
| 25:BA:881:G:H3' | 25:BA:882:G:H4' | 1.98 | 0.43 |
| 25:BA:2212:A:H1' | 25:BA:2215:G:C4 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:1479:G:C2 | 25:BA:1480:G:C4 | 3.05 | 0.43 |
| 32:BK:77:LEU:O | 32:BK:77:LEU:HD12 | 2.18 | 0.43 |
| 25:BA:999:U:H5'' | 25:BA:1154:G:O6 | 2.18 | 0.43 |
| 2:CE:95:GLN:HB2 | 2:CE:148:TYR:HA | 2.00 | 0.43 |
| 9:CL:53:VAL:HG11 | 9:CL:92:TYR:CD2 | 2.53 | 0.43 |
| 35:DO:83:VAL:HG11 | 35:DO:112:LEU:HD21 | 1.99 | 0.43 |
| 1:CA:1067:A:H4' | 1:CA:1068:G:O5' | 2.18 | 0.43 |
| 49:BX:4:LEU:O | 49:BX:36:VAL:HA | 2.17 | 0.43 |
| 1:AA:406:G:N2 | 1:AA:437:U:O2 | 2.51 | 0.43 |
| 1:AA:191:G:N3 | 20:AW:105:SER:HB2 | 2.33 | 0.43 |
| 25:DA:84:A:H2' | 25:DA:99:U:O4 | 2.18 | 0.43 |
| 5:AH:47:LYS:HE2 | 5:AH:47:LYS:HB2 | 1.90 | 0.43 |
| 29:DF:178:PRO:HG2 | 29:DF:179:GLU:OE1 | 2.18 | 0.43 |
| 25:BA:654(S):G:H4' | 25:BA:654(T):A:OP1 | 2.17 | 0.43 |
| 1:CA:408:A:H2' | 1:CA:409:G:O4' | 2.18 | 0.43 |
| 1:CA:926:G:C6 | 1:CA:1505:G:C5 | 3.06 | 0.43 |
| 1:AA:101:A:C4 | 1:AA:102:G:C8 | 3.06 | 0.43 |
| 26:BB:11:C:O5' | 26:BB:12:C:H5 | 2.01 | 0.43 |
| 3:CF:18:TRP:N | 3:CF:18:TRP:CE3 | 2.85 | 0.43 |
| 25:BA:2331:G:C4' | 46:B3:42:GLY:HA3 | 2.48 | 0.43 |
| 38:BQ:93:LYS:HG3 | 38:BQ:94:TYR:N | 2.33 | 0.43 |
| 25:DA:873:G:N2 | 25:DA:905:U:O2 | 2.50 | 0.43 |
| 31:DH:131:VAL:HG12 | 31:DH:132:ARG:N | 2.33 | 0.43 |
| 1:AA:487:A:H5'' | 1:AA:488:C:OP2 | 2.18 | 0.43 |
| 25:DA:639:U:H2' | 25:DA:640:C:H6 | 1.78 | 0.43 |
| 5:AH:57:LYS:H | 5:AH:57:LYS:HG2 | 1.52 | 0.43 |
| 4:CG:61:LYS:CA | 4:CG:203:VAL:HG22 | 2.47 | 0.43 |
| 25:BA:270(P):C:O2' | 25:BA:270(Q):C:H5' | 2.18 | 0.43 |
| 25:BA:155:C:H5'' | 25:BA:155:C:H6 | 1.83 | 0.43 |
| 46:D3:25:ARG:HD2 | 46:D3:29:GLN:HE22 | 1.82 | 0.43 |
| 25:DA:1181:C:H2' | 25:DA:1182:A:H8 | 1.83 | 0.43 |
| 25:DA:2544:G:H8 | 25:DA:2544:G:O5' | 2.01 | 0.43 |
| 25:BA:1582:C:O2' | 25:BA:1586:A:C8 | 2.67 | 0.43 |
| 22:AB:27:G:H5' | 22:AB:28:C:OP2 | 2.18 | 0.43 |
| 27:DD:48:ARG:CG | 27:DD:48:ARG:HH11 | 2.30 | 0.43 |
| 25:DA:869:G:C2 | 25:DA:870:A:C8 | 3.06 | 0.43 |
| 10:CM:8:LEU:HG | 10:CM:96:ILE:HG23 | 1.99 | 0.43 |
| 43:BT:70:LEU:HD23 | 43:BT:70:LEU:H | 1.82 | 0.43 |
| 25:BA:815:C:H2' | 25:BA:816:C:C6 | 2.50 | 0.43 |
| 7:AJ:36:LYS:HB2 | 7:AJ:36:LYS:NZ | 2.34 | 0.43 |
| 25:DA:723:G:H2' | 25:DA:724:U:O4' | 2.18 | 0.43 |
| 30:DG:125:PHE:HB3 | 30:DG:166:ASP:HB2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:2505:G:H2' | 25:BA:2576:G:O6 | 2.17 | 0.43 |
| 23:AC:24:C:H2' | 23:AC:25:U:H6 | 1.82 | 0.43 |
| 1:AA:132:C:N3 | 1:AA:231:G:C2 | 2.86 | 0.43 |
| 25:DA:1759:A:C8 | 25:DA:2696:U:O2 | 2.71 | 0.43 |
| 9:AL:25:LYS:HE3 | 9:AL:25:LYS:HB2 | 1.79 | 0.43 |
| 6:CI:19:LEU:HD11 | 6:CI:59:TYR:CE1 | 2.53 | 0.43 |
| 31:BH:111:HIS:HB2 | 31:BH:112:PRO:HD2 | 2.00 | 0.43 |
| 25:BA:2533:A:H2' | 25:BA:2534:A:H5' | 1.99 | 0.43 |
| 25:DA:280:C:C2 | 25:DA:361:G:N2 | 2.86 | 0.43 |
| 31:DH:99:VAL:HG12 | 31:DH:100:GLY:N | 2.33 | 0.43 |
| 13:AP:55:ARG:HG3 | 13:AP:55:ARG:HH11 | 1.83 | 0.43 |
| 31:BH:129:THR:OG1 | 31:BH:129:THR:O | 2.33 | 0.43 |
| 44:DU:41:GLY:O | 44:DU:64:GLU:HB3 | 2.17 | 0.43 |
| 1:CA:1499:A:H1' | 1:CA:1520:G:H5' | 1.99 | 0.43 |
| 23:CC:15:G:N3 | 23:CC:60:A:C2 | 2.87 | 0.43 |
| 1:CA:983:A:H5' | 14:CQ:2:ALA:CB | 2.48 | 0.43 |
| 1:AA:1032(B):G:H2' | 1:AA:1033:G:H8 | 1.83 | 0.43 |
| 23:AC:77:A:C8 | 23:AC:77:A:C5' | 3.02 | 0.43 |
| 1:CA:1305:G:H5'' | 21:CX:4:GLY:CA | 2.49 | 0.43 |
| 30:BG:121:ASN:HA | 30:BG:122:PRO:HD2 | 1.83 | 0.43 |
| 25:BA:2749:A:O3' | 31:BH:62:LYS:HE3 | 2.18 | 0.43 |
| 25:DA:1464:C:C2 | 25:DA:1465:G:C8 | 3.06 | 0.43 |
| 15:AR:56:LEU:HD12 | 15:AR:60:VAL:HG23 | 1.99 | 0.43 |
| 48:BW:15:LYS:H | 48:BW:67:LYS:CE | 2.31 | 0.43 |
| 33:BM:55:VAL:O | 33:BM:56:ASN:C | 2.56 | 0.43 |
| 13:CP:3:ARG:N | 50:D4:34:GLU:HG3 | 2.33 | 0.43 |
| 9:CL:95:LYS:CD | 9:CL:96:LEU:N | 2.73 | 0.43 |
| 25:BA:658:C:H2' | 25:BA:659:C:C6 | 2.53 | 0.43 |
| 47:BZ:92:LYS:HA | 47:BZ:95:LEU:HD12 | 2.00 | 0.43 |
| 25:BA:900:A:H3' | 25:BA:901:A:H8 | 1.83 | 0.43 |
| 9:AL:4:TYR:CD2 | 9:AL:88:TYR:HB2 | 2.54 | 0.43 |
| 45:DV:26:GLY:C | 45:DV:37:VAL:HG22 | 2.39 | 0.43 |
| 25:BA:304:G:N2 | 25:BA:314:A:C4 | 2.86 | 0.43 |
| 25:BA:101:G:H3' | 25:BA:102:G:C5' | 2.48 | 0.43 |
| 5:CH:140:ARG:O | 5:CH:143:ARG:NH2 | 2.51 | 0.43 |
| 23:AD:10:G:N1 | 23:AD:27:G:C2 | 2.87 | 0.43 |
| 25:DA:26:G:C6 | 25:DA:27:G:N1 | 2.85 | 0.43 |
| 19:CV:78:ARG:NH1 | 19:CV:79:THR:HA | 2.33 | 0.43 |
| 3:AF:65:ALA:O | 3:AF:66:VAL:C | 2.56 | 0.43 |
| 43:DT:5:TYR:HB3 | 48:DW:33:MET:SD | 2.58 | 0.43 |
| 25:BA:2312:U:C6 | 25:BA:2312:U:O5' | 2.70 | 0.43 |
| 31:DH:20:ALA:HB1 | 31:DH:21:PRO:HD2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:1071:C:O2 | 1:CA:1072:G:C8 | 2.71 | 0.43 |
| 49:BX:19:GLN:NE2 | 49:BX:52:HIS:CE1 | 2.84 | 0.43 |
| 25:BA:2205:C:O2 | 25:BA:2205:C:H2' | 2.18 | 0.43 |
| 25:DA:2517:C:C6 | 25:DA:2542:A:C2 | 3.05 | 0.43 |
| 1:CA:769:G:H4' | 1:CA:1513:A:H4' | 1.99 | 0.43 |
| 1:CA:838:G:C2' | 1:CA:841:U:H5' | 2.47 | 0.43 |
| 11:AN:82:VAL:CG2 | 11:AN:98:LEU:HD13 | 2.48 | 0.43 |
| 31:DH:143:GLN:HE21 | 31:DH:143:GLN:CA | 2.31 | 0.43 |
| 25:DA:277:C:OP2 | 25:DA:278:A:N6 | 2.40 | 0.43 |
| 38:BQ:4:LEU:HB3 | 38:BQ:5:THR:H | 1.71 | 0.43 |
| 8:AK:27:PRO:HG3 | 8:AK:58:TYR:HE2 | 1.82 | 0.43 |
| 25:DA:1639:U:H4' | 25:DA:2699:C:H4' | 1.99 | 0.43 |
| 25:BA:1279:G:N2 | 25:BA:1292:U:C2 | 2.86 | 0.43 |
| 9:CL:43:ALA:HA | 9:CL:74:ILE:HD13 | 2.00 | 0.43 |
| 34:DN:79:PHE:CD2 | 39:DR:72:VAL:HG22 | 2.53 | 0.43 |
| 20:CW:67:ALA:O | 20:CW:73:HIS:CE1 | 2.71 | 0.43 |
| 1:CA:39:G:N7 | 1:CA:547:A:C8 | 2.86 | 0.43 |
| 25:BA:2345:G:N3 | 25:BA:2381:C:H2' | 2.32 | 0.43 |
| 1:CA:529:G:O2' | 1:CA:533:A:C6 | 2.67 | 0.43 |
| 25:BA:1281:G:O2' | 25:BA:1282:U:H5' | 2.18 | 0.43 |
| 29:BF:155:LEU:HD13 | 29:BF:174:VAL:CG2 | 2.48 | 0.43 |
| 1:AA:317:G:C6 | 1:AA:318:G:C5 | 3.06 | 0.43 |
| 4:CG:73:ARG:HA | 4:CG:73:ARG:HD2 | 1.84 | 0.43 |
| 31:DH:105:LEU:HD22 | 31:DH:105:LEU:H | 1.82 | 0.43 |
| 1:AA:515:G:N2 | 1:AA:537:G:C4 | 2.86 | 0.43 |
| 11:CN:45:GLY:O | 11:CN:50:TYR:HB2 | 2.18 | 0.43 |
| 44:DU:54:LYS:HD2 | 44:DU:55:TYR:CZ | 2.54 | 0.43 |
| 34:BN:115:VAL:HG23 | 34:BN:116:SER:N | 2.33 | 0.43 |
| 1:AA:453:A:C6 | 1:AA:454:C:C4 | 3.06 | 0.43 |
| 25:BA:120:U:O2 | 25:BA:120:U:O4' | 2.35 | 0.43 |
| 1:AA:1159:U:O2 | 1:AA:1160:G:O6 | 2.36 | 0.43 |
| 25:DA:2629:A:O2' | 25:DA:2630:G:C5' | 2.65 | 0.43 |
| 25:DA:2375:G:O2' | 25:DA:2377:A:N7 | 2.47 | 0.43 |
| 38:DQ:83:LYS:HZ3 | 38:DQ:109:GLY:H | 1.65 | 0.43 |
| 40:D1:98:LEU:C | 40:D1:100:VAL:N | 2.69 | 0.43 |
| 28:BE:82:ARG:O | 28:BE:83:ASP:C | 2.55 | 0.43 |
| 1:CA:1004:A:C5' | 1:CA:1025:U:N3 | 2.81 | 0.43 |
| 25:BA:299:A:H62 | 25:BA:300:A:N6 | 2.16 | 0.43 |
| 25:BA:299:A:H5' | 25:BA:300:A:OP2 | 2.19 | 0.43 |
| 44:BU:97:ARG:HH21 | 44:BU:98:VAL:CG2 | 2.31 | 0.43 |
| 1:CA:1227:A:OP2 | 13:CP:111:LYS:HD3 | 2.17 | 0.43 |
| 45:DV:175:VAL:C | 45:DV:177:PRO:HD3 | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:973:G:H3' | 1:CA:974:A:H5'' | 2.00 | 0.43 |
| 22:CB:69:A:H4' | 22:CB:70:G:OP1 | 2.18 | 0.43 |
| 45:BV:61:LEU:HD12 | 45:BV:62:PRO:O | 2.19 | 0.43 |
| 25:DA:2250:G:OP1 | 25:DA:2275:C:H2' | 2.18 | 0.43 |
| 25:DA:2275:C:O2' | 36:DP:84:GLY:HA2 | 2.14 | 0.43 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:C6 | 2.51 | 0.43 |
| 25:DA:747:U:C5 | 51:D5:3:LYS:CB | 2.88 | 0.43 |
| 25:BA:1138:G:H21 | 33:BM:106:MET:CE | 2.17 | 0.43 |
| 9:CL:18:PHE:CD1 | 9:CL:62:TYR:HD2 | 2.30 | 0.43 |
| 9:CL:17:VAL:HG22 | 9:CL:63:ILE:HG12 | 1.99 | 0.43 |
| 1:AA:254:G:H21 | 17:AT:16:GLN:HE21 | 1.66 | 0.43 |
| 4:AG:8:VAL:HG11 | 4:AG:21:LEU:HB2 | 2.01 | 0.43 |
| 1:AA:690:G:N2 | 11:AN:55:LYS:NZ | 2.67 | 0.43 |
| 25:BA:1359:A:N1 | 25:BA:1372:U:O4 | 2.51 | 0.43 |
| 1:CA:1299:A:C6 | 1:CA:1301:U:C2 | 3.06 | 0.43 |
| 25:DA:2320:A:H4' | 25:DA:2321:G:N7 | 2.33 | 0.43 |
| 25:DA:654(S):G:C1' | 25:DA:654(T):A:OP1 | 2.66 | 0.43 |
| 32:BK:7:GLU:HA | 32:BK:15:VAL:HG12 | 1.98 | 0.43 |
| 1:CA:171:A:N6 | 1:CA:172:A:N6 | 2.67 | 0.43 |
| 3:AF:131:ARG:HH11 | 3:AF:131:ARG:HG3 | 1.83 | 0.43 |
| 2:CE:178:ARG:HH11 | 2:CE:178:ARG:CB | 2.24 | 0.43 |
| 28:BE:116:VAL:HG13 | 28:BE:122:PHE:CD2 | 2.54 | 0.43 |
| 45:BV:121:HIS:C | 45:BV:123:ASP:N | 2.71 | 0.43 |
| 1:CA:1372:U:H2' | 1:CA:1373:G:H5' | 1.99 | 0.43 |
| 1:CA:926:G:C5' | 1:CA:927:G:O5' | 2.66 | 0.43 |
| 25:BA:612:G:C6 | 25:BA:613:U:C4 | 3.06 | 0.43 |
| 25:BA:2314:C:O2' | 25:BA:2315:G:H5' | 2.19 | 0.43 |
| 42:BS:70:TYR:CE2 | 42:BS:108:GLY:HA3 | 2.54 | 0.43 |
| 1:CA:1054:C:O2' | 1:CA:1055:A:C5' | 2.66 | 0.43 |
| 37:B0:44:LEU:HD22 | 37:B0:48:VAL:HG22 | 2.00 | 0.43 |
| 25:DA:2820:A:C6 | 37:D0:4:LEU:HD11 | 2.53 | 0.43 |
| 28:DE:169:ASN:OD1 | 28:DE:201:THR:HG21 | 2.18 | 0.43 |
| 25:BA:371:A:O3' | 25:BA:372:G:H4' | 2.18 | 0.43 |
| 1:AA:313:A:H2' | 1:AA:314:C:C6 | 2.53 | 0.43 |
| 11:CN:99:GLN:HG2 | 11:CN:105:VAL:CG2 | 2.46 | 0.43 |
| 1:CA:1028(A):C:C2 | 1:CA:1028(B):C:C5 | 3.06 | 0.43 |
| 23:CD:20:G:C2' | 23:CD:20:G:N3 | 2.79 | 0.43 |
| 36:BP:81:VAL:O | 36:BP:82:ARG:NE | 2.50 | 0.43 |
| 25:BA:2389:G:H5'' | 25:BA:2390:U:C5' | 2.47 | 0.43 |
| 5:AH:43:LEU:HD13 | 5:AH:109:ILE:HD11 | 2.00 | 0.43 |
| 43:BT:80:ILE:HG13 | 43:BT:80:ILE:O | 2.18 | 0.43 |
| 27:BD:68:LYS:HB3 | 27:BD:70:TRP:CH2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:CF:69:HIS:HA | 3:CF:104:GLN:HB2 | 1.99 | 0.43 |
| 10:CM:24:VAL:HG21 | 10:CM:37:PRO:HD3 | 1.99 | 0.43 |
| 7:AJ:155:ARG:O | 7:AJ:155:ARG:HD3 | 2.18 | 0.43 |
| 35:BO:106:LEU:HD23 | 35:BO:106:LEU:HA | 1.48 | 0.43 |
| 25:BA:2275:C:H5' | 25:BA:2275:C:H6 | 1.83 | 0.43 |
| 3:CF:121:ALA:HB2 | 3:CF:198:VAL:HG21 | 2.01 | 0.43 |
| 1:CA:1213:A:C6 | 1:CA:1215:G:H1' | 2.52 | 0.43 |
| 25:DA:971:C:H2' | 25:DA:972:G:H5' | 2.00 | 0.43 |
| 1:CA:1486:G:H2' | 1:CA:1487:G:C1' | 2.48 | 0.43 |
| 25:DA:460:A:OP1 | 53:D7:41:ARG:NH2 | 2.47 | 0.43 |
| 25:BA:185:U:H4' | 25:BA:218:A:H4' | 2.00 | 0.43 |
| 10:AM:42:THR:HG22 | 10:AM:67:THR:O | 2.18 | 0.43 |
| 29:DF:161:GLU:HB3 | 29:DF:162:LEU:HD12 | 2.00 | 0.43 |
| 25:DA:2342:C:O2' | 25:DA:2374:C:H5'' | 2.18 | 0.43 |
| 33:BM:85:ILE:HA | 33:BM:86:PRO:HD3 | 1.84 | 0.43 |
| 25:DA:608:A:H2' | 25:DA:609:A:C8 | 2.54 | 0.43 |
| 1:AA:1030:C:H2' | 1:AA:1031:G:O4' | 2.18 | 0.43 |
| 25:BA:503:A:C6 | 25:BA:505:A:C6 | 3.06 | 0.43 |
| 25:BA:59:U:O2' | 25:BA:73:A:H2' | 2.18 | 0.43 |
| 1:CA:105:G:H2' | 1:CA:106:C:C6 | 2.53 | 0.43 |
| 25:BA:307:G:N2 | 25:BA:310:A:C8 | 2.86 | 0.43 |
| 15:CR:25:THR:HG21 | 15:CR:70:LEU:HB2 | 2.00 | 0.43 |
| 1:CA:837:G:C2 | 1:CA:850:U:O2 | 2.71 | 0.43 |
| 5:CH:13:ILE:HG12 | 5:CH:13:ILE:O | 2.18 | 0.43 |
| 25:DA:2324:C:H5'' | 25:DA:2325:G:O5' | 2.17 | 0.43 |
| 9:CL:14:VAL:O | 9:CL:14:VAL:HG12 | 2.18 | 0.43 |
| 12:AO:60:LEU:HD21 | 12:AO:66:VAL:HG22 | 2.01 | 0.43 |
| 1:AA:1175:G:C2 | 1:AA:1176:A:C6 | 3.07 | 0.43 |
| 38:DQ:83:LYS:HB3 | 38:DQ:84:GLN:HG2 | 1.99 | 0.43 |
| 39:DR:61:PHE:CE2 | 39:DR:76:PHE:HB2 | 2.53 | 0.43 |
| 1:AA:1055:A:C5 | 1:AA:1206:G:C2 | 3.06 | 0.43 |
| 25:BA:299:A:C5' | 25:BA:300:A:OP2 | 2.66 | 0.43 |
| 36:BP:104:PHE:O | 36:BP:105:GLU:HB3 | 2.19 | 0.43 |
| 28:DE:137:HIS:CB | 28:DE:138:PRO:HD2 | 2.48 | 0.43 |
| 39:DR:21:GLU:O | 39:DR:91:ARG:NH2 | 2.52 | 0.43 |
| 25:BA:893:C:N4 | 25:BA:894:C:N4 | 2.66 | 0.43 |
| 29:DF:29:ASN:N | 29:DF:112:MET:CE | 2.81 | 0.43 |
| 26:DB:40:U:C4 | 26:DB:43:C:OP2 | 2.71 | 0.43 |
| 30:DG:64:THR:OG1 | 30:DG:94:LEU:HD13 | 2.18 | 0.43 |
| 25:DA:2126:A:H4' | 25:DA:2127:G:OP1 | 2.18 | 0.43 |
| 25:DA:2135:A:N6 | 25:DA:2156:G:H21 | 2.15 | 0.43 |
| 25:BA:2172:U:H5' | 25:BA:2173:A:OP2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 26:DB:88:C:C6 | 26:DB:89:G:C8 | 3.07 | 0.43 |
| 39:DR:3:ARG:NE | 39:DR:6:LEU:HD13 | 2.34 | 0.43 |
| 1:CA:812:C:C2' | 1:CA:813:U:OP2 | 2.66 | 0.43 |
| 1:AA:18:C:H2' | 1:AA:19:C:O4' | 2.18 | 0.43 |
| 1:CA:1095:U:H2' | 1:CA:1096:C:O4' | 2.18 | 0.43 |
| 1:AA:1504:G:H1' | 1:AA:1505:G:OP2 | 2.18 | 0.43 |
| 25:BA:528:A:N1 | 25:BA:2043:C:H4' | 2.33 | 0.43 |
| 45:DV:70:LEU:HD11 | 45:DV:98:MET:CE | 2.48 | 0.43 |
| 19:CV:78:ARG:CD | 19:CV:79:THR:N | 2.81 | 0.43 |
| 3:AF:92:ALA:O | 3:AF:95:THR:O | 2.36 | 0.43 |
| 25:BA:2688:U:O5' | 25:BA:2688:U:O2 | 2.35 | 0.43 |
| 25:BA:2590:A:H2' | 25:BA:2591:C:C6 | 2.53 | 0.43 |
| 1:AA:1277:C:HO2' | 1:AA:1279:A:C1' | 2.32 | 0.43 |
| 28:BE:182:LEU:C | 28:BE:183:LEU:HD12 | 2.38 | 0.43 |
| 29:DF:36:VAL:HG11 | 29:DF:183:VAL:CG1 | 2.48 | 0.43 |
| 3:CF:27:LYS:HB3 | 3:CF:27:LYS:HZ2 | 1.83 | 0.43 |
| 1:CA:689:C:O2' | 1:CA:690:G:H5' | 2.17 | 0.43 |
| 9:AL:42:ARG:HE | 9:AL:42:ARG:HB2 | 1.44 | 0.43 |
| 13:CP:7:VAL:HG23 | 30:DG:115:ARG:NH2 | 2.33 | 0.43 |
| 1:AA:516:U:C4 | 1:AA:517:G:C6 | 3.06 | 0.43 |
| 4:AG:99:SER:O | 4:AG:140:VAL:HG22 | 2.18 | 0.43 |
| 22:AB:28:C:H2' | 22:AB:29:U:H6 | 1.83 | 0.43 |
| 25:DA:867:C:C5 | 25:DA:868:U:H5 | 2.35 | 0.43 |
| 25:DA:669:G:O2' | 25:DA:670:A:OP1 | 2.35 | 0.43 |
| 3:CF:21:ARG:HH11 | 3:CF:21:ARG:CB | 2.31 | 0.43 |
| 10:CM:13:HIS:HB3 | 10:CM:68:HIS:NE2 | 2.34 | 0.43 |
| 1:AA:158:G:H2' | 1:AA:159:G:C8 | 2.54 | 0.43 |
| 1:AA:1406:U:O2 | 1:AA:1517:G:N2 | 2.52 | 0.43 |
| 25:BA:2189:U:H3' | 25:BA:2190:G:H5'' | 2.00 | 0.43 |
| 14:CQ:4:LYS:HG3 | 14:CQ:7:ILE:HD11 | 1.99 | 0.43 |
| 25:DA:375:C:H2' | 25:DA:376:C:H6 | 1.80 | 0.43 |
| 25:BA:727:A:C6 | 25:BA:728:G:C6 | 3.06 | 0.43 |
| 53:D7:34:ARG:NH1 | 53:D7:41:ARG:O | 2.51 | 0.43 |
| 25:BA:2206:C:H2' | 25:BA:2207:C:C6 | 2.51 | 0.43 |
| 25:BA:318:C:O2' | 25:BA:319:C:H5' | 2.18 | 0.43 |
| 25:DA:2239:G:H5' | 27:DD:251:GLY:CA | 2.48 | 0.43 |
| 1:CA:853:G:H2' | 1:CA:854:G:H8 | 1.83 | 0.43 |
| 1:CA:783:C:H2' | 1:CA:784:C:H6 | 1.83 | 0.43 |
| 1:AA:622:A:C8 | 1:AA:623:C:C6 | 3.07 | 0.43 |
| 1:AA:455:C:H42 | 1:AA:477:G:H1 | 1.66 | 0.43 |
| 25:BA:2830:G:N3 | 25:BA:2883:A:H2 | 2.17 | 0.43 |
| 3:AF:147:LYS:HB3 | 3:AF:203:PHE:CD2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:459:U:H2' | 25:BA:460:A:H8 | 1.84 | 0.43 |
| 23:AC:34:U:O2 | 23:AC:36:A:C8 | 2.72 | 0.43 |
| 17:CT:29:HIS:CG | 17:CT:30:PRO:HD2 | 2.53 | 0.43 |
| 1:CA:1483:A:H1' | 25:DA:1948:G:H1' | 2.01 | 0.43 |
| 23:AC:75:C:O2 | 25:BA:2252:G:N2 | 2.45 | 0.43 |
| 20:AW:49:ALA:O | 20:AW:52:ALA:HB3 | 2.18 | 0.43 |
| 25:DA:1122:G:H2' | 25:DA:1122:G:N3 | 2.34 | 0.43 |
| 27:BD:118:VAL:HG22 | 27:BD:119:ALA:N | 2.33 | 0.43 |
| 32:BK:93:THR:O | 32:BK:96:ASP:HB2 | 2.18 | 0.43 |
| 1:AA:1530:G:H2' | 1:AA:1531:A:C8 | 2.52 | 0.43 |
| 30:BG:83:ARG:CB | 30:BG:86:MET:HE2 | 2.48 | 0.43 |
| 47:BZ:87:PRO:HG2 | 47:BZ:88:LYS:H | 1.82 | 0.43 |
| 25:BA:50:U:H3' | 25:BA:51:G:H5' | 2.00 | 0.43 |
| 1:AA:1176:A:N6 | 1:AA:1177:G:C5 | 2.87 | 0.43 |
| 40:D1:94:ASN:O | 40:D1:97:ASP:HB3 | 2.18 | 0.43 |
| 28:BE:64:LYS:O | 28:BE:70:ALA:HB2 | 2.18 | 0.43 |
| 23:AC:19:G:C2 | 23:AC:59:A:C4 | 3.06 | 0.43 |
| 25:BA:1899:G:O2' | 25:BA:1900:A:O5' | 2.31 | 0.43 |
| 29:DF:83:PHE:C | 29:DF:84:VAL:HG13 | 2.21 | 0.43 |
| 39:DR:19:LEU:HA | 39:DR:20:PRO:HD3 | 1.81 | 0.43 |
| 1:CA:983:A:H2 | 1:CA:984:C:C5 | 2.37 | 0.43 |
| 1:CA:1060:C:H4' | 10:CM:51:ARG:HB3 | 1.99 | 0.43 |
| 19:AV:41:VAL:HG23 | 19:AV:67:VAL:HG22 | 2.01 | 0.43 |
| 19:AV:9:VAL:O | 19:AV:9:VAL:CG1 | 2.66 | 0.43 |
| 25:DA:1342:A:N1 | 25:DA:1397:U:C4 | 2.86 | 0.43 |
| 36:BP:34:LEU:HD23 | 36:BP:104:PHE:HD1 | 1.83 | 0.43 |
| 25:DA:1608:A:H1' | 25:DA:1610:A:OP2 | 2.18 | 0.43 |
| 29:DF:25:PRO:HB2 | 29:DF:27:GLU:N | 2.32 | 0.43 |
| 25:DA:2272:U:H5'' | 25:DA:2273:A:OP1 | 2.19 | 0.43 |
| 31:DH:4:ILE:HG12 | 31:DH:7:LEU:HG | 2.01 | 0.43 |
| 25:DA:2303:G:C2 | 25:DA:2314:C:C2 | 3.06 | 0.43 |
| 17:CT:68:ARG:H | 17:CT:70:ARG:NH1 | 2.17 | 0.43 |
| 5:CH:83:GLU:HB3 | 5:CH:88:LYS:CG | 2.34 | 0.43 |
| 9:CL:3:GLN:NE2 | 9:CL:20:ARG:NH1 | 2.66 | 0.43 |
| 26:DB:8:U:C5' | 26:DB:8:U:H6 | 2.31 | 0.43 |
| 38:DQ:25:ARG:NH2 | 38:DQ:40:ILE:HD12 | 2.33 | 0.43 |
| 35:BO:18:ARG:NH1 | 35:BO:21:ARG:HH11 | 2.16 | 0.43 |
| 25:BA:2124:G:H2' | 25:BA:2125:G:H5' | 1.99 | 0.43 |
| 39:BR:53:ARG:NH1 | 39:BR:60:THR:OG1 | 2.51 | 0.43 |
| 25:DA:856:C:O2' | 25:DA:857:C:P | 2.76 | 0.43 |
| 26:DB:88:C:H3' | 26:DB:88:C:H6 | 1.84 | 0.43 |
| 25:DA:138:G:C2' | 25:DA:139:G:H5' | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 27:BD:25:THR:HG21 | 27:BD:81:ALA:HA | 2.01 | 0.43 |
| 39:BR:50:ILE:HA | 39:BR:50:ILE:HD12 | 1.66 | 0.43 |
| 51:B5:40:LYS:CB | 51:B5:46:CYS:SG | 3.06 | 0.43 |
| 25:DA:2154:G:C2 | 25:DA:2155:G:C5 | 3.06 | 0.43 |
| 1:AA:439:A:C4 | 1:AA:496:A:C2 | 3.06 | 0.43 |
| 19:CV:29:ARG:O | 19:CV:30:LEU:HG | 2.17 | 0.43 |
| 54:B8:60:LEU:O | 54:B8:61:LEU:C | 2.56 | 0.43 |
| 25:BA:525:U:H5' | 25:BA:556:G:OP1 | 2.19 | 0.43 |
| 25:DA:2554:U:C5' | 25:DA:2554:U:H6 | 2.30 | 0.43 |
| 28:BE:116:VAL:HG13 | 28:BE:122:PHE:HB2 | 1.99 | 0.43 |
| 25:BA:1049:C:C4 | 25:BA:1050:A:N1 | 2.87 | 0.43 |
| 1:CA:1531:A:H5'' | 1:CA:1531:A:H8 | 1.84 | 0.43 |
| 37:B0:74:LYS:H | 37:B0:74:LYS:HG2 | 1.49 | 0.43 |
| 25:BA:2312:U:H5' | 30:BG:88:ILE:CG2 | 2.48 | 0.43 |
| 1:AA:562:C:C4 | 1:AA:884:U:C5 | 3.06 | 0.43 |
| 45:DV:19:ARG:NH1 | 45:DV:84:GLU:O | 2.51 | 0.43 |
| 4:CG:178:VAL:CG1 | 4:CG:179:GLU:H | 2.31 | 0.43 |
| 25:DA:833:U:H1' | 35:DO:55:ARG:NH1 | 2.34 | 0.43 |
| 1:AA:985:C:C2 | 1:AA:1221:G:C2 | 3.06 | 0.43 |
| 1:AA:619:U:C2 | 4:AG:135:LEU:HD22 | 2.53 | 0.43 |
| 1:CA:1380:U:C2 | 7:CJ:3:ARG:NH1 | 2.87 | 0.43 |
| 1:CA:652:U:C5 | 1:CA:752:G:N3 | 2.86 | 0.43 |
| 20:AW:9:ASN:C | 20:AW:9:ASN:ND2 | 2.71 | 0.43 |
| 25:BA:2850:A:C2' | 25:BA:2851:A:O5' | 2.67 | 0.43 |
| 13:AP:25:ILE:HD11 | 13:AP:60:VAL:HG11 | 2.00 | 0.43 |
| 34:DN:68:GLU:CB | 34:DN:78:ARG:HB3 | 2.48 | 0.43 |
| 25:BA:142:G:H1' | 43:BT:37:THR:HG22 | 1.99 | 0.43 |
| 25:BA:270(P):C:H2' | 25:BA:270(Q):C:C6 | 2.53 | 0.43 |
| 7:AJ:35:LYS:O | 7:AJ:38:LEU:N | 2.51 | 0.43 |
| 1:CA:87:A:C2 | 1:CA:88:C:C5 | 3.06 | 0.43 |
| 26:BB:89:G:C6 | 26:BB:89(A):A:N1 | 2.87 | 0.43 |
| 13:CP:17:VAL:O | 13:CP:20:THR:N | 2.46 | 0.43 |
| 1:AA:655:A:C2 | 1:AA:754:C:N4 | 2.87 | 0.43 |
| 25:BA:2097:C:H2' | 25:BA:2098:U:O4' | 2.18 | 0.43 |
| 7:AJ:24:THR:HA | 7:AJ:27:ILE:HG13 | 2.01 | 0.43 |
| 37:D0:23:ASN:N | 37:D0:23:ASN:ND2 | 2.66 | 0.43 |
| 25:BA:2025:C:H2' | 25:BA:2026:C:H6 | 1.83 | 0.43 |
| 1:AA:835:U:P | 18:AU:60:ALA:HB3 | 2.58 | 0.43 |
| 25:BA:2364:C:O2' | 25:BA:2365:G:H5' | 2.18 | 0.43 |
| 27:DD:71:ASP:N | 27:DD:71:ASP:OD2 | 2.52 | 0.43 |
| 42:BS:32:ALA:O | 42:BS:36:LEU:HG | 2.17 | 0.43 |
| 25:BA:2194:G:H2' | 25:BA:2195:C:H6 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:DA:609:A:H2' | 25:DA:609(A):G:O4' | 2.18 | 0.43 |
| 25:DA:374:A:C2 | 25:DA:401:A:C4 | 3.06 | 0.43 |
| 2:AE:147:LYS:HE2 | 2:AE:148:TYR:CE1 | 2.53 | 0.43 |
| 25:BA:2771:C:H2' | 25:BA:2772:C:C6 | 2.53 | 0.43 |
| 25:BA:1680:U:C4 | 25:BA:1681:G:C6 | 3.07 | 0.43 |
| 7:AJ:72:ARG:HG3 | 7:AJ:142:GLU:OE1 | 2.19 | 0.43 |
| 37:D0:102:GLU:HG2 | 37:D0:102:GLU:O | 2.17 | 0.43 |
| 25:BA:1087:G:C5 | 25:BA:1089:G:H1' | 2.53 | 0.43 |
| 27:DD:61:LEU:HA | 27:DD:61:LEU:HD12 | 1.82 | 0.43 |
| 25:BA:2309:A:N6 | 25:BA:2310:A:N6 | 2.67 | 0.43 |
| 27:BD:92:ILE:HD12 | 27:BD:104:TYR:CD2 | 2.54 | 0.43 |
| 27:BD:34:VAL:C | 27:BD:35:LYS:HG3 | 2.39 | 0.43 |
| 25:BA:2318:G:N2 | 38:BQ:2:ALA:CA | 2.82 | 0.43 |
| 33:BM:114:ARG:O | 33:BM:115:ARG:HB2 | 2.18 | 0.43 |
| 28:DE:3:GLY:HA3 | 28:DE:81:ILE:HD13 | 2.01 | 0.43 |
| 28:DE:33:VAL:HG11 | 28:DE:88:GLY:CA | 2.48 | 0.43 |
| 30:BG:67:LYS:CE | 50:B4:6:HIS:NE2 | 2.82 | 0.43 |
| 1:CA:961:U:O2 | 1:CA:1201:A:N1 | 2.51 | 0.43 |
| 1:AA:1036:G:C8 | 1:AA:1037:C:C4 | 3.07 | 0.43 |
| 21:AX:15:ARG:CG | 21:AX:15:ARG:NH1 | 2.66 | 0.43 |
| 25:DA:66:C:C4 | 25:DA:67:U:C5 | 3.07 | 0.43 |
| 36:BP:66:ILE:O | 36:BP:104:PHE:N | 2.51 | 0.43 |
| 1:AA:345:C:O2' | 1:AA:346:G:N2 | 2.51 | 0.43 |
| 1:CA:1162:C:C2 | 1:CA:1175:G:N2 | 2.86 | 0.43 |
| 45:BV:6:LYS:O | 45:BV:7:ALA:HB2 | 2.17 | 0.43 |
| 39:BR:22:PHE:CE1 | 39:BR:52:ILE:HD11 | 2.53 | 0.43 |
| 23:CD:59:A:O2' | 23:CD:61:U:H5 | 2.02 | 0.43 |
| 25:DA:527:C:H4' | 25:DA:528:A:O5' | 2.19 | 0.43 |
| 22:AB:85:C:C5 | 25:BA:2555:U:C2 | 3.07 | 0.43 |
| 25:BA:996:A:H4' | 40:B1:92:ARG:NE | 2.34 | 0.43 |
| 25:DA:2130:U:O2' | 25:DA:2133:G:O2' | 2.34 | 0.43 |
| 27:BD:172:TYR:CD1 | 27:BD:186:HIS:HA | 2.53 | 0.43 |
| 25:DA:2571:C:H6 | 25:DA:2571:C:H5'' | 1.84 | 0.43 |
| 35:DO:97:PRO:HB3 | 35:DO:106:LEU:HD21 | 2.00 | 0.43 |
| 37:B0:104:ARG:HD3 | 37:B0:111:LEU:HD21 | 2.01 | 0.43 |
| 51:B5:40:LYS:HZ3 | 51:B5:46:CYS:CB | 2.32 | 0.43 |
| 29:BF:40:GLN:OE1 | 29:BF:184:TYR:CB | 2.67 | 0.43 |
| 41:B2:3:ALA:HB1 | 41:B2:38:LEU:HD11 | 2.01 | 0.43 |
| 25:DA:1006:C:C2 | 25:DA:1138:G:C2 | 3.07 | 0.43 |
| 7:CJ:78:ARG:HB2 | 7:CJ:156:TRP:HZ3 | 1.82 | 0.43 |
| 1:CA:1324:A:C6 | 1:CA:1325:C:C4 | 3.07 | 0.43 |
| 25:DA:1239:G:H2' | 25:DA:1240:U:O4' | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:CD:22:A:N1 | 23:CD:47:G:H2' | 2.33 | 0.43 |
| 37:B0:72:ASP:O | 37:B0:76:VAL:HG23 | 2.19 | 0.43 |
| 25:BA:611:C:C2' | 25:BA:612:G:H5' | 2.49 | 0.43 |
| 10:CM:75:ILE:HG13 | 10:CM:76:ASN:N | 2.33 | 0.43 |
| 25:DA:986:C:O2' | 25:DA:987:G:H5' | 2.19 | 0.43 |
| 1:AA:66:G:H22 | 1:AA:172:A:H2 | 1.65 | 0.43 |
| 25:DA:1168:G:C2 | 25:DA:1182:A:C2 | 3.05 | 0.43 |
| 25:BA:2283:C:N3 | 25:BA:2389:G:C2 | 2.86 | 0.43 |
| 10:CM:16:LEU:O | 10:CM:20:ALA:HB3 | 2.19 | 0.43 |
| 1:AA:611:A:H61 | 1:AA:629:G:H1 | 1.67 | 0.43 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:H6 | 1.83 | 0.43 |
| 25:BA:989:G:N7 | 49:BX:13:ILE:HD11 | 2.34 | 0.43 |
| 25:BA:411:G:H4' | 25:BA:412:A:OP1 | 2.19 | 0.43 |
| 7:CJ:138:LYS:HE2 | 7:CJ:142:GLU:CD | 2.39 | 0.43 |
| 33:BM:89:LYS:O | 33:BM:93:THR:HG22 | 2.17 | 0.43 |
| 25:BA:2645:G:N2 | 25:BA:2767:C:OP2 | 2.51 | 0.43 |
| 1:AA:1275:A:C6 | 1:AA:1276:G:C5 | 3.07 | 0.43 |
| 1:CA:115:G:H1' | 1:CA:116:A:N7 | 2.34 | 0.43 |
| 8:AK:103:VAL:HG21 | 8:AK:110:ALA:HB2 | 2.01 | 0.43 |
| 43:DT:67:GLY:O | 43:DT:69:TYR:N | 2.47 | 0.43 |
| 1:AA:834:C:O2' | 1:AA:835:U:H5' | 2.19 | 0.43 |
| 25:DA:460:A:P | 53:D7:41:ARG:HH22 | 2.41 | 0.43 |
| 30:DG:23:PHE:HB2 | 30:DG:25:TYR:CZ | 2.54 | 0.43 |
| 25:BA:1271:G:O3' | 25:BA:1272:A:H4' | 2.18 | 0.43 |
| 1:AA:958:A:C6 | 1:AA:959:A:N1 | 2.87 | 0.43 |
| 1:CA:949:A:H1' | 1:CA:1364:U:H3 | 1.83 | 0.43 |
| 20:CW:36:LEU:HA | 20:CW:36:LEU:HD13 | 1.92 | 0.43 |
| 2:CE:21:ARG:HB3 | 2:CE:39:ILE:HA | 1.98 | 0.43 |
| 1:CA:853:G:C2 | 1:CA:854:G:C8 | 3.07 | 0.43 |
| 35:DO:68:GLN:CG | 54:D8:12:LYS:HG2 | 2.48 | 0.43 |
| 1:CA:38:G:H4' | 1:CA:547:A:N6 | 2.33 | 0.43 |
| 16:CS:34:GLU:OE2 | 16:CS:55:ARG:HD3 | 2.19 | 0.43 |
| 1:CA:1057:G:C5 | 1:CA:1204:A:C2 | 3.06 | 0.43 |
| 9:CL:14:VAL:O | 9:CL:65:VAL:HA | 2.18 | 0.43 |
| 1:AA:273:A:N6 | 1:AA:274:A:C6 | 2.87 | 0.43 |
| 10:CM:3:LYS:HE2 | 10:CM:77:PRO:CD | 2.48 | 0.43 |
| 25:DA:807:U:C2 | 25:DA:808:G:C8 | 3.06 | 0.43 |
| 18:AU:43:PHE:O | 18:AU:51:LEU:HG | 2.19 | 0.43 |
| 43:BT:9:LEU:O | 48:BW:36:ARG:NE | 2.51 | 0.43 |
| 44:DU:12:THR:OG1 | 44:DU:26:LYS:HE2 | 2.17 | 0.43 |
| 25:BA:2517:C:C2 | 25:BA:2542:A:N6 | 2.87 | 0.43 |
| 45:BV:82:ARG:HG3 | 45:BV:82:ARG:O | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 15:AR:66:LEU:HD12 | 15:AR:66:LEU:HA | 1.82 | 0.43 |
| 44:BU:33:LYS:H | 44:BU:33:LYS:HG3 | 1.58 | 0.43 |
| 36:DP:112:GLU:H | 36:DP:112:GLU:HG2 | 1.51 | 0.43 |
| 25:DA:1593:G:C2 | 25:DA:1594:G:C4 | 3.06 | 0.43 |
| 36:DP:139:GLU:OE1 | 45:DV:76:LEU:HD21 | 2.18 | 0.43 |
| 54:D8:30:ARG:CG | 54:D8:30:ARG:O | 2.67 | 0.43 |
| 30:BG:77:ILE:O | 30:BG:78:SER:C | 2.57 | 0.43 |
| 25:DA:778:G:H2' | 25:DA:779:U:H6 | 1.83 | 0.43 |
| 25:DA:1225:C:H5'' | 41:D2:85:LYS:HD3 | 1.99 | 0.43 |
| 27:BD:48:ARG:O | 27:BD:50:THR:HG23 | 2.18 | 0.43 |
| 27:BD:33:LEU:CD1 | 27:BD:34:VAL:N | 2.82 | 0.43 |
| 23:AC:59:A:N6 | 23:AC:62:C:O2 | 2.52 | 0.43 |
| 1:CA:1002:G:H1 | 1:CA:1038:C:N4 | 2.17 | 0.43 |
| 28:DE:47:VAL:O | 28:DE:80:GLU:CB | 2.67 | 0.43 |
| 23:CC:18:C:O2' | 23:CC:19:G:C5' | 2.66 | 0.43 |
| 27:DD:85:ASP:HA | 27:DD:86:PRO:HD2 | 1.85 | 0.43 |
| 25:BA:898:C:C3' | 25:BA:899:A:H5' | 2.49 | 0.43 |
| 9:AL:111:ARG:O | 9:AL:113:LYS:HD2 | 2.18 | 0.43 |
| 31:BH:30:LYS:NZ | 31:BH:83:TYR:HE2 | 2.16 | 0.43 |
| 30:DG:161:THR:HG22 | 30:DG:163:ALA:N | 2.13 | 0.43 |
| 25:DA:1041:C:H2' | 25:DA:1042:G:H8 | 1.83 | 0.43 |
| 25:DA:1559:G:O2' | 25:DA:1560:G:H5' | 2.18 | 0.43 |
| 30:BG:32:PRO:HG3 | 30:BG:163:ALA:HB2 | 2.01 | 0.43 |
| 29:DF:102:PRO:O | 29:DF:105:VAL:N | 2.52 | 0.43 |
| 1:AA:691:G:H1' | 1:AA:696:A:N6 | 2.34 | 0.43 |
| 25:BA:2115:G:H2' | 25:BA:2116:G:C8 | 2.43 | 0.43 |
| 12:CO:47:LYS:CB | 12:CO:48:PRO:CD | 2.95 | 0.43 |
| 25:DA:2721:A:H1' | 25:DA:2873:A:O2' | 2.19 | 0.43 |
| 39:BR:91:ARG:O | 39:BR:116:ALA:HA | 2.18 | 0.43 |
| 39:BR:16:ARG:NH1 | 39:BR:16:ARG:HG3 | 2.33 | 0.43 |
| 1:AA:406:G:C6 | 1:AA:495:A:C8 | 3.06 | 0.43 |
| 1:AA:606:G:N3 | 1:AA:606:G:H2' | 2.34 | 0.43 |
| 1:AA:1449:C:H2' | 1:AA:1450:U:O4' | 2.18 | 0.43 |
| 25:DA:2015:A:N3 | 51:D5:6:VAL:HG23 | 2.33 | 0.43 |
| 19:AV:37:ARG:HG3 | 19:AV:37:ARG:H | 1.48 | 0.43 |
| 1:CA:1252:A:H2' | 1:CA:1253:G:O5' | 2.19 | 0.43 |
| 29:DF:182:ASN:O | 29:DF:186:ILE:HG12 | 2.19 | 0.43 |
| 25:DA:2211:G:H3' | 25:DA:2212:A:C2 | 2.52 | 0.43 |
| 25:DA:2656:U:C4 | 25:DA:2664:G:N2 | 2.86 | 0.43 |
| 35:BO:29:LYS:HB3 | 35:BO:30:THR:H | 1.47 | 0.43 |
| 1:CA:586:C:O2' | 1:CA:878:G:H4' | 2.19 | 0.43 |
| 25:DA:26:G:O2' | 25:DA:27:G:H5' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 32:DK:76:THR:CG2 | 32:DK:139:GLN:O | 2.66 | 0.43 |
| 1:AA:1320:C:N4 | 19:AV:36:ARG:HG3 | 2.33 | 0.43 |
| 25:DA:2682:U:H5' | 28:DE:11:MET:HB3 | 2.00 | 0.43 |
| 25:BA:404:C:C1' | 25:BA:405:U:OP2 | 2.66 | 0.43 |
| 25:BA:2591:C:P | 27:BD:239:ARG:HG3 | 2.58 | 0.43 |
| 25:DA:797:C:H2' | 25:DA:798:G:O4' | 2.19 | 0.43 |
| 19:CV:45:VAL:HA | 19:CV:62:ILE:CG2 | 2.47 | 0.43 |
| 25:DA:1262:A:C2 | 51:D5:10:LYS:HE3 | 2.54 | 0.43 |
| 28:DE:201:THR:C | 28:DE:202:LYS:HD2 | 2.38 | 0.43 |
| 34:DN:68:GLU:HB3 | 34:DN:78:ARG:HB3 | 2.00 | 0.43 |
| 25:DA:479:A:N3 | 25:DA:481:G:H5'' | 2.33 | 0.43 |
| 32:DK:128:LEU:HD13 | 32:DK:128:LEU:HA | 1.85 | 0.43 |
| 25:BA:2389:G:H5'' | 25:BA:2390:U:O4' | 2.18 | 0.43 |
| 8:AK:100:ILE:HA | 8:AK:101:PRO:HD3 | 1.89 | 0.43 |
| 6:CI:2:ARG:NH2 | 6:CI:69:GLU:HG3 | 2.33 | 0.43 |
| 25:DA:184:C:H2' | 25:DA:185:U:C6 | 2.54 | 0.43 |
| 27:DD:31:LYS:HZ2 | 27:DD:31:LYS:HB2 | 1.82 | 0.43 |
| 3:CF:54:ARG:HB2 | 3:CF:69:HIS:CG | 2.54 | 0.43 |
| 1:AA:1047:G:O2' | 1:AA:1048:G:H5' | 2.18 | 0.43 |
| 20:CW:41:ILE:HG13 | 20:CW:41:ILE:H | 1.59 | 0.43 |
| 25:DA:1545:A:N7 | 25:DA:1545(A):A:C6 | 2.87 | 0.43 |
| 2:AE:82:ARG:HG2 | 2:AE:92:TYR:CE1 | 2.54 | 0.43 |
| 2:AE:82:ARG:HG2 | 2:AE:92:TYR:OH | 2.18 | 0.43 |
| 25:BA:1818:U:H4' | 25:BA:1821:A:H1' | 2.00 | 0.43 |
| 25:BA:943:U:OP2 | 35:BO:36:LYS:HE3 | 2.19 | 0.43 |
| 25:BA:2364:C:H2' | 25:BA:2365:G:O4' | 2.18 | 0.43 |
| 3:AF:15:THR:HG23 | 3:AF:15:THR:O | 2.19 | 0.43 |
| 25:DA:616:A:C4 | 29:DF:180:GLY:HA2 | 2.54 | 0.43 |
| 1:CA:39:G:N7 | 1:CA:547:A:H8 | 2.16 | 0.43 |
| 47:DZ:67:ILE:N | 47:DZ:68:PRO:CD | 2.80 | 0.43 |
| 18:CU:87:ARG:HA | 18:CU:87:ARG:HD3 | 1.70 | 0.43 |
| 25:DA:2658:C:H5'' | 31:DH:158:HIS:HE1 | 1.82 | 0.43 |
| 1:AA:1376:U:H2' | 1:AA:1377:A:C8 | 2.53 | 0.43 |
| 1:CA:15:G:H4' | 5:CH:24:ARG:HH12 | 1.83 | 0.43 |
| 51:D5:34:PRO:HG2 | 51:D5:35:GLU:OE2 | 2.19 | 0.43 |
| 25:DA:1247:A:C2 | 25:DA:1249:U:C6 | 3.07 | 0.43 |
| 1:CA:24:U:H2' | 1:CA:25:C:C6 | 2.54 | 0.43 |
| 25:DA:577:G:O2' | 25:DA:1254:A:OP1 | 2.37 | 0.43 |
| 25:DA:1356:G:C6 | 25:DA:1357:U:C4 | 3.06 | 0.43 |
| 30:BG:145:THR:O | 30:BG:146:TYR:HB3 | 2.18 | 0.43 |
| 1:CA:123:C:O5' | 1:CA:123:C:H6 | 2.00 | 0.43 |
| 19:CV:48:THR:HG22 | 19:CV:61:TYR:CD1 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 27:BD:45:ASN:C | 27:BD:45:ASN:OD1 | 2.56 | 0.43 |
| 43:DT:65:ARG:HB3 | 43:DT:70:LEU:HA | 2.01 | 0.43 |
| 25:DA:590:A:H2' | 25:DA:591:C:O4' | 2.19 | 0.43 |
| 1:AA:241:C:H42 | 1:AA:285:G:H1 | 1.66 | 0.43 |
| 36:DP:23:GLY:HA2 | 36:DP:24:GLY:HA3 | 1.74 | 0.43 |
| 52:D6:28:ARG:HD2 | 52:D6:30:THR:O | 2.19 | 0.43 |
| 25:DA:846:C:N1 | 25:DA:847:U:C5 | 2.87 | 0.43 |
| 25:DA:2629:A:C8 | 25:DA:2895:U:C5 | 3.07 | 0.43 |
| 25:BA:2810:A:H61 | 25:BA:2891:G:C2' | 2.32 | 0.43 |
| 28:BE:34:VAL:HG23 | 28:BE:34:VAL:O | 2.19 | 0.43 |
| 23:CC:18:C:O2' | 23:CC:19:G:H5'' | 2.19 | 0.43 |
| 31:DH:109:PHE:CZ | 31:DH:152:ARG:CD | 3.01 | 0.43 |
| 30:BG:67:LYS:HE2 | 50:B4:6:HIS:NE2 | 2.27 | 0.43 |
| 3:CF:180:ALA:HB1 | 3:CF:203:PHE:CE1 | 2.43 | 0.43 |
| 52:B6:15:GLU:OE1 | 52:B6:41:PRO:HB3 | 2.18 | 0.43 |
| 24:C1:20:U:H2' | 24:C1:21:U:C6 | 2.53 | 0.43 |
| 1:CA:1157:A:N6 | 1:CA:1178:G:C2 | 2.87 | 0.43 |
| 25:BA:1728:G:H5' | 25:BA:1729:A:OP2 | 2.19 | 0.43 |
| 51:B5:3:LYS:O | 51:B5:4:HIS:O | 2.37 | 0.43 |
| 29:BF:29:ASN:N | 29:BF:112:MET:HE3 | 2.21 | 0.43 |
| 10:AM:48:THR:HG23 | 10:AM:62:HIS:CG | 2.54 | 0.43 |
| 1:CA:633:G:C6 | 1:CA:634:C:N3 | 2.86 | 0.43 |
| 25:BA:2749:A:O2' | 31:BH:59:ARG:NE | 2.52 | 0.43 |
| 25:BA:1510:A:H2' | 25:BA:1511:A:OP2 | 2.19 | 0.43 |
| 1:AA:874:G:C6 | 1:AA:875:C:C4 | 3.07 | 0.43 |
| 25:BA:2401:U:H2' | 25:BA:2402:C:H5'' | 2.01 | 0.43 |
| 26:BB:24:G:N7 | 26:BB:56:G:H2' | 2.33 | 0.43 |
| 25:DA:1528:A:H2' | 25:DA:1529:A:O4' | 2.19 | 0.43 |
| 27:BD:172:TYR:HD1 | 27:BD:185:VAL:C | 2.21 | 0.43 |
| 26:DB:89(A):A:C8 | 26:DB:90:C:H1' | 2.53 | 0.43 |
| 25:BA:2134:A:N6 | 25:BA:2157:G:C1' | 2.79 | 0.43 |
| 2:AE:80:ILE:CD1 | 2:AE:208:ILE:HG23 | 2.46 | 0.43 |
| 2:CE:144:ARG:HG3 | 2:CE:145:LEU:N | 2.33 | 0.43 |
| 1:AA:560:U:H5' | 1:AA:566:G:N2 | 2.34 | 0.43 |
| 25:BA:1474:C:H2' | 25:BA:1475:G:H8 | 1.82 | 0.43 |
| 9:AL:95:LYS:HB2 | 9:AL:95:LYS:HE2 | 1.67 | 0.43 |
| 25:BA:2699:C:H2' | 25:BA:2700:C:O4' | 2.19 | 0.43 |
| 5:AH:100:VAL:HG23 | 5:AH:116:THR:O | 2.18 | 0.43 |
| 30:BG:112:PRO:CB | 50:B4:37:SER:H | 2.32 | 0.43 |
| 30:BG:112:PRO:HB3 | 50:B4:37:SER:OG | 2.18 | 0.43 |
| 1:AA:475:G:H2' | 1:AA:476:G:C8 | 2.54 | 0.43 |
| 1:CA:413:G:N2 | 1:CA:429:U:C6 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 23:AD:10:G:N1 | 23:AD:27:G:N2 | 2.67 | 0.43 |
| 1:AA:376:G:C5' | 16:AS:5:ARG:HD2 | 2.45 | 0.43 |
| 28:BE:13:ARG:HG3 | 28:BE:13:ARG:H | 1.65 | 0.43 |
| 32:DK:97:ILE:HD13 | 32:DK:140:LEU:HD22 | 2.01 | 0.43 |
| 1:AA:1279:A:H5' | 10:AM:7:LYS:NZ | 2.34 | 0.43 |
| 27:DD:89:SER:HB2 | 27:DD:159:ALA:CB | 2.49 | 0.43 |
| 25:BA:2755:C:HO2' | 25:BA:2756:U:H6 | 1.67 | 0.43 |
| 27:BD:120:GLY:O | 27:BD:123:ALA:HB2 | 2.18 | 0.43 |
| 20:CW:64:ASP:OD1 | 20:CW:81:LYS:CD | 2.67 | 0.43 |
| 25:BA:271(C):U:C2' | 25:BA:271:G:OP1 | 2.66 | 0.43 |
| 22:AB:13:G:N2 | 22:AB:23:A:C8 | 2.87 | 0.43 |
| 25:BA:755:C:C2' | 25:BA:756:C:H5' | 2.49 | 0.43 |
| 25:DA:818:G:H4' | 25:DA:838:C:O3' | 2.18 | 0.43 |
| 25:DA:2563:U:O2 | 25:DA:2565:A:H8 | 2.02 | 0.43 |
| 33:DM:56:ASN:HA | 33:DM:125:GLY:H | 1.83 | 0.43 |
| 23:AD:39:A:H2' | 23:AD:40:C:O5' | 2.19 | 0.43 |
| 9:CL:70:LYS:O | 9:CL:74:ILE:HG13 | 2.18 | 0.43 |
| 25:BA:817:C:O2' | 25:BA:839:U:H5'' | 2.19 | 0.43 |
| 29:DF:157:VAL:HA | 29:DF:176:LEU:O | 2.18 | 0.43 |
| 25:BA:1701:A:H2' | 25:BA:1702:G:H5' | 2.01 | 0.43 |
| 25:DA:1356:G:C5 | 25:DA:1357:U:C5 | 3.07 | 0.43 |
| 36:BP:4:PRO:HD3 | 36:BP:70:PRO:O | 2.19 | 0.43 |
| 1:AA:31:G:O2' | 1:AA:48:C:N4 | 2.51 | 0.43 |
| 1:CA:160:A:H1' | 1:CA:344:A:C5 | 2.54 | 0.43 |
| 48:DW:50:ILE:O | 48:DW:54:LYS:HB2 | 2.18 | 0.43 |
| 2:CE:212:GLN:O | 2:CE:216:SER:HB3 | 2.19 | 0.43 |
| 25:DA:1244:G:C2' | 25:DA:1245:G:H5' | 2.48 | 0.43 |
| 27:DD:125:ILE:O | 27:DD:126:GLN:HG3 | 2.18 | 0.43 |
| 25:DA:1345:C:C2' | 25:DA:1346:G:H5' | 2.49 | 0.43 |
| 25:BA:1742:C:H5' | 25:BA:1743:G:OP2 | 2.19 | 0.43 |
| 25:BA:583:G:OP2 | 40:B1:10:ARG:HD2 | 2.19 | 0.43 |
| 20:AW:45:GLN:HB2 | 20:AW:91:LEU:HD13 | 2.00 | 0.43 |
| 25:BA:950:G:H2' | 25:BA:951:C:C6 | 2.54 | 0.43 |
| 54:D8:55:ALA:O | 54:D8:58:ILE:HG12 | 2.18 | 0.43 |
| 25:BA:1136:G:N3 | 25:BA:1136:G:H2' | 2.34 | 0.43 |
| 17:CT:65:ILE:O | 17:CT:65:ILE:HG22 | 2.18 | 0.43 |
| 25:DA:2322:A:H2' | 25:DA:2323:G:O4' | 2.19 | 0.43 |
| 18:CU:53:ARG:HH21 | 18:CU:60:ALA:N | 2.17 | 0.43 |
| 25:BA:609:A:H2' | 25:BA:609(A):G:O4' | 2.18 | 0.43 |
| 17:CT:11:VAL:HG11 | 17:CT:88:TYR:CD2 | 2.53 | 0.43 |
| 27:DD:35:LYS:CE | 27:DD:65:ILE:HG22 | 2.49 | 0.43 |
| 40:D1:58:ARG:HA | 40:D1:61:TRP:CE3 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:1225:C:O3' | 41:D2:85:LYS:HD3 | 2.18 | 0.43 |
| 28:BE:75:VAL:CG2 | 28:BE:76:ARG:H | 2.16 | 0.43 |
| 28:DE:8:LYS:CE | 28:DE:188:VAL:HG13 | 2.48 | 0.43 |
| 28:DE:36:ARG:NH2 | 28:DE:88:GLY:CA | 2.81 | 0.43 |
| 39:DR:16:ARG:HH21 | 39:DR:19:LEU:HD11 | 1.83 | 0.43 |
| 44:BU:76:CYS:CB | 44:BU:77:PRO:CD | 2.97 | 0.43 |
| 1:CA:1220:G:O3' | 19:CV:36:ARG:HD3 | 2.18 | 0.43 |
| 26:DB:75:G:N1 | 26:DB:102:G:N2 | 2.67 | 0.43 |
| 25:DA:270(Q):C:H5' | 25:DA:270(R):G:OP2 | 2.19 | 0.43 |
| 1:AA:1023:G:C3' | 1:AA:1024:G:H5'' | 2.45 | 0.43 |
| 35:BO:64:LYS:CD | 54:B8:25:MET:CE | 2.81 | 0.43 |
| 25:BA:67:U:O4 | 25:BA:74:A:N1 | 2.52 | 0.43 |
| 25:BA:2212:A:N3 | 25:BA:2215:G:C2 | 2.87 | 0.43 |
| 25:BA:1021:A:H8 | 25:BA:1021:A:H3' | 1.83 | 0.43 |
| 1:AA:856:C:H2' | 1:AA:857:C:H5' | 2.01 | 0.43 |
| 25:DA:2115:G:H1' | 25:DA:2171:A:C6 | 2.54 | 0.43 |
| 25:DA:675:A:C4 | 25:DA:804:A:C2 | 3.07 | 0.43 |
| 42:DS:59:VAL:HG13 | 42:DS:60:ASN:N | 2.33 | 0.43 |
| 1:AA:38:G:H4' | 1:AA:547:A:N6 | 2.34 | 0.43 |
| 25:DA:2688:U:H1' | 25:DA:2721:A:N6 | 2.33 | 0.43 |
| 1:CA:406:G:H5' | 4:CG:5:ILE:CG2 | 2.49 | 0.43 |
| 33:DM:128:HIS:HE2 | 33:DM:134:ARG:CD | 2.30 | 0.43 |
| 33:BM:130:HIS:HB3 | 33:BM:134:ARG:NH1 | 2.20 | 0.43 |
| 30:DG:111:LEU:O | 30:DG:117:PHE:CD2 | 2.71 | 0.43 |
| 25:BA:2262:U:H4' | 25:BA:2328:A:H2 | 1.83 | 0.43 |
| 23:AD:53:G:H1 | 23:AD:63:C:H42 | 1.67 | 0.43 |
| 1:CA:1327:C:H2' | 1:CA:1328:C:H6 | 1.82 | 0.43 |
| 1:CA:915:A:H2' | 1:CA:916:G:O5' | 2.19 | 0.43 |
| 25:BA:1263:U:H1' | 51:B5:10:LYS:HG3 | 2.00 | 0.43 |
| 27:BD:69:ARG:HH12 | 27:BD:117:VAL:HG13 | 1.84 | 0.43 |
| 47:DZ:4:VAL:HG12 | 47:DZ:11:ARG:CB | 2.46 | 0.43 |
| 22:AB:53:A:H5'' | 22:AB:54:G:OP2 | 2.18 | 0.43 |
| 29:BF:34:TRP:CH2 | 35:BO:8:PRO:HB3 | 2.54 | 0.43 |
| 3:AF:95:THR:HG22 | 3:AF:96:GLY:H | 1.84 | 0.43 |
| 1:CA:197:A:N1 | 1:CA:221:C:H4' | 2.33 | 0.43 |
| 25:DA:464:U:H4' | 53:D7:5:TRP:CZ3 | 2.54 | 0.43 |
| 4:AG:79:PHE:HE1 | 4:AG:204:ILE:CG1 | 2.29 | 0.43 |
| 1:AA:431:A:H2' | 1:AA:432:A:O4' | 2.19 | 0.43 |
| 12:AO:24:VAL:CG1 | 12:AO:98:TYR:HE2 | 2.32 | 0.43 |
| 25:DA:1000:A:N6 | 25:DA:1155:A:C8 | 2.87 | 0.43 |
| 1:AA:1263:C:O2' | 1:AA:1264:C:H5' | 2.19 | 0.43 |
| 13:AP:64:TRP:N | 13:AP:64:TRP:CD1 | 2.87 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:DD:267:SER:C | 27:DD:269:PHE:N | 2.71 | 0.43 |
| 25:BA:2147:G:H2' | 25:BA:2148:G:O4' | 2.19 | 0.43 |
| 5:AH:91:LEU:HD12 | 5:AH:120:THR:CG2 | 2.48 | 0.43 |
| 3:AF:189:ALA:O | 3:AF:190:ARG:C | 2.57 | 0.43 |
| 1:AA:1118:C:OP1 | 9:AL:9:ARG:HD3 | 2.19 | 0.43 |
| 25:BA:2037:G:H2' | 25:BA:2038:G:H8 | 1.83 | 0.43 |
| 32:BK:88:ILE:HG22 | 32:BK:90:GLY:N | 2.34 | 0.43 |
| 25:BA:2279:G:OP2 | 46:B3:11:ARG:NH2 | 2.51 | 0.43 |
| 25:BA:1952:A:C6 | 34:BN:22:ILE:CD1 | 3.02 | 0.43 |
| 36:BP:58:PHE:CD1 | 36:BP:58:PHE:O | 2.72 | 0.43 |
| 25:DA:1386:C:OP2 | 25:DA:1396:U:H5 | 2.02 | 0.43 |
| 1:CA:1205:U:H3' | 1:CA:1205:U:C6 | 2.54 | 0.43 |
| 26:BB:6:C:H2' | 26:BB:7:G:H5'' | 2.01 | 0.43 |
| 25:DA:1418:G:OP1 | 25:DA:1588:C:O2' | 2.36 | 0.43 |
| 34:DN:79:PHE:HD2 | 39:DR:72:VAL:HG22 | 1.84 | 0.43 |
| 25:BA:986:C:C2' | 25:BA:987:G:H5' | 2.48 | 0.43 |
| 27:BD:158:ALA:HB3 | 27:BD:161:THR:HG21 | 2.01 | 0.43 |
| 16:AS:12:LYS:O | 16:AS:13:HIS:HB2 | 2.18 | 0.43 |
| 1:AA:509:A:H5'' | 4:AG:55:ALA:HB2 | 2.01 | 0.43 |
| 1:AA:36:C:OP1 | 12:AO:123:LYS:NZ | 2.35 | 0.43 |
| 25:DA:2773:C:OP1 | 28:DE:166:THR:OG1 | 2.36 | 0.43 |
| 25:BA:2881:C:O2' | 37:B0:96:ARG:HA | 2.18 | 0.43 |
| 35:BO:26:GLY:O | 35:BO:28:GLY:N | 2.52 | 0.43 |
| 50:B4:48:ARG:O | 50:B4:51:ASP:HB3 | 2.18 | 0.43 |
| 54:D8:58:ILE:H | 54:D8:58:ILE:HG12 | 1.66 | 0.43 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.53 | 0.43 |
| 12:CO:117:ARG:NH2 | 12:CO:124:LYS:HA | 2.33 | 0.43 |
| 29:DF:4:VAL:CG1 | 29:DF:17:ARG:HE | 2.31 | 0.43 |
| 25:BA:8:A:H2' | 25:BA:9:U:O4' | 2.18 | 0.43 |
| 25:BA:382:G:N2 | 25:BA:393:C:C2 | 2.86 | 0.43 |
| 46:B3:24:LYS:O | 46:B3:25:ARG:HD3 | 2.18 | 0.43 |
| 32:DK:41:GLU:H | 32:DK:41:GLU:HG3 | 1.53 | 0.43 |
| 14:AQ:3:ARG:HD3 | 14:AQ:3:ARG:HA | 1.49 | 0.43 |
| 44:BU:38:ILE:HG12 | 44:BU:38:ILE:O | 2.19 | 0.43 |
| 16:AS:20:VAL:HG22 | 16:AS:32:TYR:HB2 | 2.01 | 0.43 |
| 23:AC:17:C:O2' | 23:AC:18:C:OP1 | 2.32 | 0.43 |
| 29:DF:51:THR:CG2 | 29:DF:92:PRO:HD2 | 2.48 | 0.43 |
| 28:DE:48:GLN:CG | 28:DE:78:LEU:HB2 | 2.49 | 0.43 |
| 25:BA:1026:U:O2 | 25:BA:1027:A:H3' | 2.18 | 0.43 |
| 36:DP:61:GLY:HA2 | 36:DP:62:GLY:HA3 | 1.71 | 0.43 |
| 22:CB:70:G:C3' | 22:CB:71:U:C6 | 3.01 | 0.43 |
| 47:DZ:6:GLU:O | 47:DZ:91:LYS:HE2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 19:AV:42:PRO:HD3 | 50:B4:63:TYR:CE1 | 2.54 | 0.43 |
| 19:AV:44:MET:O | 19:AV:47:HIS:HB2 | 2.19 | 0.43 |
| 32:DK:145:VAL:O | 32:DK:146:ALA:HB3 | 2.19 | 0.43 |
| 25:DA:1005:C:O2 | 25:DA:1143:A:C6 | 2.71 | 0.43 |
| 9:CL:97:LYS:HG3 | 9:CL:98:PRO:CD | 2.49 | 0.43 |
| 1:AA:974:A:O2' | 1:AA:975:A:OP2 | 2.34 | 0.43 |
| 13:CP:19:LEU:O | 13:CP:22:ILE:HG13 | 2.19 | 0.43 |
| 23:CD:8:U:C5 | 23:CD:13:C:C4 | 3.06 | 0.43 |
| 25:DA:1048:A:OP2 | 25:DA:1109:C:N4 | 2.52 | 0.43 |
| 25:DA:1557:C:OP2 | 25:DA:1558:A:O2' | 2.36 | 0.43 |
| 1:AA:823:G:H21 | 8:AK:1:MET:CE | 2.19 | 0.43 |
| 25:DA:1300:U:C4' | 25:DA:1301:A:H5'' | 2.44 | 0.43 |
| 25:DA:329:G:C5 | 44:DU:19:LYS:HG2 | 2.54 | 0.43 |
| 25:DA:2134:A:O2' | 25:DA:2159:G:N2 | 2.52 | 0.43 |
| 9:CL:45:ALA:O | 9:CL:48:GLU:HB2 | 2.19 | 0.43 |
| 35:BO:21:ARG:HB3 | 35:BO:22:GLY:H | 1.57 | 0.43 |
| 1:AA:1028(A):C:N3 | 1:AA:1028(B):C:N4 | 2.66 | 0.43 |
| 1:AA:547:A:OP2 | 4:AG:2:GLY:HA2 | 2.18 | 0.43 |
| 50:D4:32:TYR:HB3 | 50:D4:33:VAL:H | 1.59 | 0.43 |
| 31:BH:161:GLY:O | 31:BH:163:TYR:CD1 | 2.72 | 0.43 |
| 35:DO:97:PRO:HG3 | 35:DO:112:LEU:HB2 | 2.01 | 0.43 |
| 25:DA:654(A):A:C2 | 25:DA:654(U):A:N3 | 2.87 | 0.43 |
| 25:DA:2136:C:H2' | 25:DA:2137:C:C6 | 2.54 | 0.43 |
| 4:AG:4:TYR:CZ | 4:AG:5:ILE:O | 2.72 | 0.43 |
| 14:AQ:26:ARG:HD2 | 14:AQ:47:LEU:HD11 | 2.00 | 0.43 |
| 54:B8:61:LEU:O | 54:B8:62:LEU:HB2 | 2.18 | 0.43 |
| 25:BA:2701:C:H2' | 25:BA:2702:U:H2' | 2.01 | 0.43 |
| 6:AI:75:LEU:HD22 | 6:AI:79:LEU:HG | 2.00 | 0.43 |
| 42:BS:29:LEU:O | 42:BS:33:ARG:HG3 | 2.19 | 0.43 |
| 52:D6:34:LEU:O | 52:D6:35:GLU:HB2 | 2.18 | 0.43 |
| 34:BN:23:ARG:HG3 | 34:BN:24:VAL:H | 1.83 | 0.43 |
| 23:AD:8:U:C5 | 23:AD:13:C:N4 | 2.86 | 0.43 |
| 25:DA:1416:G:C2' | 25:DA:1417:C:H6 | 2.32 | 0.43 |
| 25:DA:1416:G:HO2' | 25:DA:1417:C:H6 | 1.67 | 0.43 |
| 1:CA:1342:C:H4' | 9:CL:125:TYR:HB3 | 2.01 | 0.43 |
| 48:DW:17:SER:CB | 48:DW:21:LEU:H | 2.32 | 0.43 |
| 25:BA:76:C:HO2' | 48:BW:62:THR:HG21 | 1.83 | 0.43 |
| 39:BR:124:ASP:O | 39:BR:127:ALA:N | 2.52 | 0.43 |
| 1:AA:102:G:C6 | 1:AA:103:C:C4 | 3.07 | 0.43 |
| 25:BA:1925:C:O2' | 25:BA:1926:U:H5' | 2.18 | 0.43 |
| 25:BA:1448:G:N2 | 25:BA:1449:A:N6 | 2.67 | 0.43 |
| 12:CO:110:VAL:HG21 | 12:CO:120:TYR:HB3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:CA:720:C:O2 | 18:CU:71:LYS:NZ | 2.43 | 0.43 |
| 1:AA:232:G:H1' | 1:AA:262:A:N1 | 2.33 | 0.43 |
| 3:CF:182:ILE:HG23 | 3:CF:202:ILE:O | 2.19 | 0.43 |
| 12:AO:38:THR:O | 12:AO:79:GLU:HG3 | 2.18 | 0.43 |
| 3:CF:164:ARG:HH12 | 3:CF:166:GLU:CD | 2.22 | 0.43 |
| 25:BA:856:C:H2' | 25:BA:857:C:O5' | 2.18 | 0.43 |
| 25:BA:1582:C:H2' | 25:BA:1583:A:O4' | 2.18 | 0.43 |
| 32:BK:73:GLU:HG3 | 32:BK:137:PRO:CD | 2.46 | 0.43 |
| 26:BB:89(A):A:H8 | 26:BB:89(A):A:O5' | 2.00 | 0.43 |
| 25:DA:5:A:H61 | 25:DA:2898:U:H3 | 1.66 | 0.43 |
| 25:BA:989:G:C5 | 49:BX:13:ILE:HD12 | 2.54 | 0.43 |
| 4:CG:126:ILE:HG22 | 4:CG:127:THR:N | 2.34 | 0.43 |
| 23:CD:23:G:C2 | 23:CD:24:C:C2 | 3.07 | 0.43 |
| 25:BA:495:G:H1' | 42:BS:57:ASN:HD21 | 1.83 | 0.43 |
| 1:CA:578:C:C2 | 1:CA:579:G:C8 | 3.07 | 0.43 |
| 25:DA:755:C:H2' | 25:DA:756:C:H6 | 1.83 | 0.43 |
| 34:BN:22:ILE:HA | 34:BN:22:ILE:HD12 | 1.63 | 0.43 |
| 6:CI:14:LEU:HB2 | 6:CI:18:GLN:OE1 | 2.19 | 0.43 |
| 25:DA:2574:G:O2' | 28:DE:143:ASN:HB3 | 2.19 | 0.43 |
| 19:AV:30:LEU:H | 19:AV:30:LEU:CD1 | 2.31 | 0.43 |
| 25:DA:1445:C:H2' | 25:DA:1446:C:C6 | 2.53 | 0.43 |
| 18:CU:70:ILE:O | 18:CU:74:ARG:HG3 | 2.19 | 0.43 |
| 25:BA:1590:U:H2' | 25:BA:1591:G:H8 | 1.81 | 0.43 |
| 34:DN:2:ILE:HD11 | 34:DN:82:ASN:ND2 | 2.34 | 0.43 |
| 9:AL:22:GLY:O | 9:AL:57:GLY:O | 2.37 | 0.43 |
| 25:BA:834:C:C2' | 25:BA:835:A:H5' | 2.49 | 0.43 |
| 50:D4:42:PHE:O | 50:D4:43:TYR:HB3 | 2.18 | 0.43 |
| 43:BT:26:TYR:HB3 | 43:BT:92:LEU:HD12 | 2.00 | 0.43 |
| 25:DA:558:G:P | 33:DM:111:PRO:HD2 | 2.59 | 0.43 |
| 25:DA:2092:U:H4' | 25:DA:2093:G:O5' | 2.19 | 0.43 |
| 11:AN:99:GLN:HG2 | 11:AN:105:VAL:HG21 | 2.01 | 0.43 |
| 25:BA:2881:C:N4 | 25:BA:2882:A:N6 | 2.66 | 0.43 |
| 25:DA:30:G:C5 | 25:DA:31:C:C4 | 3.07 | 0.43 |
| 1:AA:1111:A:N6 | 3:AF:177:THR:HA | 2.33 | 0.43 |
| 25:BA:455:C:N3 | 25:BA:472:A:H2' | 2.34 | 0.43 |
| 25:DA:2658:C:H5" | 31:DH:158:HIS:CE1 | 2.54 | 0.43 |
| 25:DA:1319:G:C6 | 25:DA:1320:C:N4 | 2.87 | 0.43 |
| 17:AT:26:GLN:HG2 | 17:AT:37:LYS:HG2 | 2.00 | 0.43 |
| 25:BA:1541:U:O2' | 25:BA:1542:G:H5' | 2.19 | 0.43 |
| 3:AF:108:ASN:ND2 | 3:AF:144:SER:OG | 2.51 | 0.43 |
| 34:DN:119:PRO:HB2 | 39:DR:68:TYR:CE2 | 2.54 | 0.43 |
| 31:DH:37:VAL:HG22 | 31:DH:38:SER:H | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:15:G:C2 | 25:DA:16:G:C8 | 3.06 | 0.43 |
| 25:DA:454:A:H4' | 25:DA:455:C:OP2 | 2.18 | 0.43 |
| 39:DR:33:LYS:HE2 | 39:DR:42:ILE:HD11 | 2.01 | 0.43 |
| 25:DA:392:C:H5'' | 25:DA:409:C:H5'' | 2.00 | 0.43 |
| 47:DZ:82:LEU:HB2 | 47:DZ:83:GLU:H | 1.69 | 0.43 |
| 6:AI:23:LYS:HB2 | 6:AI:23:LYS:NZ | 2.34 | 0.43 |
| 38:DQ:93:LYS:HB2 | 38:DQ:93:LYS:HE3 | 1.72 | 0.43 |
| 53:B7:23:ARG:HH11 | 53:B7:23:ARG:HG2 | 1.83 | 0.43 |
| 4:CG:118:ARG:HB2 | 4:CG:118:ARG:HH21 | 1.83 | 0.43 |
| 1:CA:397:A:H3' | 1:CA:397:A:N3 | 2.34 | 0.43 |
| 41:D2:19:LYS:H | 41:D2:19:LYS:HG3 | 1.49 | 0.43 |
| 25:BA:2822:G:H2' | 25:BA:2823:A:H5'' | 2.01 | 0.43 |
| 1:AA:24:U:O2' | 1:AA:25:C:H5' | 2.19 | 0.43 |
| 51:B5:36:CYS:SG | 51:B5:48:GLU:O | 2.77 | 0.43 |
| 25:DA:1779:U:C6 | 25:DA:1783:A:N7 | 2.87 | 0.43 |
| 25:BA:618:G:H2' | 25:BA:618(A):C:O4' | 2.19 | 0.43 |
| 25:BA:1062:G:C2' | 25:BA:1063:G:C8 | 2.98 | 0.42 |
| 54:D8:32:LEU:HB2 | 54:D8:33:ASN:H | 1.64 | 0.42 |
| 38:BQ:106:ARG:HH22 | 38:BQ:107:GLU:HB2 | 1.77 | 0.42 |
| 25:DA:777:A:C2 | 25:DA:778:G:C8 | 3.07 | 0.42 |
| 23:CC:14:A:C6 | 23:CC:23:G:C5 | 3.07 | 0.42 |
| 31:DH:89:ILE:HG21 | 31:DH:129:THR:HG22 | 2.01 | 0.42 |
| 9:CL:114:TYR:CE1 | 10:CM:60:ARG:O | 2.71 | 0.42 |
| 1:CA:974:A:P | 14:CQ:41:ARG:HH22 | 2.42 | 0.42 |
| 25:DA:270(H):C:H2' | 25:DA:270(I):G:H8 | 1.84 | 0.42 |
| 25:DA:270(R):G:H2' | 25:DA:270(S):G:H8 | 1.84 | 0.42 |
| 25:BA:882:G:H1 | 25:BA:894:C:H42 | 1.67 | 0.42 |
| 48:DW:15:LYS:HA | 48:DW:67:LYS:NZ | 2.34 | 0.42 |
| 1:AA:1202:G:H2' | 1:AA:1203:C:O5' | 2.18 | 0.42 |
| 25:DA:1043:C:H42 | 25:DA:1112:G:H1 | 1.67 | 0.42 |
| 32:BK:92:VAL:O | 32:BK:92:VAL:HG22 | 2.19 | 0.42 |
| 1:CA:1128:C:O2' | 1:CA:1129:C:P | 2.73 | 0.42 |
| 25:DA:311:A:C6 | 25:DA:328:U:C4 | 3.07 | 0.42 |
| 25:DA:607:U:C2 | 25:DA:621:A:N1 | 2.86 | 0.42 |
| 41:B2:8:GLY:O | 41:B2:10:LYS:HE3 | 2.19 | 0.42 |
| 4:AG:108:LEU:HD12 | 4:AG:174:LEU:HD13 | 2.01 | 0.42 |
| 1:AA:687:A:H2' | 1:AA:701:C:H41 | 1.84 | 0.42 |
| 25:BA:2116:G:OP1 | 25:BA:2165:G:N2 | 2.50 | 0.42 |
| 19:CV:11:VAL:HG21 | 19:CV:16:LEU:HD11 | 2.01 | 0.42 |
| 25:BA:2156:G:H2' | 25:BA:2157:G:N3 | 2.34 | 0.42 |
| 25:DA:2690:C:H6 | 25:DA:2690:C:OP2 | 2.02 | 0.42 |
| 25:DA:943:U:OP2 | 35:DO:36:LYS:CE | 2.66 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 13:CP:2:ALA:N | 50:D4:32:TYR:HH | 2.17 | 0.42 |
| 33:BM:134:ARG:O | 33:BM:136:GLU:N | 2.52 | 0.42 |
| 1:CA:959:A:H5'' | 1:CA:960:U:OP2 | 2.19 | 0.42 |
| 32:BK:14:ASP:C | 32:BK:15:VAL:HG22 | 2.39 | 0.42 |
| 25:BA:1468:C:O2' | 25:BA:1469:A:H5' | 2.19 | 0.42 |
| 25:BA:1209:G:N2 | 25:BA:1210:A:H62 | 2.14 | 0.42 |
| 31:BH:10:PRO:C | 31:BH:11:VAL:HG13 | 2.39 | 0.42 |
| 54:D8:37:SER:O | 54:D8:39:LYS:O | 2.37 | 0.42 |
| 9:AL:77:ILE:O | 9:AL:81:ILE:HG12 | 2.19 | 0.42 |
| 25:BA:1263:U:O2' | 51:B5:11:THR:HG23 | 2.18 | 0.42 |
| 41:B2:35:LEU:C | 41:B2:37:VAL:N | 2.72 | 0.42 |
| 1:CA:422:C:O2' | 1:CA:423:G:N3 | 2.51 | 0.42 |
| 44:DU:61:ILE:HG22 | 44:DU:62:GLU:OE2 | 2.18 | 0.42 |
| 53:D7:43:THR:HG23 | 53:D7:44:PRO:HD2 | 2.01 | 0.42 |
| 3:CF:95:THR:HG22 | 3:CF:95:THR:O | 2.19 | 0.42 |
| 25:DA:833:U:O2 | 35:DO:55:ARG:NH2 | 2.51 | 0.42 |
| 1:CA:1084:G:C5 | 1:CA:1085:U:C4 | 3.07 | 0.42 |
| 1:CA:255:G:O3' | 17:CT:17:LYS:HD2 | 2.20 | 0.42 |
| 25:DA:483:A:H5'' | 44:DU:49:VAL:HA | 2.01 | 0.42 |
| 25:DA:909:A:C4 | 25:DA:912:C:C5 | 3.07 | 0.42 |
| 25:BA:2428:G:H5'' | 25:BA:2429:G:OP1 | 2.19 | 0.42 |
| 25:DA:2548:G:C2' | 25:DA:2549:G:O5' | 2.67 | 0.42 |
| 35:BO:106:LEU:HD22 | 35:BO:106:LEU:O | 2.19 | 0.42 |
| 25:DA:1639:U:C2' | 25:DA:1640:C:H5' | 2.49 | 0.42 |
| 25:BA:221:A:C4 | 25:BA:266:G:N7 | 2.87 | 0.42 |
| 36:BP:26:TYR:CE2 | 36:BP:28:ALA:HB2 | 2.52 | 0.42 |
| 18:CU:44:LEU:CD2 | 18:CU:79:LEU:HD13 | 2.49 | 0.42 |
| 40:D1:112:ARG:HD3 | 41:D2:47:VAL:HG11 | 2.01 | 0.42 |
| 38:DQ:49:VAL:HG23 | 38:DQ:80:LEU:HD12 | 2.01 | 0.42 |
| 43:BT:11:PRO:HB3 | 43:BT:92:LEU:CD2 | 2.49 | 0.42 |
| 43:DT:64:LYS:HD3 | 43:DT:73:ARG:CZ | 2.49 | 0.42 |
| 40:D1:17:ILE:HG23 | 40:D1:39:LEU:HD12 | 2.01 | 0.42 |
| 17:AT:27:PHE:CE1 | 17:AT:36:ILE:HD11 | 2.54 | 0.42 |
| 26:DB:80:U:H2' | 26:DB:81:G:H21 | 1.83 | 0.42 |
| 42:BS:45:TYR:CD2 | 42:BS:45:TYR:C | 2.91 | 0.42 |
| 25:BA:1825:A:O4' | 27:BD:254:THR:HG21 | 2.19 | 0.42 |
| 1:AA:1417:G:N2 | 1:AA:1482:G:H2' | 2.34 | 0.42 |
| 4:AG:145:GLU:HB2 | 4:AG:184:LYS:HZ2 | 1.84 | 0.42 |
| 25:BA:96:G:C2 | 25:BA:97:C:C6 | 3.06 | 0.42 |
| 25:DA:2667:C:N3 | 31:DH:110:SER:OG | 2.43 | 0.42 |
| 25:DA:2464:C:C2 | 25:DA:2487:G:C2 | 3.07 | 0.42 |
| 25:BA:984:A:H5'' | 25:BA:985:C:H5 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:AA:1310:G:O2' | 1:AA:1311:G:H5' | 2.18 | 0.42 |
| 1:CA:1294:G:C2' | 1:CA:1295:G:H5' | 2.49 | 0.42 |
| 25:DA:1919:A:H5'' | 25:DA:1920:C:OP2 | 2.19 | 0.42 |
| 19:AV:43:GLU:H | 19:AV:43:GLU:HG2 | 1.42 | 0.42 |
| 40:B1:47:TYR:CD2 | 40:B1:47:TYR:C | 2.92 | 0.42 |
| 25:DA:207:A:H2' | 25:DA:208:C:O4' | 2.19 | 0.42 |
| 25:BA:343:C:O2' | 25:BA:344:G:H5' | 2.18 | 0.42 |
| 25:DA:2393:A:H4' | 35:DO:62:LEU:N | 2.33 | 0.42 |
| 36:DP:28:ALA:O | 36:DP:29:PHE:CG | 2.71 | 0.42 |
| 28:DE:54:GLN:NE2 | 28:DE:54:GLN:HA | 2.34 | 0.42 |
| 23:CC:14:A:C4 | 23:CC:23:G:C2 | 3.07 | 0.42 |
| 30:BG:61:ALA:O | 50:B4:7:PRO:HG3 | 2.18 | 0.42 |
| 44:BU:96:ILE:HG23 | 44:BU:101:LYS:CG | 2.36 | 0.42 |
| 25:BA:2286:A:H8 | 52:B6:37:ARG:HH11 | 1.66 | 0.42 |
| 1:CA:1199:U:H4' | 10:CM:54:PHE:CD1 | 2.54 | 0.42 |
| 1:CA:543:C:C2' | 1:CA:544:G:H5' | 2.48 | 0.42 |
| 4:CG:59:ARG:NH2 | 4:CG:66:ARG:HH12 | 2.17 | 0.42 |
| 39:BR:74:ARG:CG | 39:BR:74:ARG:NH1 | 2.73 | 0.42 |
| 28:DE:131:ALA:HB1 | 28:DE:135:HIS:CE1 | 2.53 | 0.42 |
| 25:DA:1019:U:HO2' | 25:DA:1021:A:H2 | 1.59 | 0.42 |
| 25:DA:1140:C:H4' | 25:DA:1143:A:N7 | 2.34 | 0.42 |
| 25:DA:1043:C:H2' | 25:DA:1044:G:C5' | 2.49 | 0.42 |
| 25:BA:1005:C:O2' | 33:BM:28:THR:HG21 | 2.19 | 0.42 |
| 1:CA:1127:G:H22 | 1:CA:1144:G:N2 | 2.18 | 0.42 |
| 40:B1:92:ARG:HH21 | 41:B2:10:LYS:HG2 | 1.85 | 0.42 |
| 1:CA:1097:C:OP1 | 2:CE:137:ARG:NH2 | 2.53 | 0.42 |
| 25:BA:1525:G:O2' | 25:BA:1526:G:O5' | 2.20 | 0.42 |
| 25:BA:2401:U:O2 | 25:BA:2402:C:C5 | 2.72 | 0.42 |
| 31:BH:6:ARG:NE | 31:BH:54:ARG:HH12 | 2.17 | 0.42 |
| 1:CA:1300:G:C6 | 1:CA:1334:G:C5 | 3.06 | 0.42 |
| 25:BA:2168:G:N2 | 25:BA:2170:A:C8 | 2.87 | 0.42 |
| 53:B7:15:THR:HG22 | 53:B7:16:HIS:CE1 | 2.54 | 0.42 |
| 25:DA:1360:A:N6 | 25:DA:1371:G:H1' | 2.35 | 0.42 |
| 7:AJ:21:VAL:HG23 | 7:AJ:22:LEU:N | 2.34 | 0.42 |
| 1:CA:502:G:C2 | 1:CA:503:C:C2 | 3.07 | 0.42 |
| 51:B5:40:LYS:CG | 51:B5:46:CYS:HB3 | 2.48 | 0.42 |
| 41:B2:39:LEU:O | 41:B2:40:LEU:CD2 | 2.67 | 0.42 |
| 25:DA:2439:A:H5' | 25:DA:2439:A:H8 | 1.75 | 0.42 |
| 2:AE:178:ARG:HH11 | 2:AE:178:ARG:HB2 | 1.84 | 0.42 |
| 25:DA:2015:A:N3 | 51:D5:6:VAL:CG2 | 2.83 | 0.42 |
| 15:AR:74:ASP:CB | 15:AR:77:ARG:HG2 | 2.48 | 0.42 |
| 25:DA:1416:G:O2' | 25:DA:1417:C:C6 | 2.72 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 50:B4:15:ILE:HG13 | 50:B4:32:TYR:HA | 2.00 | 0.42 |
| 25:DA:1935:G:H1' | 25:DA:1964:G:N2 | 2.34 | 0.42 |
| 51:B5:42:PRO:O | 51:B5:44:THR:N | 2.52 | 0.42 |
| 32:DK:104:GLN:HB2 | 32:DK:104:GLN:HE21 | 1.68 | 0.42 |
| 25:BA:1931:U:C5 | 25:BA:1969:A:N7 | 2.81 | 0.42 |
| 16:CS:43:LYS:HA | 16:CS:48:TRP:HB3 | 2.01 | 0.42 |
| 1:CA:76:G:C6 | 1:CA:77:C:C4 | 3.07 | 0.42 |
| 25:BA:2199:A:H3' | 25:BA:2205:C:C6 | 2.49 | 0.42 |
| 1:CA:1386:G:H2' | 1:CA:1387:G:H8 | 1.84 | 0.42 |
| 1:AA:533:A:C2 | 1:AA:536:C:C6 | 3.07 | 0.42 |
| 25:BA:2250:G:C5 | 36:BP:82:ARG:HD3 | 2.54 | 0.42 |
| 38:DQ:97:ARG:O | 38:DQ:100:ALA:HB3 | 2.19 | 0.42 |
| 25:BA:2875:C:O2' | 39:BR:5:ALA:CB | 2.67 | 0.42 |
| 22:AB:24:C:C6 | 22:AB:24:C:C3' | 3.02 | 0.42 |
| 1:AA:1434:A:H2' | 1:AA:1435:G:O4' | 2.20 | 0.42 |
| 1:CA:1152:A:OP1 | 10:CM:68:HIS:CE1 | 2.72 | 0.42 |
| 51:D5:31:VAL:CG1 | 51:D5:42:PRO:HG3 | 2.48 | 0.42 |
| 25:DA:362:U:C6 | 25:DA:362:U:C3' | 3.03 | 0.42 |
| 26:DB:41:U:C4 | 30:DG:70:VAL:HG23 | 2.54 | 0.42 |
| 1:CA:1250:A:H4' | 9:CL:68:GLY:H | 1.83 | 0.42 |
| 25:DA:2209:C:C2 | 25:DA:2216:G:C2 | 3.07 | 0.42 |
| 29:DF:79:GLY:HA2 | 29:DF:86:GLY:CA | 2.48 | 0.42 |
| 43:DT:66:LEU:HD23 | 43:DT:66:LEU:HA | 1.81 | 0.42 |
| 1:AA:1219:U:OP1 | 14:AQ:19:ARG:NH2 | 2.39 | 0.42 |
| 23:CC:50:G:N1 | 23:CC:51:U:O2 | 2.51 | 0.42 |
| 25:DA:1131:G:N2 | 25:DA:1132:A:N3 | 2.67 | 0.42 |
| 25:BA:1976:U:O5' | 25:BA:1976:U:H6 | 2.02 | 0.42 |
| 2:CE:168:THR:HG23 | 2:CE:192:SER:CB | 2.49 | 0.42 |
| 25:BA:947:G:N3 | 25:BA:984:A:H2 | 2.17 | 0.42 |
| 25:BA:908:C:O2' | 25:BA:909:A:H5' | 2.19 | 0.42 |
| 25:BA:1458:C:H4' | 25:BA:1459:G:O5' | 2.18 | 0.42 |
| 25:DA:702:G:C2 | 25:DA:731:C:C2 | 3.07 | 0.42 |
| 8:CK:13:ILE:O | 8:CK:17:THR:HG23 | 2.19 | 0.42 |
| 25:BA:2528:U:H2' | 25:BA:2530:A:O5' | 2.19 | 0.42 |
| 25:BA:2050:C:H2' | 25:BA:2051:A:C8 | 2.55 | 0.42 |
| 25:BA:116:C:C2' | 25:BA:117:G:O5' | 2.67 | 0.42 |
| 1:AA:782:A:C8 | 1:AA:783:C:C5 | 3.07 | 0.42 |
| 8:CK:58:TYR:O | 8:CK:59:LEU:HD23 | 2.18 | 0.42 |
| 1:CA:593:G:C2 | 1:CA:647:C:O2 | 2.72 | 0.42 |
| 45:BV:171:ILE:O | 45:BV:171:ILE:HG22 | 2.19 | 0.42 |
| 10:CM:46:ARG:HA | 10:CM:64:GLU:HA | 2.01 | 0.42 |
| 25:BA:1070:A:H2' | 25:BA:1097:U:OP1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:BD:181:GLU:CB | 27:BD:272:ALA:HB3 | 2.49 | 0.42 |
| 38:DQ:42:ASP:C | 38:DQ:44:LYS:H | 2.22 | 0.42 |
| 33:BM:39:ARG:HA | 33:BM:40:PRO:HD3 | 1.85 | 0.42 |
| 1:AA:1125:U:O4 | 10:AM:5:ARG:CD | 2.68 | 0.42 |
| 1:CA:484:G:C8 | 1:CA:486:U:C2 | 3.07 | 0.42 |
| 47:DZ:92:LYS:O | 47:DZ:94:LEU:N | 2.52 | 0.42 |
| 36:BP:66:ILE:H | 36:BP:104:PHE:HA | 1.83 | 0.42 |
| 23:AC:77:A:H8 | 23:AC:77:A:C5' | 2.32 | 0.42 |
| 51:B5:3:LYS:CE | 51:B5:3:LYS:HA | 2.40 | 0.42 |
| 25:DA:363(B):G:C2 | 25:DA:363(C):G:C4 | 3.08 | 0.42 |
| 23:CD:15:G:C5 | 23:CD:16:C:H5 | 2.36 | 0.42 |
| 1:CA:1148:U:C4 | 1:CA:1149:C:C2 | 3.07 | 0.42 |
| 17:AT:67:LYS:O | 17:AT:68:ARG:HB3 | 2.19 | 0.42 |
| 26:DB:40:U:H1' | 26:DB:46:A:N1 | 2.34 | 0.42 |
| 25:BA:2401:U:H2' | 25:BA:2402:C:H6 | 1.85 | 0.42 |
| 25:BA:783:A:C3' | 25:BA:783:A:C8 | 3.02 | 0.42 |
| 25:BA:2169:A:C5 | 25:BA:2170:A:C2 | 3.07 | 0.42 |
| 53:B7:8:ASN:ND2 | 53:B7:11:LYS:N | 2.52 | 0.42 |
| 35:DO:21:ARG:CA | 35:DO:21:ARG:HE | 2.20 | 0.42 |
| 35:DO:97:PRO:HG3 | 35:DO:112:LEU:HD12 | 1.99 | 0.42 |
| 45:BV:164:ALA:O | 45:BV:165:VAL:CG1 | 2.66 | 0.42 |
| 32:BK:14:ASP:O | 32:BK:15:VAL:HG22 | 2.18 | 0.42 |
| 3:AF:126:ARG:NH1 | 3:AF:126:ARG:CG | 2.65 | 0.42 |
| 25:DA:2335:A:N7 | 25:DA:2337:G:C5 | 2.87 | 0.42 |
| 1:CA:1368:G:C2' | 1:CA:1369:C:H5' | 2.50 | 0.42 |
| 1:CA:1286:A:C2 | 21:CX:18:TYR:OH | 2.72 | 0.42 |
| 1:AA:1372:U:OP1 | 9:AL:72:GLY:N | 2.50 | 0.42 |
| 22:CB:26:C:C4 | 22:CB:27:G:C2 | 3.08 | 0.42 |
| 43:DT:63:LYS:CE | 43:DT:63:LYS:H | 2.27 | 0.42 |
| 45:BV:105:VAL:CG1 | 45:BV:140:ASP:HB3 | 2.50 | 0.42 |
| 25:DA:1204:A:N1 | 25:DA:1241:A:N1 | 2.67 | 0.42 |
| 8:AK:51:VAL:HG23 | 8:AK:52:ASP:N | 2.34 | 0.42 |
| 23:CD:31:G:N2 | 23:CD:42:C:N3 | 2.66 | 0.42 |
| 36:DP:102:VAL:O | 36:DP:102:VAL:CG1 | 2.66 | 0.42 |
| 36:DP:43:THR:HG22 | 36:DP:94:VAL:HG12 | 2.00 | 0.42 |
| 44:BU:42:VAL:CG2 | 44:BU:67:LEU:HD11 | 2.49 | 0.42 |
| 8:AK:64:LYS:O | 8:AK:65:TYR:CD1 | 2.72 | 0.42 |
| 32:DK:76:THR:HG23 | 32:DK:77:LEU:N | 2.34 | 0.42 |
| 28:DE:66:HIS:CE1 | 28:DE:71:GLY:HA2 | 2.54 | 0.42 |
| 1:CA:937:A:C2 | 1:CA:1379:G:O6 | 2.72 | 0.42 |
| 25:DA:2012:G:P | 42:DS:11:ARG:HH22 | 2.42 | 0.42 |
| 1:CA:16:A:N1 | 1:CA:919:A:C2 | 2.85 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:977:G:O6 | 25:DA:987:G:C6 | 2.72 | 0.42 |
| 19:AV:66:MET:HB3 | 19:AV:74:PHE:HZ | 1.83 | 0.42 |
| 1:CA:1084:G:C4 | 1:CA:1085:U:C5 | 3.08 | 0.42 |
| 1:CA:342:C:H42 | 1:CA:347:G:H1 | 1.68 | 0.42 |
| 1:CA:188:U:O2' | 1:CA:189:U:C5' | 2.65 | 0.42 |
| 1:AA:1149:C:P | 9:AL:9:ARG:NH2 | 2.91 | 0.42 |
| 1:CA:900:A:H2' | 1:CA:901:A:C8 | 2.54 | 0.42 |
| 1:CA:302:G:H4' | 12:CO:17:LYS:HE3 | 2.01 | 0.42 |
| 4:AG:100:ARG:NH1 | 4:AG:137:SER:HA | 2.35 | 0.42 |
| 8:CK:112:LEU:HD12 | 8:CK:114:THR:CG2 | 2.50 | 0.42 |
| 25:DA:2121:G:H2' | 25:DA:2122:U:C6 | 2.54 | 0.42 |
| 25:BA:2584:U:O4' | 25:BA:2584:U:O2 | 2.37 | 0.42 |
| 25:BA:24:G:O2' | 25:BA:25:U:H5' | 2.19 | 0.42 |
| 1:AA:540:G:H2' | 1:AA:541:G:O4' | 2.19 | 0.42 |
| 48:BW:42:GLY:C | 48:BW:44:LEU:H | 2.21 | 0.42 |
| 25:BA:1705:G:C6 | 25:BA:1706:U:C4 | 3.07 | 0.42 |
| 2:AE:95:GLN:HE21 | 2:AE:147:LYS:HE3 | 1.84 | 0.42 |
| 37:B0:98:LEU:HD11 | 51:B5:54:GLY:HA3 | 2.01 | 0.42 |
| 23:AD:23:G:H2' | 23:AD:24:C:H6 | 1.84 | 0.42 |
| 38:BQ:66:ALA:O | 38:BQ:69:VAL:HG13 | 2.19 | 0.42 |
| 1:AA:60:A:H4' | 1:AA:61:G:OP1 | 2.18 | 0.42 |
| 1:CA:450:G:H2' | 1:CA:451:A:OP1 | 2.19 | 0.42 |
| 25:DA:1575:C:H2' | 25:DA:1576:U:C6 | 2.55 | 0.42 |
| 25:BA:1665:A:C2' | 25:BA:1666:G:H5' | 2.49 | 0.42 |
| 3:CF:90:GLU:O | 3:CF:93:LYS:HB3 | 2.19 | 0.42 |
| 8:AK:10:LEU:N | 8:AK:10:LEU:HD23 | 2.34 | 0.42 |
| 11:AN:91:ARG:HG3 | 11:AN:91:ARG:HH11 | 1.83 | 0.42 |
| 4:CG:4:TYR:O | 4:CG:4:TYR:CG | 2.72 | 0.42 |
| 53:D7:1:MET:HA | 53:D7:1:MET:CE | 2.49 | 0.42 |
| 12:CO:28:LYS:O | 12:CO:29:GLY:C | 2.57 | 0.42 |
| 45:DV:76:LEU:CD2 | 45:DV:76:LEU:N | 2.81 | 0.42 |
| 25:BA:1063:G:C4 | 25:BA:1064:C:C5 | 3.07 | 0.42 |
| 25:BA:2394:C:OP1 | 35:BO:62:LEU:CA | 2.67 | 0.42 |
| 38:DQ:88:ASP:CG | 38:DQ:89:ARG:N | 2.72 | 0.42 |
| 40:D1:92:ARG:NE | 41:D2:11:GLN:HB2 | 2.34 | 0.42 |
| 23:AC:19:G:C6 | 23:AC:59:A:C6 | 3.07 | 0.42 |
| 35:BO:75:ILE:CG1 | 35:BO:77:ARG:NH1 | 2.82 | 0.42 |
| 29:DF:66:PRO:O | 29:DF:67:GLN:CG | 2.67 | 0.42 |
| 28:DE:47:VAL:HG23 | 28:DE:84:PHE:O | 2.20 | 0.42 |
| 23:CC:15:G:C4 | 23:CC:60:A:C2 | 3.08 | 0.42 |
| 23:CC:61:U:H2' | 23:CC:61:U:H6 | 1.65 | 0.42 |
| 45:DV:115:GLY:N | 45:DV:177:PRO:HG2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 26:DB:75:G:C5' | 26:DB:75:G:C8 | 2.98 | 0.42 |
| 25:DA:2415:G:C3' | 35:DO:66:GLY:HA3 | 2.50 | 0.42 |
| 52:B6:28:ARG:HH12 | 52:B6:30:THR:HG22 | 1.84 | 0.42 |
| 36:DP:75:THR:CG2 | 36:DP:88:GLY:HA3 | 2.49 | 0.42 |
| 29:DF:116:ASP:OD2 | 35:DO:1:MET:N | 2.53 | 0.42 |
| 1:AA:1368:G:H5'' | 9:AL:112:LYS:HB3 | 2.00 | 0.42 |
| 1:AA:1060:C:P | 14:AQ:45:ARG:HH22 | 2.42 | 0.42 |
| 13:CP:34:LEU:HD13 | 13:CP:41:PRO:HA | 2.02 | 0.42 |
| 13:CP:29:ARG:HD3 | 13:CP:64:TRP:CE2 | 2.54 | 0.42 |
| 1:CA:1281:U:H3' | 1:CA:1282:C:H5 | 1.83 | 0.42 |
| 30:DG:4:ASP:O | 30:DG:5:VAL:HB | 2.19 | 0.42 |
| 30:BG:7:LEU:HB2 | 30:BG:104:GLU:CD | 2.39 | 0.42 |
| 1:AA:858:G:N1 | 1:AA:870:U:OP2 | 2.48 | 0.42 |
| 44:BU:45:VAL:HG12 | 44:BU:60:PHE:CD1 | 2.54 | 0.42 |
| 25:BA:1498:C:O4' | 25:BA:1577:C:H4' | 2.19 | 0.42 |
| 4:AG:19:LEU:HD21 | 4:AG:21:LEU:HD12 | 2.01 | 0.42 |
| 1:AA:690:G:H22 | 11:AN:55:LYS:NZ | 2.17 | 0.42 |
| 38:BQ:70:GLY:HA2 | 38:BQ:101:LEU:HD13 | 2.01 | 0.42 |
| 25:DA:1952:A:C6 | 34:DN:22:ILE:HD12 | 2.54 | 0.42 |
| 12:CO:47:LYS:HB3 | 12:CO:48:PRO:CD | 2.42 | 0.42 |
| 2:CE:163:PHE:HE1 | 2:CE:215:LEU:HD22 | 1.85 | 0.42 |
| 39:DR:3:ARG:HG2 | 39:DR:6:LEU:HB2 | 2.01 | 0.42 |
| 35:DO:9:ASN:O | 35:DO:10:PRO:C | 2.56 | 0.42 |
| 31:BH:154:PRO:O | 31:BH:155:SER:CB | 2.67 | 0.42 |
| 30:DG:116:ASP:O | 30:DG:117:PHE:HB3 | 2.19 | 0.42 |
| 35:DO:147:LEU:O | 35:DO:148:LEU:HD23 | 2.19 | 0.42 |
| 25:BA:1471:A:N3 | 25:BA:1471:A:H2' | 2.35 | 0.42 |
| 25:BA:2697:G:H2' | 25:BA:2698:U:O4' | 2.19 | 0.42 |
| 25:DA:1484:G:C6 | 25:DA:1485:G:C5 | 3.07 | 0.42 |
| 1:CA:1252:A:C2' | 1:CA:1253:G:O5' | 2.67 | 0.42 |
| 4:CG:24:GLU:OE1 | 4:CG:112:VAL:HG21 | 2.19 | 0.42 |
| 25:DA:2211:G:C2' | 25:DA:2211:G:N3 | 2.82 | 0.42 |
| 32:DK:101:LEU:CD2 | 32:DK:101:LEU:N | 2.82 | 0.42 |
| 5:CH:147:ASP:OD2 | 5:CH:147:ASP:N | 2.49 | 0.42 |
| 12:CO:100:ILE:HG22 | 12:CO:101:VAL:N | 2.33 | 0.42 |
| 25:DA:319:C:C2 | 25:DA:333:G:N2 | 2.87 | 0.42 |
| 44:DU:61:ILE:CG2 | 44:DU:62:GLU:H | 2.29 | 0.42 |
| 5:AH:152:ARG:HA | 8:AK:64:LYS:HZ2 | 1.84 | 0.42 |
| 1:AA:1254:C:H41 | 10:AM:43:ARG:NH1 | 2.12 | 0.42 |
| 37:B0:117:VAL:HG13 | 37:B0:118:GLU:N | 2.35 | 0.42 |
| 25:BA:1449:A:H8 | 25:BA:1449:A:OP2 | 2.00 | 0.42 |
| 1:CA:720:C:O5' | 1:CA:720:C:H6 | 2.03 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:2205:C:H42 | 25:BA:2219:G:H1 | 1.68 | 0.42 |
| 25:BA:2219:G:H2' | 25:BA:2224:G:C5' | 2.50 | 0.42 |
| 4:AG:162:LEU:CD1 | 4:AG:181:MET:HB3 | 2.49 | 0.42 |
| 1:AA:1342:C:H2' | 1:AA:1343:G:C8 | 2.55 | 0.42 |
| 43:BT:29:TRP:CZ3 | 43:BT:78:LYS:CG | 3.02 | 0.42 |
| 1:CA:189:U:C4 | 17:CT:72:ARG:CZ | 3.03 | 0.42 |
| 4:CG:110:PHE:CZ | 4:CG:182:LYS:HA | 2.54 | 0.42 |
| 1:AA:967:C:H4' | 9:AL:125:TYR:CE2 | 2.53 | 0.42 |
| 26:BB:59:A:H2' | 26:BB:60:C:C6 | 2.51 | 0.42 |
| 25:BA:540:G:H3' | 25:BA:541:C:H6 | 1.84 | 0.42 |
| 7:AJ:23:VAL:HG13 | 7:AJ:43:PHE:CE2 | 2.55 | 0.42 |
| 3:CF:173:VAL:HG12 | 3:CF:175:LEU:CD2 | 2.49 | 0.42 |
| 26:BB:82:G:C2' | 26:BB:83:G:H5' | 2.49 | 0.42 |
| 4:AG:86:LYS:HD2 | 4:AG:86:LYS:N | 2.34 | 0.42 |
| 25:DA:1614:A:H61 | 42:DS:88:ARG:H | 1.67 | 0.42 |
| 1:CA:754:C:H1' | 15:CR:69:TYR:CG | 2.54 | 0.42 |
| 34:BN:26:LYS:O | 34:BN:27:GLY:O | 2.38 | 0.42 |
| 28:DE:7:VAL:CG2 | 39:DR:1:MET:HE3 | 2.49 | 0.42 |
| 25:DA:1915:U:H2' | 25:DA:1916:A:O4' | 2.20 | 0.42 |
| 39:BR:11:GLU:CA | 39:BR:11:GLU:OE1 | 2.67 | 0.42 |
| 28:BE:152:LYS:HD3 | 33:BM:77:GLY:HA3 | 2.02 | 0.42 |
| 1:AA:685:G:H5' | 11:AN:39:PRO:O | 2.19 | 0.42 |
| 1:AA:647:C:C4 | 1:AA:648:A:N7 | 2.88 | 0.42 |
| 25:BA:2746:U:C2' | 25:BA:2747:G:H5' | 2.50 | 0.42 |
| 25:DA:2324:C:H5'' | 25:DA:2325:G:H5' | 2.02 | 0.42 |
| 46:B3:64:ASP:HB2 | 46:B3:85:ALA:HB2 | 2.02 | 0.42 |
| 33:DM:73:THR:HA | 33:DM:83:LYS:O | 2.20 | 0.42 |
| 11:AN:30:VAL:HG21 | 11:AN:65:ALA:HA | 2.00 | 0.42 |
| 1:AA:799:G:C6 | 1:AA:800:G:C4 | 3.07 | 0.42 |
| 8:CK:5:PRO:O | 8:CK:8:ASP:HB3 | 2.19 | 0.42 |
| 25:BA:2525:G:N3 | 25:BA:2525:G:H2' | 2.34 | 0.42 |
| 28:BE:8:LYS:HD2 | 28:BE:188:VAL:HG22 | 2.00 | 0.42 |
| 25:BA:1056:G:HO2' | 25:BA:1057:A:P | 2.42 | 0.42 |
| 1:AA:1128:C:C5 | 1:AA:1139:G:C5 | 3.07 | 0.42 |
| 28:DE:3:GLY:HA3 | 28:DE:81:ILE:HD11 | 2.01 | 0.42 |
| 26:BB:42:C:O3' | 30:BG:67:LYS:CE | 2.68 | 0.42 |
| 4:CG:32:ALA:HA | 4:CG:35:ARG:HB2 | 2.01 | 0.42 |
| 1:AA:1038:C:C2' | 1:AA:1039:C:H5' | 2.50 | 0.42 |
| 11:AN:77:MET:CE | 11:AN:80:VAL:HG12 | 2.49 | 0.42 |
| 25:DA:1088:A:H3' | 25:DA:1088:A:N3 | 2.34 | 0.42 |
| 2:AE:21:ARG:HB2 | 2:AE:39:ILE:CA | 2.50 | 0.42 |
| 43:DT:81:VAL:HG23 | 43:DT:81:VAL:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:DA:1005:C:C2 | 25:DA:1143:A:C2 | 3.07 | 0.42 |
| 25:BA:879:G:C8 | 25:BA:879:G:OP2 | 2.73 | 0.42 |
| 41:B2:47:VAL:O | 41:B2:48:GLY:O | 2.37 | 0.42 |
| 1:AA:789:U:O2 | 1:AA:789:U:O4' | 2.34 | 0.42 |
| 25:BA:2212:A:H2' | 25:BA:2213:U:OP2 | 2.19 | 0.42 |
| 1:CA:1127:G:C1' | 1:CA:1147:C:H42 | 2.31 | 0.42 |
| 30:DG:67:LYS:HE3 | 50:D4:6:HIS:CD2 | 2.54 | 0.42 |
| 25:DA:311:A:H2 | 25:DA:331:A:H5'' | 1.85 | 0.42 |
| 9:CL:3:GLN:O | 9:CL:88:TYR:HE1 | 2.03 | 0.42 |
| 2:CE:114:ARG:O | 2:CE:118:LEU:HG | 2.20 | 0.42 |
| 26:DB:109:G:C4 | 26:DB:110:G:C8 | 3.08 | 0.42 |
| 25:DA:2572:A:N7 | 28:DE:144:ARG:HD2 | 2.35 | 0.42 |
| 33:BM:22:THR:O | 33:BM:61:ARG:O | 2.37 | 0.42 |
| 27:BD:79:VAL:HG12 | 27:BD:113:VAL:HA | 2.01 | 0.42 |
| 25:BA:1533:C:H3' | 25:BA:1534:G:H5'' | 2.01 | 0.42 |
| 38:DQ:35:ILE:CD1 | 38:DQ:101:LEU:HD23 | 2.41 | 0.42 |
| 31:DH:136:ILE:H | 31:DH:136:ILE:CD1 | 2.31 | 0.42 |
| 39:BR:16:ARG:HG3 | 39:BR:16:ARG:HH11 | 1.85 | 0.42 |
| 54:B8:58:ILE:HA | 54:B8:61:LEU:HD11 | 2.01 | 0.42 |
| 25:BA:2335:A:O2' | 25:BA:2336:A:OP2 | 2.29 | 0.42 |
| 25:BA:1188:U:C4' | 41:B2:79:VAL:CG2 | 2.97 | 0.42 |
| 1:AA:1346:A:O3' | 1:AA:1347:G:H4' | 2.19 | 0.42 |
| 27:DD:132:PRO:HG3 | 27:DD:190:TYR:CE1 | 2.55 | 0.42 |
| 36:DP:3:MET:HA | 36:DP:4:PRO:HD3 | 1.89 | 0.42 |
| 23:AD:15:G:C2 | 23:AD:49:C:O2 | 2.72 | 0.42 |
| 25:DA:146:G:H2' | 25:DA:147:U:O4' | 2.19 | 0.42 |
| 25:DA:1204:A:HO2' | 25:DA:1205:U:P | 2.42 | 0.42 |
| 27:BD:147:LEU:HD13 | 27:BD:155:LEU:HD11 | 2.01 | 0.42 |
| 13:CP:88:ARG:O | 13:CP:92:HIS:ND1 | 2.46 | 0.42 |
| 25:DA:125:G:H1' | 53:D7:13:ALA:HB1 | 2.01 | 0.42 |
| 26:BB:90:C:OP2 | 36:BP:16:ARG:NH2 | 2.51 | 0.42 |
| 10:CM:69:ASN:O | 10:CM:70:ARG:CG | 2.66 | 0.42 |
| 41:B2:24:LYS:HA | 41:B2:92:THR:HG23 | 2.00 | 0.42 |
| 25:DA:867:C:C4 | 25:DA:868:U:C5 | 3.08 | 0.42 |
| 25:DA:669:G:O2' | 25:DA:670:A:O5' | 2.36 | 0.42 |
| 25:BA:1789:A:H2' | 25:BA:1790:C:O4' | 2.19 | 0.42 |
| 12:CO:23:LYS:CE | 12:CO:23:LYS:H | 2.32 | 0.42 |
| 25:DA:2141:G:C2' | 25:DA:2142:C:H5' | 2.50 | 0.42 |
| 23:CD:23:G:N2 | 23:CD:24:C:C2 | 2.87 | 0.42 |
| 17:AT:17:LYS:CG | 17:AT:47:PRO:HA | 2.48 | 0.42 |
| 25:BA:280:C:N3 | 25:BA:361:G:C2 | 2.87 | 0.42 |
| 1:CA:298:A:H5'' | 1:CA:299:G:OP2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:2751:G:N1 | 31:BH:3:ARG:HB3 | 2.34 | 0.42 |
| 1:CA:1225:A:C8 | 1:CA:1225:A:OP2 | 2.71 | 0.42 |
| 18:AU:53:ARG:HH21 | 18:AU:60:ALA:N | 2.17 | 0.42 |
| 25:DA:729:G:H2' | 25:DA:1775:U:H1' | 2.00 | 0.42 |
| 26:DB:10:C:C2' | 26:DB:11:C:H5' | 2.49 | 0.42 |
| 8:AK:94:TYR:CE1 | 8:AK:132:GLU:HB2 | 2.53 | 0.42 |
| 1:CA:219:C:H2' | 1:CA:220:G:O4' | 2.20 | 0.42 |
| 42:DS:27:LYS:O | 42:DS:71:VAL:HG23 | 2.20 | 0.42 |
| 25:DA:360:G:O2' | 25:DA:361:G:H5' | 2.20 | 0.42 |
| 38:BQ:65:VAL:O | 38:BQ:69:VAL:HG12 | 2.20 | 0.42 |
| 32:BK:86:THR:HA | 32:BK:123:LEU:HD12 | 2.01 | 0.42 |
| 1:AA:981:U:H5 | 1:AA:982:U:HO2' | 1.67 | 0.42 |
| 25:BA:270(B):A:N7 | 25:BA:270(X):G:N2 | 2.63 | 0.42 |
| 38:DQ:18:ILE:O | 38:DQ:21:THR:CG2 | 2.68 | 0.42 |
| 25:DA:892:G:N7 | 25:DA:893:C:N4 | 2.67 | 0.42 |
| 7:AJ:9:VAL:HG13 | 7:AJ:94:ARG:NE | 2.34 | 0.42 |
| 14:CQ:34:TYR:CE2 | 14:CQ:44:LEU:HD21 | 2.55 | 0.42 |
| 36:DP:42:ILE:HD13 | 36:DP:97:VAL:CG2 | 2.50 | 0.42 |
| 42:DS:72:LYS:HB3 | 42:DS:106:ILE:O | 2.20 | 0.42 |
| 45:BV:172:ALA:O | 45:BV:173:ALA:HB2 | 2.20 | 0.42 |
| 25:DA:1835:G:H5'' | 25:DA:1836:C:OP2 | 2.19 | 0.42 |
| 2:AE:112:VAL:O | 2:AE:115:LEU:N | 2.52 | 0.42 |
| 17:CT:89:LEU:HD23 | 17:CT:89:LEU:HA | 1.91 | 0.42 |
| 6:AI:43:LEU:N | 6:AI:43:LEU:CD1 | 2.82 | 0.42 |
| 30:BG:62:LEU:HD12 | 30:BG:62:LEU:HA | 1.80 | 0.42 |
| 9:AL:29:ASN:OD1 | 9:AL:65:VAL:N | 2.48 | 0.42 |
| 31:DH:109:PHE:HZ | 31:DH:152:ARG:CD | 2.32 | 0.42 |
| 22:CB:37:G:C5 | 22:CB:38:G:N7 | 2.88 | 0.42 |
| 19:AV:40:ILE:HG12 | 19:AV:41:VAL:N | 2.35 | 0.42 |
| 25:DA:1060:U:O4' | 25:DA:1062:G:H5' | 2.20 | 0.42 |
| 2:AE:21:ARG:HB2 | 2:AE:38:GLY:C | 2.39 | 0.42 |
| 43:DT:7:VAL:HG12 | 43:DT:30:VAL:HG12 | 2.00 | 0.42 |
| 25:DA:1005:C:C1' | 25:DA:1143:A:H2 | 2.21 | 0.42 |
| 25:BA:879:G:N2 | 25:BA:898:C:N3 | 2.59 | 0.42 |
| 1:CA:1177:G:H2' | 1:CA:1178:G:N3 | 2.34 | 0.42 |
| 9:AL:114:TYR:HD1 | 10:AM:60:ARG:H | 1.61 | 0.42 |
| 1:CA:1148:U:H2' | 1:CA:1149:C:O4' | 2.19 | 0.42 |
| 25:DA:329:G:N7 | 44:DU:19:LYS:HG2 | 2.35 | 0.42 |
| 26:DB:15:A:H1' | 26:DB:109:G:N9 | 2.34 | 0.42 |
| 42:BS:8:ARG:O | 42:BS:9:TYR:HB2 | 2.19 | 0.42 |
| 5:CH:79:GLU:HA | 5:CH:91:LEU:O | 2.20 | 0.42 |
| 28:BE:111:ARG:HG2 | 37:B0:1:MET:SD | 2.60 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 7:AJ:26:PHE:CB | 7:AJ:62:PHE:HZ | 2.32 | 0.42 |
| 25:BA:674:G:H1' | 29:BF:74:ARG:HH11 | 1.85 | 0.42 |
| 12:CO:26:ALA:O | 12:CO:27:LEU:HD12 | 2.20 | 0.42 |
| 25:BA:1475:G:C2 | 25:BA:1519:G:C2 | 3.08 | 0.42 |
| 25:DA:2332:U:H5' | 46:D3:43:THR:CG2 | 2.50 | 0.42 |
| 3:AF:70:VAL:HG12 | 3:AF:71:ALA:N | 2.34 | 0.42 |
| 40:B1:78:THR:O | 40:B1:79:PHE:C | 2.57 | 0.42 |
| 1:CA:914:A:C2' | 1:CA:915:A:H5' | 2.49 | 0.42 |
| 2:CE:7:VAL:HG22 | 2:CE:8:LYS:N | 2.27 | 0.42 |
| 36:DP:4:PRO:HD3 | 36:DP:70:PRO:O | 2.19 | 0.42 |
| 23:AD:15:G:C2' | 23:AD:60:A:C2 | 3.03 | 0.42 |
| 25:BA:2681:C:C1' | 25:BA:2682:U:OP2 | 2.67 | 0.42 |
| 37:B0:74:LYS:O | 37:B0:76:VAL:N | 2.50 | 0.42 |
| 35:BO:19:VAL:HG21 | 35:BO:32:THR:HB | 2.00 | 0.42 |
| 44:BU:42:VAL:CG1 | 44:BU:65:ALA:HB3 | 2.49 | 0.42 |
| 25:BA:2312:U:O2' | 30:BG:40:ASN:ND2 | 2.45 | 0.42 |
| 26:BB:13:A:N6 | 26:BB:70:C:H5' | 2.35 | 0.42 |
| 40:D1:75:ASN:HD22 | 40:D1:78:THR:HG23 | 1.83 | 0.42 |
| 1:AA:1256:A:N6 | 1:AA:1278:U:OP2 | 2.52 | 0.42 |
| 1:AA:652:U:O2' | 1:AA:653:A:C5' | 2.68 | 0.42 |
| 46:D3:56:ASP:OD1 | 46:D3:58:THR:OG1 | 2.38 | 0.42 |
| 25:BA:1171:G:C6 | 25:BA:1174:A:N6 | 2.87 | 0.42 |
| 1:AA:49:U:O2' | 1:AA:50:A:OP1 | 2.36 | 0.42 |
| 2:CE:197:VAL:HG12 | 2:CE:200:ILE:CG1 | 2.49 | 0.42 |
| 25:DA:383:U:O2 | 25:DA:385:C:N4 | 2.53 | 0.42 |
| 25:DA:817:C:O2' | 25:DA:839:U:OP1 | 2.36 | 0.42 |
| 35:DO:138:LEU:C | 35:DO:138:LEU:HD13 | 2.39 | 0.42 |
| 25:BA:288:C:H2' | 25:BA:289:A:C8 | 2.55 | 0.42 |
| 25:BA:1162:G:H1' | 41:B2:23:GLU:OE2 | 2.19 | 0.42 |
| 23:CD:4:G:N2 | 23:CD:71:G:C4 | 2.88 | 0.42 |
| 10:CM:63:PHE:CD1 | 14:CQ:57:ARG:O | 2.70 | 0.42 |
| 25:DA:1944:U:O2 | 25:DA:1955:U:H5'' | 2.19 | 0.42 |
| 25:BA:21:A:C2' | 25:BA:22:C:H5' | 2.49 | 0.42 |
| 1:AA:745:C:OP1 | 1:AA:851:G:O2' | 2.37 | 0.42 |
| 31:DH:41:MET:HB3 | 31:DH:42:ARG:H | 1.68 | 0.42 |
| 25:BA:962:G:H2' | 25:BA:963:U:C6 | 2.54 | 0.42 |
| 34:DN:2:ILE:HG13 | 34:DN:8:LEU:HD11 | 2.01 | 0.42 |
| 34:BN:98:VAL:HG23 | 34:BN:99:PHE:N | 2.34 | 0.42 |
| 1:CA:52:G:O2' | 1:CA:53:A:H5' | 2.20 | 0.42 |
| 25:BA:322:A:C5 | 25:BA:340:A:C2 | 3.08 | 0.42 |
| 43:DT:64:LYS:HB3 | 43:DT:64:LYS:HE2 | 1.68 | 0.42 |
| 25:BA:760:G:H4' | 25:BA:1776:G:OP1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 26:DB:79:C:H2' | 26:DB:80:U:O4' | 2.20 | 0.42 |
| 25:DA:2300:G:C2 | 25:DA:2317:C:O2 | 2.73 | 0.42 |
| 25:DA:2625:G:H2' | 25:DA:2626:C:C6 | 2.55 | 0.42 |
| 25:DA:1067:A:H5'' | 25:DA:1068:G:OP2 | 2.18 | 0.42 |
| 10:AM:33:GLN:HB2 | 10:AM:75:ILE:HD11 | 2.01 | 0.42 |
| 31:BH:68:THR:O | 31:BH:72:ILE:HG13 | 2.19 | 0.42 |
| 25:DA:2348:U:O4 | 25:DA:2382:G:N1 | 2.52 | 0.42 |
| 25:BA:2877:G:O2' | 25:BA:2878:U:H5' | 2.18 | 0.42 |
| 11:AN:104:GLN:O | 11:AN:104:GLN:HG3 | 2.18 | 0.42 |
| 52:B6:21:TYR:N | 52:B6:21:TYR:CD2 | 2.88 | 0.42 |
| 3:AF:91:LEU:HD23 | 3:AF:91:LEU:HA | 1.88 | 0.42 |
| 25:DA:1914:C:O4' | 25:DA:1914:C:O2 | 2.37 | 0.42 |
| 22:CB:5:A:H61 | 22:CB:79:U:H3 | 1.66 | 0.42 |
| 25:BA:1056:G:O2' | 25:BA:1057:A:OP2 | 2.31 | 0.42 |
| 25:BA:1060:U:C4 | 25:BA:1062:G:H4' | 2.54 | 0.42 |
| 54:B8:8:LYS:HA | 54:B8:8:LYS:HD2 | 1.67 | 0.42 |
| 25:DA:2681:C:C5 | 25:DA:2727:G:C2 | 3.07 | 0.42 |
| 52:D6:16:CYS:O | 52:D6:44:ARG:NH2 | 2.52 | 0.42 |
| 52:B6:28:ARG:HB3 | 52:B6:30:THR:H | 1.83 | 0.42 |
| 1:CA:485:G:H2' | 1:CA:486:U:OP2 | 2.20 | 0.42 |
| 35:BO:10:PRO:HB2 | 35:BO:11:GLY:H | 1.64 | 0.42 |
| 25:DA:953:A:H2' | 25:DA:954:G:H8 | 1.85 | 0.42 |
| 1:AA:1498:U:H1' | 1:AA:1499:A:OP2 | 2.19 | 0.42 |
| 25:DA:1729:A:C2 | 25:DA:1730:U:H5 | 2.38 | 0.42 |
| 1:CA:1145:C:H5' | 1:CA:1146:A:OP1 | 2.18 | 0.42 |
| 1:AA:255:G:O6 | 1:AA:266:G:O6 | 2.37 | 0.42 |
| 25:DA:2311:A:O2' | 30:DG:88:ILE:HD12 | 2.18 | 0.42 |
| 32:BK:101:LEU:HA | 32:BK:104:GLN:HB2 | 2.02 | 0.42 |
| 23:AD:19:G:N2 | 23:AD:56:U:O2 | 2.53 | 0.42 |
| 23:AD:57:C:H2' | 23:AD:58:A:O4' | 2.20 | 0.42 |
| 25:BA:2061:G:N2 | 25:BA:2062:A:C2 | 2.85 | 0.42 |
| 48:BW:17:SER:CB | 48:BW:18:PRO:CD | 2.98 | 0.42 |
| 28:BE:181:LEU:HA | 28:BE:181:LEU:HD12 | 1.70 | 0.42 |
| 1:CA:812:C:H4' | 1:CA:813:U:H5' | 2.01 | 0.42 |
| 2:AE:88:ALA:O | 2:AE:226:ARG:NH1 | 2.51 | 0.42 |
| 19:AV:65:ASN:N | 19:AV:65:ASN:HD22 | 2.04 | 0.42 |
| 25:DA:459:U:H5'' | 53:D7:40:TRP:CG | 2.55 | 0.42 |
| 50:D4:58:ARG:C | 50:D4:61:ARG:H | 2.23 | 0.42 |
| 25:BA:901:A:H5' | 25:BA:902:C:OP2 | 2.20 | 0.42 |
| 25:BA:2334:G:H4' | 25:BA:2335:A:OP2 | 2.20 | 0.42 |
| 33:DM:30:ILE:HG21 | 33:DM:120:LEU:CD1 | 2.49 | 0.42 |
| 1:AA:5:U:H1' | 1:AA:6:G:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 32:DK:107:VAL:HG13 | 32:DK:108:THR:N | 2.35 | 0.42 |
| 15:CR:56:LEU:HD21 | 25:DA:715:G:C2 | 2.55 | 0.42 |
| 25:BA:1265:A:C8 | 25:BA:1267:U:C2 | 3.08 | 0.42 |
| 45:BV:139:VAL:HG13 | 45:BV:155:LEU:HD21 | 2.01 | 0.42 |
| 19:CV:79:THR:OG1 | 19:CV:79:THR:O | 2.29 | 0.42 |
| 8:AK:104:ARG:HD2 | 8:AK:138:TRP:CG | 2.54 | 0.42 |
| 5:AH:152:ARG:HA | 8:AK:64:LYS:NZ | 2.35 | 0.42 |
| 25:DA:1093:G:H2' | 25:DA:1094:U:H5' | 2.02 | 0.42 |
| 26:BB:13:A:C6 | 26:BB:70:C:H5' | 2.54 | 0.42 |
| 5:CH:9:LYS:HD2 | 5:CH:9:LYS:HA | 1.81 | 0.42 |
| 1:AA:1256:A:N3 | 1:AA:1277:C:C4 | 2.88 | 0.42 |
| 25:DA:2292:C:P | 38:DQ:17:ARG:NH2 | 2.93 | 0.42 |
| 25:DA:977:G:C2 | 25:DA:978:G:C8 | 3.07 | 0.42 |
| 25:BA:1870:C:O2 | 25:BA:1870:C:C2' | 2.63 | 0.42 |
| 25:DA:1777:U:C2 | 25:DA:1778:U:C5 | 3.08 | 0.42 |
| 3:AF:188:LEU:HD22 | 3:AF:188:LEU:HA | 1.77 | 0.42 |
| 2:CE:17:PHE:HD1 | 2:CE:17:PHE:HA | 1.71 | 0.42 |
| 25:BA:2147:G:H3' | 25:BA:2147:G:H8 | 1.83 | 0.42 |
| 45:DV:11:GLU:O | 45:DV:36:LYS:NZ | 2.47 | 0.42 |
| 25:DA:384:U:H2' | 25:DA:385:C:H6 | 1.84 | 0.42 |
| 41:B2:91:TYR:CD1 | 41:B2:91:TYR:C | 2.93 | 0.42 |
| 7:CJ:149:ARG:HD3 | 11:CN:59:TYR:CZ | 2.55 | 0.42 |
| 30:DG:146:TYR:CD2 | 30:DG:146:TYR:O | 2.73 | 0.42 |
| 30:DG:81:LYS:HB3 | 30:DG:82:LEU:H | 1.68 | 0.42 |
| 3:CF:28:GLN:CB | 3:CF:32:LEU:HD12 | 2.49 | 0.42 |
| 10:CM:28:ARG:CZ | 10:CM:34:VAL:HB | 2.49 | 0.42 |
| 22:CB:76:U:O4 | 22:CB:77:C:C4 | 2.73 | 0.42 |
| 1:CA:1414:U:H2' | 1:CA:1415:G:C8 | 2.55 | 0.42 |
| 25:DA:1639:U:O2' | 25:DA:1640:C:H5' | 2.19 | 0.42 |
| 1:CA:1104:G:C4 | 1:CA:1105:A:C8 | 3.07 | 0.42 |
| 25:BA:1591:G:H2' | 25:BA:1592:C:C6 | 2.55 | 0.42 |
| 2:AE:134:GLU:O | 2:AE:138:LEU:HG | 2.18 | 0.42 |
| 1:CA:787:A:C2' | 1:CA:788:U:H5' | 2.49 | 0.42 |
| 25:BA:986:C:O2' | 25:BA:987:G:H5' | 2.20 | 0.42 |
| 25:DA:273(E):U:C2' | 25:DA:273(F):C:H5' | 2.50 | 0.42 |
| 25:BA:249:C:H4' | 25:BA:250:G:O5' | 2.20 | 0.42 |
| 3:AF:23:TYR:CD2 | 3:AF:23:TYR:C | 2.93 | 0.42 |
| 25:BA:1701:A:C2' | 25:BA:1702:G:H5' | 2.50 | 0.42 |
| 25:DA:1758:G:C2 | 25:DA:2696:U:H5' | 2.54 | 0.42 |
| 2:CE:168:THR:HG23 | 2:CE:192:SER:HB3 | 2.00 | 0.42 |
| 1:CA:1103:C:O2' | 2:CE:108:ILE:HD13 | 2.20 | 0.42 |
| 25:BA:1773:A:C2' | 25:BA:1774:C:H5' | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:AA:31:G:H2' | 1:AA:48:C:N4 | 2.35 | 0.42 |
| 25:BA:116:C:H2' | 25:BA:117:G:O5' | 2.20 | 0.42 |
| 25:DA:2228:G:OP1 | 27:DD:261:LYS:NZ | 2.43 | 0.42 |
| 11:CN:115:PRO:C | 11:CN:117:ASN:H | 2.22 | 0.42 |
| 6:AI:1:MET:HB3 | 6:AI:66:GLU:HG3 | 2.01 | 0.42 |
| 53:D7:26:GLY:O | 53:D7:30:VAL:HG23 | 2.20 | 0.42 |
| 23:CC:27:G:H1 | 23:CC:46:G:N2 | 2.17 | 0.42 |
| 25:BA:1973:G:H2' | 25:BA:1974:C:C6 | 2.53 | 0.42 |
| 11:CN:31:THR:HG23 | 11:CN:31:THR:O | 2.20 | 0.42 |
| 37:D0:21:TYR:OH | 37:D0:43:GLU:HG2 | 2.19 | 0.42 |
| 29:DF:38:ARG:HH11 | 29:DF:38:ARG:HG3 | 1.84 | 0.42 |
| 25:BA:2063:C:O2 | 25:BA:2450:A:N1 | 2.53 | 0.42 |
| 44:DU:102:CYS:HB3 | 44:DU:103:GLY:H | 1.41 | 0.42 |
| 16:AS:14:ASN:O | 16:AS:15:PRO:O | 2.38 | 0.42 |
| 25:BA:1083:U:H3' | 25:BA:1083:U:H6 | 1.85 | 0.42 |
| 25:BA:2361:A:OP1 | 54:B8:27:THR:HG23 | 2.19 | 0.42 |
| 52:D6:25:LYS:CB | 54:D8:34:TRP:CZ3 | 2.85 | 0.42 |
| 40:D1:76:TYR:C | 40:D1:76:TYR:CD2 | 2.93 | 0.42 |
| 25:DA:1010:A:H5' | 40:D1:62:ILE:HG21 | 2.01 | 0.42 |
| 25:DA:1153:C:H2' | 25:DA:1154:G:O4' | 2.19 | 0.42 |
| 33:DM:36:GLY:N | 33:DM:42:TRP:CZ3 | 2.88 | 0.42 |
| 35:BO:16:ARG:CG | 35:BO:16:ARG:NH1 | 2.80 | 0.42 |
| 1:AA:1054:C:O2' | 1:AA:1055:A:O5' | 2.32 | 0.42 |
| 23:CC:31:G:H2' | 23:CC:32:G:O5' | 2.19 | 0.42 |
| 4:AG:13:ARG:H | 4:AG:13:ARG:HG2 | 1.35 | 0.42 |
| 28:DE:5:LEU:CD2 | 28:DE:79:ARG:HG2 | 2.49 | 0.42 |
| 28:DE:3:GLY:CA | 28:DE:81:ILE:CD1 | 2.97 | 0.42 |
| 31:DH:153:LYS:HA | 31:DH:153:LYS:HD2 | 1.38 | 0.42 |
| 1:CA:978:A:H1' | 1:CA:1322:C:C2 | 2.55 | 0.42 |
| 25:BA:2346:A:H5'' | 25:BA:2383:G:C1' | 2.49 | 0.42 |
| 1:CA:485:G:O2' | 1:CA:486:U:P | 2.77 | 0.42 |
| 4:AG:70:ILE:HG23 | 4:AG:75:PHE:HB2 | 2.02 | 0.42 |
| 32:DK:123:LEU:HD22 | 32:DK:143:SER:CB | 2.49 | 0.42 |
| 25:BA:878:A:N1 | 25:BA:879:G:C2 | 2.88 | 0.42 |
| 25:BA:883:G:H2' | 25:BA:884:C:C4' | 2.49 | 0.42 |
| 1:CA:1158:C:N3 | 1:CA:1160:G:N7 | 2.67 | 0.42 |
| 11:AN:34:ASP:HA | 11:AN:40:ILE:HD11 | 2.01 | 0.42 |
| 9:AL:111:ARG:NH2 | 10:AM:62:HIS:CE1 | 2.88 | 0.42 |
| 1:CA:1496:C:H2' | 1:CA:1497:G:O4' | 2.19 | 0.42 |
| 25:DA:1041:C:H2' | 25:DA:1042:G:C8 | 2.55 | 0.42 |
| 32:BK:92:VAL:HG13 | 32:BK:120:ILE:CG2 | 2.34 | 0.42 |
| 1:CA:1128:C:H4' | 9:CL:16:ARG:NH2 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 20:AW:71:THR:O | 20:AW:72:LEU:C | 2.58 | 0.42 |
| 1:AA:201:C:N4 | 1:AA:209:U:C2 | 2.87 | 0.42 |
| 25:BA:1266:G:C8 | 42:BS:15:ARG:NH2 | 2.88 | 0.42 |
| 26:DB:13:A:H5'' | 26:DB:15:A:N6 | 2.34 | 0.42 |
| 25:DA:2126:A:H1' | 25:DA:2127:G:H5'' | 2.02 | 0.42 |
| 45:BV:27:VAL:HG12 | 45:BV:87:ASP:CB | 2.46 | 0.42 |
| 5:CH:102:ALA:HB1 | 5:CH:106:PRO:HG2 | 2.02 | 0.42 |
| 13:CP:3:ARG:H | 50:D4:34:GLU:HG3 | 1.85 | 0.42 |
| 33:DM:133:GLN:NE2 | 33:DM:135:PRO:HG3 | 2.34 | 0.42 |
| 15:CR:74:ASP:HB3 | 15:CR:77:ARG:HG2 | 2.02 | 0.42 |
| 25:BA:931:G:C4 | 25:BA:933:A:C8 | 3.07 | 0.42 |
| 1:AA:5:U:C2' | 1:AA:5:U:O2 | 2.61 | 0.42 |
| 25:DA:1277:G:O2' | 37:D0:24:GLN:HG2 | 2.20 | 0.42 |
| 25:BA:654(B):C:H2' | 25:BA:654(C):G:O4' | 2.19 | 0.42 |
| 41:B2:35:LEU:HB2 | 41:B2:37:VAL:CG2 | 2.49 | 0.42 |
| 24:A1:13:U:O2 | 24:A1:13:U:C2' | 2.63 | 0.42 |
| 50:B4:53:GLU:O | 50:B4:54:GLY:C | 2.57 | 0.42 |
| 25:BA:1241:A:O4' | 25:BA:1241:A:N3 | 2.53 | 0.42 |
| 25:DA:26:G:C6 | 25:DA:27:G:C6 | 3.08 | 0.42 |
| 25:BA:1734:C:C3' | 25:BA:1735:C:H5'' | 2.50 | 0.42 |
| 25:BA:1735:C:O2' | 25:BA:1741:C:H5' | 2.20 | 0.42 |
| 37:B0:17:ARG:O | 37:B0:20:LEU:HB3 | 2.20 | 0.42 |
| 4:AG:107:ARG:NH2 | 4:AG:194:LEU:HD11 | 2.33 | 0.42 |
| 1:AA:49:U:O2' | 1:AA:50:A:P | 2.78 | 0.42 |
| 1:AA:1240:U:OP2 | 7:AJ:116:ALA:N | 2.41 | 0.42 |
| 7:AJ:113:GLU:HG2 | 7:AJ:113:GLU:H | 1.62 | 0.42 |
| 25:DA:1165:U:O2' | 25:DA:1166:C:H5' | 2.20 | 0.42 |
| 43:BT:57:LEU:HD11 | 43:BT:78:LYS:HB2 | 2.02 | 0.42 |
| 9:AL:18:PHE:HB2 | 9:AL:62:TYR:HB3 | 2.02 | 0.42 |
| 25:BA:1337:G:C4 | 25:BA:1338:G:C8 | 3.08 | 0.42 |
| 36:BP:80:GLU:OE2 | 36:BP:80:GLU:CA | 2.67 | 0.42 |
| 46:D3:68:GLU:OE1 | 46:D3:82:ARG:HG3 | 2.19 | 0.42 |
| 29:BF:64:ILE:HG23 | 29:BF:65:TRP:NE1 | 2.35 | 0.42 |
| 42:DS:51:LEU:O | 42:DS:54:ALA:HB3 | 2.20 | 0.42 |
| 14:CQ:7:ILE:HG22 | 14:CQ:23:ARG:HD2 | 2.01 | 0.42 |
| 1:CA:1349:A:P | 9:CL:118:LYS:NZ | 2.92 | 0.42 |
| 25:DA:2699:C:H2' | 25:DA:2700:C:O4' | 2.20 | 0.42 |
| 3:CF:186:PHE:HD1 | 3:CF:198:VAL:O | 2.01 | 0.42 |
| 3:CF:186:PHE:HE1 | 3:CF:197:GLY:HA2 | 1.84 | 0.42 |
| 25:DA:249:C:H4' | 25:DA:250:G:O5' | 2.20 | 0.42 |
| 25:BA:1502:C:O2' | 25:BA:1503:U:H5' | 2.19 | 0.42 |
| 13:AP:45:VAL:O | 13:AP:48:LEU:HD22 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:107:C:H2' | 25:BA:108:U:C6 | 2.55 | 0.42 |
| 7:AJ:51:GLN:O | 7:AJ:54:THR:O | 2.38 | 0.42 |
| 1:CA:450:G:N7 | 1:CA:481:G:C6 | 2.88 | 0.42 |
| 27:BD:133:LEU:HD13 | 27:BD:173:VAL:HG22 | 2.01 | 0.42 |
| 25:DA:1844:C:C2 | 25:DA:1897:G:C2 | 3.08 | 0.42 |
| 25:BA:278:A:H2' | 25:BA:279:C:C6 | 2.54 | 0.42 |
| 25:DA:1750:G:C2' | 25:DA:1751:C:H5' | 2.50 | 0.42 |
| 25:DA:2282:G:OP1 | 25:DA:2283:C:H1' | 2.19 | 0.42 |
| 7:AJ:115:ARG:O | 7:AJ:118:VAL:HG12 | 2.20 | 0.42 |
| 25:DA:52:A:O2' | 25:DA:53:A:H5' | 2.19 | 0.42 |
| 10:AM:45:ARG:O | 10:AM:64:GLU:HA | 2.18 | 0.42 |
| 30:BG:165:THR:OG1 | 30:BG:168:GLU:HG3 | 2.20 | 0.42 |
| 47:BZ:25:LYS:HE3 | 47:BZ:25:LYS:HB2 | 1.59 | 0.42 |
| 4:CG:192:GLU:H | 4:CG:192:GLU:HG3 | 1.65 | 0.42 |
| 2:AE:158:LEU:HD12 | 2:AE:158:LEU:O | 2.20 | 0.42 |
| 27:BD:35:LYS:HE2 | 27:BD:104:TYR:HB2 | 2.01 | 0.42 |
| 28:BE:35:GLN:C | 28:BE:36:ARG:HG2 | 2.41 | 0.42 |
| 28:BE:45:THR:O | 28:BE:83:ASP:N | 2.51 | 0.42 |
| 28:BE:4:ILE:C | 28:BE:5:LEU:HD23 | 2.40 | 0.42 |
| 28:BE:5:LEU:O | 28:BE:28:ALA:HA | 2.20 | 0.42 |
| 33:BM:40:PRO:HA | 40:B1:67:ALA:HB3 | 2.01 | 0.42 |
| 28:DE:32:PRO:O | 28:DE:49:LEU:HA | 2.20 | 0.42 |
| 28:DE:33:VAL:O | 28:DE:67:PHE:CZ | 2.73 | 0.42 |
| 44:BU:97:ARG:N | 44:BU:97:ARG:HD3 | 2.35 | 0.42 |
| 45:DV:146:ILE:CG1 | 45:DV:147:GLY:N | 2.59 | 0.42 |
| 15:CR:17:ARG:NH1 | 15:CR:17:ARG:CG | 2.62 | 0.42 |
| 43:DT:8:ILE:O | 48:DW:36:ARG:NH2 | 2.53 | 0.42 |
| 1:CA:1162:C:C2 | 1:CA:1175:G:C2 | 3.07 | 0.42 |
| 31:DH:3:ARG:HG3 | 31:DH:4:ILE:N | 2.35 | 0.42 |
| 25:DA:560:C:H2' | 25:DA:561:G:O4' | 2.20 | 0.42 |
| 9:CL:17:VAL:CG1 | 9:CL:81:ILE:HD13 | 2.49 | 0.42 |
| 9:CL:17:VAL:HG11 | 9:CL:81:ILE:HD13 | 2.01 | 0.42 |
| 30:DG:38:VAL:O | 30:DG:38:VAL:HG12 | 2.18 | 0.42 |
| 26:DB:109:G:C5 | 26:DB:110:G:N7 | 2.88 | 0.42 |
| 2:AE:74:LYS:NZ | 2:AE:206:ASP:OD2 | 2.43 | 0.42 |
| 1:CA:625:G:H2' | 1:CA:626:U:C6 | 2.55 | 0.42 |
| 2:CE:185:ILE:CG2 | 2:CE:199:TYR:HD1 | 2.31 | 0.42 |
| 15:AR:88:ARG:H | 15:AR:88:ARG:HG2 | 1.57 | 0.42 |
| 37:B0:1:MET:HB3 | 37:B0:2:ARG:H | 1.60 | 0.42 |
| 51:B5:58:LEU:HB2 | 51:B5:60:VAL:HB | 2.01 | 0.42 |
| 25:DA:654(A):A:C2 | 25:DA:654(T):A:N1 | 2.88 | 0.42 |
| 52:D6:53:LYS:HG3 | 52:D6:53:LYS:H | 1.49 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 25:BA:1595:G:C2' | 25:BA:1596:A:H5' | 2.50 | 0.42 |
| 29:DF:122:LYS:O | 29:DF:123:LEU:HB3 | 2.19 | 0.42 |
| 29:BF:67:GLN:HB2 | 29:BF:67:GLN:HE21 | 1.72 | 0.42 |
| 25:BA:1187:G:H5'' | 41:B2:81:TYR:CE2 | 2.55 | 0.42 |
| 13:AP:37:THR:OG1 | 13:AP:39:ILE:HG13 | 2.20 | 0.42 |
| 9:AL:4:TYR:CE1 | 9:AL:88:TYR:HB2 | 2.54 | 0.42 |
| 3:CF:47:LEU:HD22 | 3:CF:47:LEU:HA | 1.93 | 0.42 |
| 25:DA:2665:A:H2' | 25:DA:2666:C:O4' | 2.20 | 0.42 |
| 23:AD:8:U:C1' | 23:AD:49:C:H4' | 2.49 | 0.42 |
| 25:BA:2180:U:H2' | 25:BA:2181:G:O4' | 2.19 | 0.42 |
| 1:CA:586:C:H1' | 1:CA:878:G:O2' | 2.20 | 0.42 |
| 7:CJ:139:GLU:O | 7:CJ:143:ARG:HB2 | 2.20 | 0.42 |
| 8:AK:64:LYS:C | 8:AK:65:TYR:CD1 | 2.94 | 0.42 |
| 25:BA:2094:G:OP1 | 32:BK:22:LYS:HG3 | 2.19 | 0.42 |
| 1:AA:960:U:C2 | 1:AA:1225:A:C5 | 3.08 | 0.42 |
| 52:B6:50:ARG:HB3 | 52:B6:51:GLU:H | 1.48 | 0.42 |
| 1:AA:91:C:H2' | 1:AA:92:G:O4' | 2.20 | 0.42 |
| 28:DE:120:TRP:O | 28:DE:121:ASN:HB2 | 2.18 | 0.42 |
| 39:BR:45:PHE:CZ | 39:BR:65:LYS:HG2 | 2.55 | 0.42 |
| 25:BA:265:A:C8 | 25:BA:266:G:H1' | 2.54 | 0.42 |
| 25:DA:497:A:H2' | 25:DA:498:G:O4' | 2.20 | 0.42 |
| 26:BB:95:U:C2 | 26:BB:96:G:C8 | 3.08 | 0.42 |
| 37:B0:42:LYS:HA | 37:B0:45:ARG:HD2 | 2.00 | 0.42 |
| 25:DA:2065:C:H1' | 25:DA:2449:U:H3 | 1.85 | 0.42 |
| 28:DE:203:LYS:O | 28:DE:204:ALA:HB3 | 2.19 | 0.42 |
| 28:DE:98:PRO:HD3 | 28:DE:175:VAL:CG1 | 2.50 | 0.42 |
| 23:AC:41:C:C2' | 23:AC:42:C:H5' | 2.50 | 0.42 |
| 1:CA:784:C:H2' | 1:CA:785:G:O4' | 2.20 | 0.42 |
| 41:D2:21:ARG:HD3 | 41:D2:91:TYR:HB3 | 2.01 | 0.42 |
| 1:CA:833:U:H2' | 1:CA:834:C:C6 | 2.55 | 0.42 |
| 1:CA:437:U:H5' | 4:CG:155:LEU:HD21 | 2.00 | 0.42 |
| 24:A1:20:U:H2' | 24:A1:21:U:H6 | 1.85 | 0.42 |
| 1:CA:1057:G:C4 | 1:CA:1204:A:C2 | 3.08 | 0.42 |
| 46:B3:25:ARG:HG3 | 46:B3:37:LEU:HD23 | 2.02 | 0.42 |
| 25:DA:1133:U:H2' | 25:DA:1137:G:OP1 | 2.20 | 0.42 |
| 42:DS:82:LEU:HB2 | 42:DS:98:LYS:HB2 | 2.01 | 0.42 |
| 43:DT:41:ASN:O | 43:DT:45:THR:HG23 | 2.19 | 0.42 |
| 40:D1:83:LEU:HG | 40:D1:88:ILE:HD11 | 2.00 | 0.42 |
| 42:DS:110:LYS:HD2 | 42:DS:110:LYS:HA | 1.79 | 0.42 |
| 39:BR:17:THR:OG1 | 39:BR:17:THR:O | 2.38 | 0.42 |
| 32:DK:131:LYS:H | 32:DK:131:LYS:HD2 | 1.84 | 0.42 |
| 29:BF:165:ARG:HG3 | 29:BF:165:ARG:HH11 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 30:BG:44:GLY:C | 30:BG:46:ALA:N | 2.72 | 0.42 |
| 25:BA:1077:A:C2' | 25:BA:1077:A:N3 | 2.82 | 0.42 |
| 52:D6:10:LEU:HD12 | 52:D6:10:LEU:H | 1.84 | 0.42 |
| 27:DD:32:SER:O | 27:DD:33:LEU:HB3 | 2.20 | 0.42 |
| 28:BE:31:CYS:HA | 28:BE:32:PRO:HD3 | 1.75 | 0.42 |
| 28:BE:52:LEU:O | 28:BE:74:PRO:CB | 2.68 | 0.42 |
| 1:CA:1027:C:O2' | 1:CA:1028:C:C6 | 2.72 | 0.42 |
| 25:BA:2318:G:N2 | 38:BQ:2:ALA:N | 2.68 | 0.42 |
| 40:B1:59:ARG:O | 40:B1:63:VAL:HG23 | 2.20 | 0.42 |
| 1:AA:1129:C:C4 | 1:AA:1139:G:C6 | 3.08 | 0.42 |
| 23:CC:23:G:C6 | 23:CC:24:C:N4 | 2.88 | 0.42 |
| 1:CA:1223:C:P | 1:CA:1224:G:H2' | 2.60 | 0.42 |
| 1:CA:1053:G:C4 | 1:CA:1199:U:C5 | 3.07 | 0.42 |
| 25:BA:917:A:H2' | 25:BA:918:A:H5' | 2.01 | 0.42 |
| 19:AV:41:VAL:HG12 | 19:AV:44:MET:CA | 2.50 | 0.42 |
| 2:CE:74:LYS:HG3 | 2:CE:75:LYS:H | 1.85 | 0.42 |
| 1:AA:57:G:C5 | 1:AA:58:C:C4 | 3.08 | 0.42 |
| 25:DA:2271:G:C5 | 25:DA:2272:U:C4 | 3.08 | 0.42 |
| 1:AA:1349:A:P | 9:AL:118:LYS:NZ | 2.93 | 0.42 |
| 23:CD:49:C:C6 | 23:CD:60:A:O4' | 2.73 | 0.42 |
| 25:DA:1049:C:N4 | 31:DH:2:SER:HB3 | 2.34 | 0.42 |
| 1:CA:606:G:H21 | 1:CA:631:G:H2' | 1.84 | 0.42 |
| 1:CA:1127:G:HO2' | 1:CA:1128:C:H5' | 1.85 | 0.42 |
| 17:CT:63:ARG:HG2 | 17:CT:64:PRO:CD | 2.49 | 0.42 |
| 9:CL:3:GLN:O | 9:CL:88:TYR:CE1 | 2.73 | 0.42 |
| 25:DA:886:C:H1' | 25:DA:890:A:H2 | 1.81 | 0.42 |
| 1:AA:686:U:C1' | 11:AN:42:TRP:HE1 | 2.19 | 0.42 |
| 25:DA:2163:C:C5 | 25:DA:2164:C:N4 | 2.88 | 0.42 |
| 53:B7:15:THR:HG22 | 53:B7:16:HIS:ND1 | 2.35 | 0.42 |
| 7:CJ:113:GLU:CG | 7:CJ:119:ARG:HG2 | 2.50 | 0.42 |
| 35:DO:85:LEU:HB3 | 35:DO:114:ILE:HD13 | 2.00 | 0.42 |
| 25:BA:1537:C:C2' | 25:BA:1538:G:O4' | 2.68 | 0.42 |
| 25:BA:1777:U:C2' | 25:BA:1778:U:H5' | 2.50 | 0.42 |
| 1:AA:439:A:C2' | 1:AA:440:A:O5' | 2.68 | 0.42 |
| 15:CR:26:GLU:HG2 | 15:CR:26:GLU:H | 1.54 | 0.42 |
| 9:CL:106:ALA:O | 9:CL:108:VAL:HG12 | 2.20 | 0.42 |
| 7:CJ:30:ILE:O | 7:CJ:30:ILE:HG22 | 2.20 | 0.42 |
| 25:DA:84:A:H61 | 25:DA:102:G:C2' | 2.24 | 0.42 |
| 25:BA:847:U:H5 | 25:BA:933:A:C2 | 2.38 | 0.42 |
| 54:D8:41:ILE:HG22 | 54:D8:42:ARG:N | 2.35 | 0.42 |
| 45:DV:30:ASN:HD22 | 45:DV:32:HIS:H | 1.66 | 0.42 |
| 22:CB:56:G:H2' | 22:CB:57:C:C6 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:1372:U:C2' | 1:CA:1373:G:H5' | 2.49 | 0.42 |
| 1:CA:1503:A:C1' | 1:CA:1504:G:OP1 | 2.66 | 0.42 |
| 23:CD:22:A:C2 | 23:CD:47:G:H2' | 2.54 | 0.42 |
| 3:CF:92:ALA:HA | 3:CF:95:THR:O | 2.20 | 0.42 |
| 25:DA:2012:G:H8 | 25:DA:2012:G:O5' | 2.01 | 0.42 |
| 13:AP:115:LYS:O | 13:AP:116:THR:O | 2.38 | 0.42 |
| 1:CA:78:G:H2' | 1:CA:79:G:O4' | 2.20 | 0.42 |
| 1:AA:1489:G:C2' | 1:AA:1490:C:H5' | 2.49 | 0.42 |
| 37:B0:81:ASP:O | 37:B0:85:PRO:HG2 | 2.20 | 0.42 |
| 33:DM:91:LEU:O | 33:DM:95:PRO:HB3 | 2.19 | 0.42 |
| 1:AA:95:G:C6 | 1:AA:96:G:C6 | 3.07 | 0.42 |
| 25:DA:2390:U:O2' | 25:DA:2391:G:H5' | 2.20 | 0.42 |
| 23:CD:9:G:O3' | 23:CD:46:G:O2' | 2.38 | 0.42 |
| 11:CN:91:ARG:O | 11:CN:95:ILE:HG13 | 2.19 | 0.42 |
| 4:AG:121:VAL:O | 4:AG:134:ASP:HA | 2.20 | 0.42 |
| 26:BB:60:C:C2 | 26:BB:61:G:C8 | 3.07 | 0.42 |
| 7:AJ:40:ALA:O | 7:AJ:44:TYR:CD1 | 2.73 | 0.42 |
| 34:BN:35:VAL:HG11 | 34:BN:103:ALA:CB | 2.50 | 0.42 |
| 22:CB:75:G:H2' | 22:CB:76:U:C6 | 2.54 | 0.42 |
| 6:AI:63:TYR:N | 6:AI:63:TYR:CD2 | 2.88 | 0.42 |
| 32:BK:144:VAL:HG22 | 32:BK:145:VAL:H | 1.85 | 0.42 |
| 25:BA:1612:C:H5'' | 53:B7:7:PRO:HG2 | 2.02 | 0.42 |
| 12:AO:70:ILE:HD13 | 12:AO:77:LEU:HD12 | 2.01 | 0.42 |
| 25:DA:2065:C:H5'' | 25:DA:2252:G:H1' | 2.01 | 0.42 |
| 33:BM:7:LYS:HE3 | 33:BM:7:LYS:HB3 | 1.92 | 0.42 |
| 8:CK:11:THR:HA | 8:CK:14:ARG:NH1 | 2.35 | 0.42 |
| 28:DE:204:ALA:O | 28:DE:205:ALA:CB | 2.67 | 0.42 |
| 1:AA:303:A:C5 | 1:AA:304:U:C5 | 3.08 | 0.42 |
| 25:BA:1433:U:O2 | 25:BA:1561:G:C2 | 2.73 | 0.42 |
| 25:BA:2745:C:C4 | 25:BA:2746:U:C4 | 3.08 | 0.42 |
| 7:CJ:42:ILE:HD13 | 7:CJ:116:ALA:HB3 | 2.02 | 0.42 |
| 25:DA:2324:C:H5'' | 25:DA:2325:G:C5' | 2.50 | 0.42 |
| 25:BA:1261:C:C2' | 25:BA:1262:A:O5' | 2.67 | 0.42 |
| 25:DA:478:A:N1 | 25:DA:500:G:H4' | 2.35 | 0.42 |
| 42:DS:79:GLY:CA | 42:DS:100:THR:HG22 | 2.50 | 0.42 |
| 25:BA:1382:G:C2' | 25:BA:1383:C:H5' | 2.50 | 0.42 |
| 25:DA:1806:C:C4 | 25:DA:1807:G:N7 | 2.88 | 0.42 |
| 25:DA:363(F):A:OP2 | 25:DA:363(F):A:H8 | 2.03 | 0.42 |
| 25:BA:1671:U:O2' | 25:BA:1673:U:H5 | 2.02 | 0.42 |
| 25:BA:1686:C:H2' | 25:BA:1687:G:O4' | 2.20 | 0.42 |
| 25:BA:1400:G:H2' | 25:BA:1401:G:C8 | 2.55 | 0.42 |
| 17:AT:92:ARG:HA | 17:AT:92:ARG:HD3 | 1.88 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 30:BG:52:ILE:HD13 | 30:BG:52:ILE:HA | 1.84 | 0.42 |
| 35:DO:2:LYS:HB2 | 35:DO:2:LYS:HE3 | 1.85 | 0.42 |
| 25:DA:2662:A:H8 | 25:DA:2662:A:O5' | 2.03 | 0.42 |
| 37:B0:54:LEU:HA | 37:B0:54:LEU:HD12 | 1.78 | 0.42 |
| 1:AA:421:U:H3 | 3:AF:127:ARG:HH21 | 1.67 | 0.42 |
| 1:AA:711:G:O2' | 1:AA:712:A:H5' | 2.20 | 0.42 |
| 1:CA:229:U:H2' | 1:CA:230:G:O4' | 2.20 | 0.42 |
| 32:DK:115:ALA:HB3 | 32:DK:129:THR:O | 2.20 | 0.42 |
| 25:BA:1074:G:O2' | 25:BA:1075:C:H5' | 2.19 | 0.41 |
| 25:BA:2467:C:C3' | 25:BA:2468:G:C5' | 2.92 | 0.41 |
| 27:DD:34:VAL:C | 27:DD:35:LYS:O | 2.56 | 0.41 |
| 25:DA:1568:G:P | 27:DD:63:ARG:HH22 | 2.42 | 0.41 |
| 38:DQ:41:ASP:OD1 | 38:DQ:44:LYS:HE3 | 2.19 | 0.41 |
| 33:DM:33:LEU:HD12 | 33:DM:38:HIS:CD2 | 2.55 | 0.41 |
| 33:DM:42:TRP:HA | 33:DM:48:MET:CE | 2.50 | 0.41 |
| 25:BA:2810:A:H2' | 25:BA:2811:G:O4' | 2.19 | 0.41 |
| 25:BA:2811:G:OP1 | 28:BE:61:ARG:HG2 | 2.20 | 0.41 |
| 28:BE:60:ASN:HB2 | 28:BE:61:ARG:H | 1.62 | 0.41 |
| 22:CB:21:A:C1' | 22:CB:22:G:P | 3.08 | 0.41 |
| 47:DZ:95:LEU:O | 47:DZ:97:LEU:N | 2.53 | 0.41 |
| 25:DA:66:C:H2' | 25:DA:67:U:O4' | 2.19 | 0.41 |
| 51:B5:3:LYS:HB3 | 51:B5:4:HIS:H | 1.64 | 0.41 |
| 29:DF:3:GLU:HG3 | 29:DF:20:LEU:C | 2.40 | 0.41 |
| 11:AN:34:ASP:HB2 | 11:AN:35:PRO:HD2 | 2.02 | 0.41 |
| 1:AA:748:C:C4' | 1:AA:749:C:O5' | 2.49 | 0.41 |
| 30:BG:104:GLU:HG2 | 50:B4:23:GLU:CG | 2.50 | 0.41 |
| 44:DU:17:SER:CB | 44:DU:71:LYS:HD2 | 2.43 | 0.41 |
| 25:BA:2401:U:O2 | 25:BA:2402:C:H5 | 2.02 | 0.41 |
| 9:CL:75:ASP:O | 9:CL:78:LYS:HB3 | 2.20 | 0.41 |
| 23:AD:55:U:O4 | 23:AD:56:U:C4 | 2.73 | 0.41 |
| 39:BR:53:ARG:HB2 | 39:BR:60:THR:O | 2.20 | 0.41 |
| 27:BD:27:THR:O | 27:BD:28:GLU:CB | 2.55 | 0.41 |
| 46:D3:36:ILE:CD1 | 46:D3:36:ILE:N | 2.83 | 0.41 |
| 7:AJ:22:LEU:HD12 | 7:AJ:97:GLN:OE1 | 2.20 | 0.41 |
| 17:CT:45:HIS:O | 17:CT:73:VAL:HG13 | 2.20 | 0.41 |
| 11:AN:57:THR:HG22 | 11:AN:58:PRO:N | 2.35 | 0.41 |
| 32:BK:7:GLU:HG3 | 32:BK:8:PRO:HD2 | 2.02 | 0.41 |
| 19:AV:65:ASN:HA | 50:B4:56:VAL:HG22 | 2.03 | 0.41 |
| 1:AA:495:A:H4' | 1:AA:496:A:OP1 | 2.20 | 0.41 |
| 19:CV:33:THR:HG23 | 19:CV:50:ALA:O | 2.20 | 0.41 |
| 1:CA:413:G:C2' | 1:CA:414:A:OP2 | 2.67 | 0.41 |
| 12:CO:40:VAL:HG21 | 12:CO:78:GLN:CA | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 2:CE:132:LYS:HA | 2:CE:135:GLN:NE2 | 2.31 | 0.41 |
| 1:AA:153:C:N4 | 1:AA:168:G:H1 | 2.17 | 0.41 |
| 1:CA:748:C:H1' | 1:CA:749:C:OP2 | 2.19 | 0.41 |
| 4:AG:133:VAL:HG11 | 4:AG:138:TYR:CD1 | 2.53 | 0.41 |
| 31:DH:170:ARG:HA | 31:DH:170:ARG:HD3 | 1.89 | 0.41 |
| 26:DB:49:C:H2' | 26:DB:50:G:C8 | 2.55 | 0.41 |
| 25:DA:372:G:H5' | 47:DZ:66:HIS:CE1 | 2.55 | 0.41 |
| 23:CD:20:G:C8 | 23:CD:58:A:N6 | 2.86 | 0.41 |
| 54:B8:42:ARG:HG2 | 54:B8:42:ARG:HH11 | 1.85 | 0.41 |
| 1:AA:1342:C:H2' | 1:AA:1343:G:H8 | 1.85 | 0.41 |
| 2:CE:189:ASP:OD2 | 2:CE:191:ASP:HB3 | 2.19 | 0.41 |
| 32:BK:135:GLU:H | 32:BK:135:GLU:CD | 2.22 | 0.41 |
| 8:CK:64:LYS:CD | 8:CK:79:VAL:HG21 | 2.50 | 0.41 |
| 1:AA:626:U:H2' | 1:AA:627:G:H8 | 1.84 | 0.41 |
| 14:CQ:8:GLU:O | 14:CQ:12:ARG:HG3 | 2.20 | 0.41 |
| 42:BS:57:ASN:O | 42:BS:61:ASN:HB2 | 2.19 | 0.41 |
| 7:AJ:27:ILE:HD11 | 7:AJ:43:PHE:HD2 | 1.84 | 0.41 |
| 1:CA:1263:C:N4 | 1:CA:1272:G:H1 | 2.18 | 0.41 |
| 25:BA:2815:C:H5' | 51:B5:29:THR:HG21 | 2.02 | 0.41 |
| 1:CA:607:A:H2' | 1:CA:608:A:O4' | 2.19 | 0.41 |
| 40:D1:112:ARG:H | 40:D1:112:ARG:HG2 | 1.47 | 0.41 |
| 1:CA:51:A:H4' | 1:CA:52:G:H5'' | 2.02 | 0.41 |
| 48:BW:14:ARG:NH1 | 48:BW:66:GLU:OE2 | 2.53 | 0.41 |
| 1:CA:1370:G:O2' | 1:CA:1371:G:H5' | 2.20 | 0.41 |
| 25:BA:2695:C:H2' | 25:BA:2696:U:H6 | 1.84 | 0.41 |
| 25:DA:2076:U:H5 | 25:DA:2596:U:O2 | 2.03 | 0.41 |
| 12:CO:53:ARG:HH12 | 12:CO:92:ASP:CB | 2.32 | 0.41 |
| 35:DO:144:GLU:O | 35:DO:144:GLU:CD | 2.59 | 0.41 |
| 25:BA:1001:A:H2' | 25:BA:1002:G:O4' | 2.20 | 0.41 |
| 25:DA:1783:A:C2 | 25:DA:2587:A:C5 | 3.08 | 0.41 |
| 25:DA:1946:U:H2' | 25:DA:1947:C:C6 | 2.55 | 0.41 |
| 15:CR:78:TYR:O | 15:CR:82:ILE:HG23 | 2.19 | 0.41 |
| 25:DA:699:A:C2 | 25:DA:1633:G:N3 | 2.88 | 0.41 |
| 3:CF:67:THR:HG23 | 3:CF:102:ASN:HB2 | 2.02 | 0.41 |
| 27:BD:232:PRO:HB3 | 27:BD:244:ARG:CZ | 2.50 | 0.41 |
| 25:DA:2489:G:C2' | 25:DA:2490:G:H5' | 2.50 | 0.41 |
| 34:DN:11:ALA:O | 34:DN:99:PHE:N | 2.46 | 0.41 |
| 30:DG:139:LEU:C | 30:DG:139:LEU:HD12 | 2.41 | 0.41 |
| 50:B4:2:LYS:HA | 50:B4:2:LYS:HD3 | 1.88 | 0.41 |
| 37:D0:55:ALA:CB | 37:D0:79:LEU:HD22 | 2.50 | 0.41 |
| 25:BA:2545:G:H2' | 25:BA:2546:U:O4' | 2.20 | 0.41 |
| 47:BZ:21:ARG:HD3 | 47:BZ:35:THR:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:1069:A:H5'' | 25:BA:1070:A:O5' | 2.20 | 0.41 |
| 47:BZ:87:PRO:O | 47:BZ:89:GLU:N | 2.53 | 0.41 |
| 38:BQ:23:ARG:HB2 | 38:BQ:86:ALA:HB2 | 2.02 | 0.41 |
| 36:DP:35:VAL:HG23 | 36:DP:36:ALA:N | 2.36 | 0.41 |
| 28:BE:6:GLY:HA3 | 28:BE:27:LEU:O | 2.20 | 0.41 |
| 4:AG:15:GLU:OE1 | 4:AG:66:ARG:NH1 | 2.50 | 0.41 |
| 25:BA:298:G:H5'' | 25:BA:299:A:OP1 | 2.20 | 0.41 |
| 27:DD:85:ASP:HB2 | 27:DD:92:ILE:HD13 | 2.02 | 0.41 |
| 1:CA:977:A:HO2' | 1:CA:978:A:H5' | 1.84 | 0.41 |
| 22:CB:69:A:OP1 | 22:CB:69:A:H3' | 2.20 | 0.41 |
| 25:DA:1062:G:C8 | 25:DA:1062:G:OP1 | 2.68 | 0.41 |
| 25:BA:994:C:OP1 | 40:B1:53:ARG:NH2 | 2.53 | 0.41 |
| 13:CP:56:LEU:HA | 13:CP:56:LEU:HD23 | 1.93 | 0.41 |
| 54:B8:36:LYS:CD | 54:B8:40:GLU:CD | 2.87 | 0.41 |
| 25:DA:528:A:N1 | 25:DA:2043:C:H5' | 2.31 | 0.41 |
| 50:D4:24:THR:O | 50:D4:25:TYR:HB2 | 2.19 | 0.41 |
| 25:DA:2305:A:C6 | 30:DG:154:GLY:CA | 3.03 | 0.41 |
| 43:BT:24:GLY:CA | 43:BT:82:GLN:HE22 | 2.32 | 0.41 |
| 30:BG:7:LEU:HD21 | 30:BG:176:LEU:HD22 | 2.02 | 0.41 |
| 25:BA:1478:G:H2' | 25:BA:1479:G:C8 | 2.48 | 0.41 |
| 25:BA:1510:A:OP1 | 25:BA:1510:A:O3' | 2.37 | 0.41 |
| 1:CA:1446:A:C5 | 39:DR:118:ARG:CZ | 3.03 | 0.41 |
| 30:BG:129:GLY:O | 30:BG:161:THR:HB | 2.19 | 0.41 |
| 25:BA:996:A:OP2 | 40:B1:94:ASN:ND2 | 2.53 | 0.41 |
| 2:CE:90:MET:HA | 2:CE:91:PRO:HD3 | 1.87 | 0.41 |
| 4:AG:12:CYS:HA | 4:AG:19:LEU:HD21 | 2.00 | 0.41 |
| 25:BA:812:C:H5'' | 25:BA:1250:G:O2' | 2.20 | 0.41 |
| 25:BA:811:U:H2' | 35:BO:21:ARG:O | 2.19 | 0.41 |
| 26:DB:88:C:H6 | 26:DB:89:G:C8 | 2.38 | 0.41 |
| 30:DG:142:PRO:HG2 | 30:DG:143:GLU:OE2 | 2.20 | 0.41 |
| 2:CE:95:GLN:O | 2:CE:96:ARG:C | 2.59 | 0.41 |
| 25:BA:653:A:H3' | 25:BA:654:A:H5' | 2.01 | 0.41 |
| 11:AN:57:THR:HG23 | 11:AN:58:PRO:HD2 | 2.02 | 0.41 |
| 27:BD:19:ALA:HB3 | 27:BD:21:PHE:CZ | 2.55 | 0.41 |
| 28:DE:57:LYS:HD3 | 28:DE:57:LYS:HA | 1.85 | 0.41 |
| 3:AF:50:ALA:HB1 | 3:AF:70:VAL:CG1 | 2.44 | 0.41 |
| 25:BA:2703:C:O2 | 25:BA:2703:C:H2' | 2.19 | 0.41 |
| 28:DE:182:LEU:C | 28:DE:183:LEU:HD12 | 2.40 | 0.41 |
| 16:CS:19:ILE:HB | 16:CS:36:ILE:O | 2.19 | 0.41 |
| 1:CA:382:A:C6 | 1:CA:383:A:C6 | 3.08 | 0.41 |
| 8:CK:20:TYR:HA | 8:CK:65:TYR:CZ | 2.55 | 0.41 |
| 28:BE:116:VAL:HG13 | 28:BE:122:PHE:CG | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:429:U:H1' | 1:CA:430:A:H5'' | 2.02 | 0.41 |
| 49:DX:52:HIS:CE1 | 49:DX:53:LEU:HD23 | 2.56 | 0.41 |
| 25:DA:142:G:H1' | 43:DT:37:THR:HG22 | 2.02 | 0.41 |
| 23:AD:17:C:H2' | 23:AD:18:C:O2 | 2.19 | 0.41 |
| 23:AD:60:A:C5 | 23:AD:61:U:C5 | 3.07 | 0.41 |
| 1:CA:585:G:H4' | 12:CO:8:ASN:ND2 | 2.35 | 0.41 |
| 45:DV:138:GLU:O | 45:DV:156:LYS:HE3 | 2.19 | 0.41 |
| 25:DA:1204:A:N1 | 25:DA:1241:A:H2 | 2.18 | 0.41 |
| 25:DA:568:U:O5' | 25:DA:945:A:N6 | 2.52 | 0.41 |
| 13:CP:55:ARG:CG | 13:CP:55:ARG:HH11 | 2.30 | 0.41 |
| 25:BA:616:A:C4 | 29:BF:180:GLY:HA3 | 2.55 | 0.41 |
| 42:BS:79:GLY:C | 42:BS:100:THR:HG22 | 2.40 | 0.41 |
| 25:DA:603:A:C2 | 25:DA:655:A:C2 | 3.07 | 0.41 |
| 4:AG:24:GLU:O | 4:AG:27:TYR:HB2 | 2.19 | 0.41 |
| 25:BA:1448:G:H1' | 25:BA:1528:A:H62 | 1.85 | 0.41 |
| 1:AA:725:G:N3 | 1:AA:726:C:C6 | 2.88 | 0.41 |
| 20:CW:22:ARG:O | 20:CW:26:ASN:ND2 | 2.53 | 0.41 |
| 1:CA:75:C:H2' | 1:CA:76:G:O4' | 2.20 | 0.41 |
| 44:DU:2:ARG:HA | 44:DU:2:ARG:HD3 | 1.77 | 0.41 |
| 1:AA:148:G:N3 | 1:AA:149:A:C8 | 2.88 | 0.41 |
| 1:AA:73:G:C8 | 1:AA:99:C:O2 | 2.73 | 0.41 |
| 25:DA:2517:C:C2 | 25:DA:2542:A:C6 | 3.08 | 0.41 |
| 25:BA:2390:U:O2' | 25:BA:2391:G:H5' | 2.21 | 0.41 |
| 11:CN:48:ILE:HA | 11:CN:48:ILE:HD12 | 1.81 | 0.41 |
| 37:B0:34:ILE:HG22 | 37:B0:114:VAL:HB | 2.02 | 0.41 |
| 25:BA:821:A:O2' | 25:BA:945:A:H3' | 2.20 | 0.41 |
| 3:CF:82:GLU:H | 3:CF:85:ARG:HB2 | 1.85 | 0.41 |
| 29:DF:188:ARG:HG3 | 35:DO:3:LEU:HD11 | 2.01 | 0.41 |
| 25:BA:1816:G:H8 | 27:BD:62:TYR:OH | 2.03 | 0.41 |
| 1:CA:9:G:H2' | 1:CA:10:A:H8 | 1.86 | 0.41 |
| 1:CA:309:G:H1' | 1:CA:608:A:C2 | 2.55 | 0.41 |
| 25:BA:2854:G:O2' | 25:BA:2855:C:H5' | 2.19 | 0.41 |
| 42:BS:111:HIS:CD2 | 42:BS:112:GLY:H | 2.38 | 0.41 |
| 26:DB:20:C:C2' | 26:DB:21:G:H5' | 2.50 | 0.41 |
| 1:CA:799:G:C6 | 1:CA:800:G:C4 | 3.08 | 0.41 |
| 27:DD:161:THR:O | 27:DD:162:SER:HB3 | 2.20 | 0.41 |
| 25:DA:363(E):U:H5' | 25:DA:363(F):A:OP2 | 2.20 | 0.41 |
| 25:BA:2740:A:C6 | 25:BA:2764:A:C8 | 3.07 | 0.41 |
| 25:BA:1726:G:C6 | 25:BA:1727:U:C4 | 3.08 | 0.41 |
| 15:CR:11:VAL:HG21 | 15:CR:34:LEU:HD22 | 2.02 | 0.41 |
| 4:CG:54:TYR:CE1 | 4:CG:206:PHE:HE1 | 2.38 | 0.41 |
| 1:CA:186(E):C:C2 | 1:CA:191(C):G:N2 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:282:A:H2' | 1:AA:282:A:N3 | 2.34 | 0.41 |
| 15:AR:57:LEU:HD23 | 15:AR:57:LEU:HA | 1.80 | 0.41 |
| 25:DA:2099:U:H2' | 25:DA:2099:U:O2 | 2.20 | 0.41 |
| 35:BO:135:LEU:HD23 | 35:BO:135:LEU:HA | 1.81 | 0.41 |
| 45:DV:151:HIS:CD2 | 45:DV:151:HIS:N | 2.86 | 0.41 |
| 25:DA:1767:C:H2' | 25:DA:1768:U:O4' | 2.20 | 0.41 |
| 1:CA:1318:A:O2' | 19:CV:37:ARG:HG2 | 2.20 | 0.41 |
| 17:AT:13:ASP:HA | 17:AT:19:VAL:HG12 | 2.02 | 0.41 |
| 14:AQ:24:CYS:HB3 | 14:AQ:28:GLY:H | 1.85 | 0.41 |
| 25:BA:1071:G:C8 | 25:BA:1089:G:C5 | 3.08 | 0.41 |
| 25:BA:2469:A:H62 | 25:BA:2481:G:H21 | 1.67 | 0.41 |
| 38:DQ:110:LEU:HD22 | 38:DQ:112:PHE:N | 2.35 | 0.41 |
| 30:BG:77:ILE:HG22 | 30:BG:77:ILE:O | 2.18 | 0.41 |
| 27:BD:77:ALA:HB2 | 27:BD:97:TYR:CD2 | 2.55 | 0.41 |
| 28:BE:29:GLY:N | 28:BE:51:PHE:CE2 | 2.89 | 0.41 |
| 28:DE:37:ARG:O | 28:DE:45:THR:HA | 2.20 | 0.41 |
| 39:DR:16:ARG:HH21 | 39:DR:19:LEU:HD21 | 1.83 | 0.41 |
| 10:CM:54:PHE:CE1 | 10:CM:55:LYS:NZ | 2.88 | 0.41 |
| 25:DA:2748:A:C2 | 25:DA:2749:A:C8 | 3.08 | 0.41 |
| 25:DA:1021:A:C6 | 25:DA:1023:U:C4 | 3.08 | 0.41 |
| 1:CA:1161:C:O2' | 1:CA:1162:C:H5' | 2.19 | 0.41 |
| 25:DA:1330:C:O2' | 25:DA:1331:A:H5' | 2.21 | 0.41 |
| 45:BV:58:VAL:HG12 | 45:BV:66:SER:HB3 | 2.01 | 0.41 |
| 48:DW:15:LYS:H | 48:DW:67:LYS:HE2 | 1.84 | 0.41 |
| 1:CA:1329:A:OP1 | 13:CP:25:ILE:O | 2.38 | 0.41 |
| 25:DA:1111:A:H4' | 31:DH:3:ARG:CD | 2.40 | 0.41 |
| 25:DA:2312:U:C2' | 25:DA:2313:C:H5' | 2.50 | 0.41 |
| 25:BA:811:U:OP2 | 35:BO:21:ARG:O | 2.39 | 0.41 |
| 2:AE:208:ILE:HA | 2:AE:211:ILE:HG13 | 2.03 | 0.41 |
| 50:D4:13:ARG:HG3 | 50:D4:22:ILE:HG22 | 2.02 | 0.41 |
| 28:BE:119:ARG:HH12 | 28:BE:158:GLY:HA3 | 1.82 | 0.41 |
| 7:AJ:62:PHE:HA | 7:AJ:124:LEU:HD23 | 2.02 | 0.41 |
| 9:CL:52:ALA:HB3 | 9:CL:95:LYS:NZ | 2.36 | 0.41 |
| 1:CA:957:U:C3' | 1:CA:958:A:H5'' | 2.51 | 0.41 |
| 17:AT:83:ASP:OD2 | 17:AT:84:LEU:HD23 | 2.20 | 0.41 |
| 25:BA:1594:G:H2' | 25:BA:1595:G:O4' | 2.20 | 0.41 |
| 1:AA:926:G:C6 | 1:AA:1505:G:C6 | 3.08 | 0.41 |
| 1:CA:1186:G:C2 | 1:CA:1187:G:H1' | 2.55 | 0.41 |
| 9:CL:111:ARG:O | 9:CL:113:LYS:HD2 | 2.20 | 0.41 |
| 25:BA:2422:A:C4' | 25:BA:2423:U:OP1 | 2.61 | 0.41 |
| 25:BA:2646:C:O5' | 25:BA:2646:C:C6 | 2.74 | 0.41 |
| 45:BV:102:LEU:HD13 | 45:BV:139:VAL:HG21 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 2:CE:132:LYS:NZ | 2:CE:136:VAL:HG22 | 2.34 | 0.41 |
| 1:AA:280:C:O2 | 17:AT:38:ARG:HG3 | 2.20 | 0.41 |
| 32:DK:77:LEU:HG | 32:DK:78:THR:OG1 | 2.20 | 0.41 |
| 25:BA:270(E):G:C6 | 25:BA:270(F):U:C4 | 3.08 | 0.41 |
| 25:BA:2688:U:C3' | 25:BA:2688:U:O2 | 2.68 | 0.41 |
| 1:AA:411:A:C4 | 1:AA:413:G:H1' | 2.55 | 0.41 |
| 25:BA:1446:C:C2' | 25:BA:1447:G:O5' | 2.68 | 0.41 |
| 25:BA:1528:A:N6 | 25:BA:1545:A:C2 | 2.88 | 0.41 |
| 25:DA:1599:C:N3 | 25:DA:1600:C:C5 | 2.89 | 0.41 |
| 1:CA:1207:G:C5 | 1:CA:1208:C:C4 | 3.08 | 0.41 |
| 1:AA:450:G:H2' | 1:AA:451:A:OP1 | 2.21 | 0.41 |
| 1:AA:148:G:C2 | 1:AA:149:A:C8 | 3.08 | 0.41 |
| 1:CA:628:G:C2' | 1:CA:629:G:H5' | 2.50 | 0.41 |
| 25:BA:165:U:H2' | 25:BA:171:G:O4' | 2.20 | 0.41 |
| 1:AA:1342:C:O2' | 9:AL:124:GLN:HA | 2.21 | 0.41 |
| 18:AU:25:THR:HG22 | 18:AU:25:THR:O | 2.20 | 0.41 |
| 23:CD:37:U:H2' | 23:CD:38:A:C8 | 2.55 | 0.41 |
| 25:DA:277:C:H3' | 25:DA:278:A:C8 | 2.54 | 0.41 |
| 11:CN:69:ALA:HB1 | 11:CN:103:LEU:CD2 | 2.50 | 0.41 |
| 1:CA:640:A:O2' | 1:CA:641:U:H5' | 2.19 | 0.41 |
| 1:CA:814:A:H5' | 1:CA:1511:G:H4' | 2.02 | 0.41 |
| 42:DS:51:LEU:HD23 | 42:DS:105:VAL:HG11 | 2.02 | 0.41 |
| 14:CQ:7:ILE:O | 14:CQ:10:ALA:HB3 | 2.19 | 0.41 |
| 31:BH:3:ARG:NE | 31:BH:3:ARG:HA | 2.35 | 0.41 |
| 18:CU:37:VAL:O | 18:CU:41:LYS:HB2 | 2.20 | 0.41 |
| 25:DA:1475:G:H5' | 25:DA:1476:C:OP2 | 2.20 | 0.41 |
| 1:AA:836:G:C6 | 1:AA:851:G:C6 | 3.08 | 0.41 |
| 12:AO:46:LYS:CG | 12:AO:47:LYS:H | 2.33 | 0.41 |
| 5:AH:69:VAL:HG12 | 5:AH:71:LEU:HD23 | 2.03 | 0.41 |
| 26:BB:81:G:O6 | 26:BB:95:U:O2 | 2.38 | 0.41 |
| 30:DG:75:LYS:H | 30:DG:75:LYS:HG3 | 1.72 | 0.41 |
| 28:DE:105:THR:OG1 | 28:DE:166:THR:HG23 | 2.20 | 0.41 |
| 25:BA:537:C:H3' | 25:BA:539:G:H8 | 1.85 | 0.41 |
| 1:CA:438:G:H4' | 4:CG:123:HIS:ND1 | 2.35 | 0.41 |
| 1:CA:287:U:H2' | 1:CA:288:A:C8 | 2.56 | 0.41 |
| 8:CK:61:VAL:HG12 | 8:CK:63:LEU:HD13 | 2.01 | 0.41 |
| 25:BA:1665:A:H2' | 25:BA:1666:G:O4' | 2.21 | 0.41 |
| 52:B6:21:TYR:N | 52:B6:21:TYR:HD2 | 2.19 | 0.41 |
| 25:BA:807:U:O2' | 25:BA:808:G:H5' | 2.20 | 0.41 |
| 22:CB:65:U:H5'' | 36:DP:52:VAL:HG23 | 2.02 | 0.41 |
| 25:DA:704:G:H1' | 25:DA:726:G:N2 | 2.36 | 0.41 |
| 1:CA:1477:C:C2' | 1:CA:1478:C:H5' | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:1321:A:H2' | 25:BA:1322:A:O4' | 2.20 | 0.41 |
| 1:CA:681:C:C2 | 1:CA:710:G:N2 | 2.87 | 0.41 |
| 25:DA:49:A:H5'' | 25:DA:50:U:H3' | 2.01 | 0.41 |
| 1:AA:140:A:C6 | 1:AA:141:A:C5 | 3.08 | 0.41 |
| 25:DA:836:G:C5 | 25:DA:837:C:C4 | 3.07 | 0.41 |
| 41:D2:66:ARG:HG2 | 41:D2:66:ARG:H | 1.63 | 0.41 |
| 37:B0:28:LEU:HD23 | 37:B0:28:LEU:HA | 1.83 | 0.41 |
| 1:CA:1453:G:O4' | 1:CA:1453:G:N3 | 2.54 | 0.41 |
| 37:B0:51:LEU:HA | 37:B0:51:LEU:HD23 | 1.86 | 0.41 |
| 25:DA:110:G:C2 | 25:DA:111:A:C8 | 3.08 | 0.41 |
| 31:BH:38:SER:HA | 31:BH:39:PRO:HD3 | 1.89 | 0.41 |
| 25:BA:244:A:C2 | 25:BA:255:A:C4 | 3.08 | 0.41 |
| 25:BA:1070:A:H3' | 25:BA:1071:G:H5'' | 2.01 | 0.41 |
| 25:BA:49:A:C8 | 25:BA:51:G:C2 | 3.09 | 0.41 |
| 54:D8:35:GLN:C | 54:D8:36:LYS:HG3 | 2.41 | 0.41 |
| 25:BA:299:A:H62 | 25:BA:300:A:H61 | 1.67 | 0.41 |
| 13:CP:87:TYR:CD2 | 13:CP:87:TYR:C | 2.93 | 0.41 |
| 25:BA:2286:A:H2' | 52:B6:31:PRO:HG2 | 2.01 | 0.41 |
| 25:BA:2347:C:P | 52:B6:39:TYR:OH | 2.78 | 0.41 |
| 1:CA:973:G:C6 | 1:CA:974:A:N1 | 2.89 | 0.41 |
| 1:CA:447:G:H3' | 1:CA:485:G:N2 | 2.35 | 0.41 |
| 25:BA:607:U:C2 | 25:BA:621:A:N1 | 2.89 | 0.41 |
| 19:AV:40:ILE:O | 19:AV:41:VAL:HG22 | 2.21 | 0.41 |
| 25:DA:1601:G:C6 | 25:DA:1602:U:C4 | 3.08 | 0.41 |
| 25:DA:1021:A:H62 | 25:DA:1141:U:H3 | 1.68 | 0.41 |
| 25:DA:1142(A):A:N7 | 25:DA:1144:G:C5 | 2.89 | 0.41 |
| 29:DF:29:ASN:H | 29:DF:112:MET:HE1 | 1.84 | 0.41 |
| 28:BE:201:THR:HG22 | 28:BE:202:LYS:N | 2.34 | 0.41 |
| 25:DA:1899:G:H1 | 25:DA:1902:C:H41 | 1.69 | 0.41 |
| 54:B8:36:LYS:HD2 | 54:B8:40:GLU:CG | 2.51 | 0.41 |
| 1:CA:181:G:H4' | 1:CA:182:U:H5' | 2.03 | 0.41 |
| 30:DG:5:VAL:HG22 | 50:D4:25:TYR:CE2 | 2.55 | 0.41 |
| 30:DG:64:THR:HG23 | 30:DG:65:GLY:H | 1.84 | 0.41 |
| 2:CE:134:GLU:HA | 2:CE:137:ARG:HB2 | 2.02 | 0.41 |
| 1:AA:690:G:O2' | 1:AA:691:G:H5' | 2.21 | 0.41 |
| 25:DA:2164:C:C5 | 25:DA:2165:G:N7 | 2.88 | 0.41 |
| 23:CD:27:G:H2' | 23:CD:28:U:O4' | 2.20 | 0.41 |
| 1:CA:1301:U:C4 | 1:CA:1303:C:C6 | 3.08 | 0.41 |
| 1:CA:1434:A:N6 | 1:CA:1467:G:H1' | 2.33 | 0.41 |
| 33:BM:21:LYS:O | 33:BM:22:THR:O | 2.38 | 0.41 |
| 4:CG:5:ILE:HG22 | 4:CG:5:ILE:O | 2.21 | 0.41 |
| 2:AE:212:GLN:NE2 | 2:AE:212:GLN:O | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 28:BE:16:ARG:O | 28:BE:17:ASP:CB | 2.60 | 0.41 |
| 27:BD:21:PHE:O | 27:BD:24:ILE:HB | 2.20 | 0.41 |
| 41:B2:4:ILE:HB | 41:B2:40:LEU:HB2 | 2.02 | 0.41 |
| 10:CM:15:THR:HG21 | 10:CM:92:THR:CG2 | 2.43 | 0.41 |
| 23:CC:76:C:OP1 | 25:DA:2602:A:OP1 | 2.39 | 0.41 |
| 4:CG:24:GLU:CD | 4:CG:112:VAL:HG21 | 2.41 | 0.41 |
| 1:AA:187:C:O2 | 1:AA:191(A):G:C6 | 2.73 | 0.41 |
| 27:DD:68:LYS:CB | 27:DD:70:TRP:CZ3 | 3.04 | 0.41 |
| 23:AD:20:G:C5' | 23:AD:60:A:N6 | 2.81 | 0.41 |
| 23:AD:20:G:H4' | 23:AD:60:A:N6 | 2.35 | 0.41 |
| 1:CA:828:A:H5'' | 1:CA:859:A:H2 | 1.78 | 0.41 |
| 1:CA:859:A:OP2 | 1:CA:869:G:N1 | 2.41 | 0.41 |
| 41:B2:29:PRO:HA | 41:B2:61:VAL:HG22 | 2.00 | 0.41 |
| 1:CA:173:U:H5'' | 1:CA:197:A:O4' | 2.21 | 0.41 |
| 1:CA:197:A:C8 | 1:CA:198:G:C1' | 3.04 | 0.41 |
| 1:CA:1216:G:C2 | 1:CA:1217:C:C2 | 3.09 | 0.41 |
| 25:DA:2149:G:C2 | 25:DA:2150:U:C2 | 3.08 | 0.41 |
| 25:DA:1309:G:C2' | 25:DA:1310:G:H5' | 2.49 | 0.41 |
| 1:AA:562:C:N4 | 1:AA:884:U:C6 | 2.88 | 0.41 |
| 39:DR:64:ARG:O | 39:DR:64:ARG:CG | 2.67 | 0.41 |
| 1:CA:941:G:C2' | 1:CA:942:G:O5' | 2.68 | 0.41 |
| 31:DH:9:ILE:HG21 | 31:DH:51:ARG:HG2 | 2.03 | 0.41 |
| 4:AG:25:ARG:C | 4:AG:27:TYR:N | 2.74 | 0.41 |
| 12:CO:34:ARG:HD2 | 12:CO:82:VAL:CG1 | 2.49 | 0.41 |
| 25:BA:129:C:H2' | 25:BA:130:C:C6 | 2.56 | 0.41 |
| 25:BA:1652:A:C2' | 25:BA:1653:G:H5' | 2.51 | 0.41 |
| 9:CL:32:ASP:O | 9:CL:35:GLU:N | 2.49 | 0.41 |
| 44:DU:86:ARG:HB3 | 44:DU:88:LYS:NZ | 2.34 | 0.41 |
| 1:CA:79:G:OP2 | 1:CA:79:G:H8 | 2.03 | 0.41 |
| 3:CF:73:PRO:HA | 3:CF:76:VAL:HG13 | 2.03 | 0.41 |
| 33:DM:19:GLU:HG3 | 33:DM:59:LYS:CB | 2.49 | 0.41 |
| 23:AD:31:G:H1 | 23:AD:41:C:H42 | 1.67 | 0.41 |
| 1:CA:1028(A):C:C4 | 1:CA:1028(B):C:N4 | 2.86 | 0.41 |
| 33:DM:98:VAL:HG23 | 33:DM:99:LEU:N | 2.36 | 0.41 |
| 1:CA:1001:G:H1 | 1:CA:1039:C:N4 | 2.16 | 0.41 |
| 25:BA:755:C:H2' | 25:BA:756:C:C6 | 2.56 | 0.41 |
| 22:CB:8:U:H5'' | 22:CB:60:A:H5' | 2.02 | 0.41 |
| 10:CM:16:LEU:HD22 | 10:CM:16:LEU:HA | 1.76 | 0.41 |
| 25:DA:218:A:H2 | 25:DA:235:U:H4' | 1.84 | 0.41 |
| 42:BS:1:MET:HG3 | 42:BS:64:MET:HE2 | 2.02 | 0.41 |
| 12:AO:62:SER:HB2 | 12:AO:64:TYR:CD1 | 2.51 | 0.41 |
| 22:CB:34:U:C2 | 22:CB:36:A:OP2 | 2.73 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|---------------------|-------------|----------|
| 25:BA:2751:G:C8 | 25:BA:2751:G:O5' | 2.73 | 0.41 |
| 25:BA:305:U:H6 | 25:BA:305:U:O5' | 2.03 | 0.41 |
| 1:CA:956:U:C2 | 1:CA:1225:A:C2 | 3.08 | 0.41 |
| 3:AF:116:VAL:HG21 | 3:AF:202:ILE:HD11 | 2.02 | 0.41 |
| 5:CH:100:VAL:HA | 5:CH:118:ILE:HG22 | 2.02 | 0.41 |
| 25:DA:2857:G:N2 | 25:DA:2859:G:H3' | 2.36 | 0.41 |
| 39:DR:1:MET:HA | 39:DR:1:MET:CE | 2.50 | 0.41 |
| 40:D1:52:ARG:HH11 | 40:D1:52:ARG:HB3 | 1.85 | 0.41 |
| 27:DD:9:TYR:CE2 | 27:DD:13:ARG:HG2 | 2.56 | 0.41 |
| 25:DA:631:A:N6 | 25:DA:632:A:C2 | 2.88 | 0.41 |
| 25:BA:839:U:H2' | 25:BA:840:C:C6 | 2.55 | 0.41 |
| 25:BA:1444:G:C2 | 25:BA:1548:C:N3 | 2.89 | 0.41 |
| 3:AF:29:TYR:HD2 | 3:AF:29:TYR:O | 2.03 | 0.41 |
| 38:BQ:41:ASP:C | 38:BQ:41:ASP:OD1 | 2.58 | 0.41 |
| 1:AA:1310:G:N2 | 1:AA:1328:C:C2 | 2.88 | 0.41 |
| 14:CQ:44:LEU:HD12 | 14:CQ:44:LEU:C | 2.41 | 0.41 |
| 25:DA:550:G:O2' | 25:DA:1220:A:N3 | 2.42 | 0.41 |
| 18:AU:18:ARG:HB3 | 18:AU:19:LYS:H | 1.76 | 0.41 |
| 45:BV:98:MET:HE2 | 45:BV:100:VAL:HG22 | 2.02 | 0.41 |
| 27:DD:78:LYS:HA | 27:DD:115:GLN:O | 2.19 | 0.41 |
| 31:BH:125:VAL:HG12 | 31:BH:127:GLU:O | 2.20 | 0.41 |
| 31:DH:130:ARG:HB3 | 31:DH:130:ARG:NH1 | 2.35 | 0.41 |
| 45:DV:31:ARG:HE | 45:DV:31:ARG:HB2 | 1.73 | 0.41 |
| 37:D0:65:LEU:HD12 | 37:D0:65:LEU:HA | 1.86 | 0.41 |
| 18:CU:84:LYS:HE2 | 18:CU:84:LYS:HA | 2.03 | 0.41 |
| 1:AA:656:C:C6 | 1:AA:656:C:H3' | 2.56 | 0.41 |
| 25:BA:2518:A:C8 | 25:BA:2518:A:H5' | 2.56 | 0.41 |
| 25:DA:80:G:C2' | 25:DA:81:G:H5' | 2.50 | 0.41 |
| 47:BZ:83:GLU:N | 47:BZ:83:GLU:OE2 | 2.45 | 0.41 |
| 28:BE:80:GLU:C | 28:BE:82:ARG:H | 2.23 | 0.41 |
| 25:DA:2060:A:P | 29:DF:68:LYS:O | 2.74 | 0.41 |
| 28:DE:54:GLN:O | 28:DE:75:VAL:HG22 | 2.21 | 0.41 |
| 23:AD:69:C:C5 | 23:AD:70:C:C5 | 3.08 | 0.41 |
| 1:CA:1226:C:H4' | 1:CA:1227:A:OP1 | 2.20 | 0.41 |
| 1:CA:977:A:C8 | 1:CA:982:U:O4 | 2.74 | 0.41 |
| 25:DA:1342:A:C6 | 25:DA:1602:U:N3 | 2.75 | 0.41 |
| 25:DA:1063:G:N1 | 25:DA:1064:C:O2 | 2.53 | 0.41 |
| 25:DA:1019:U:OP1 | 25:DA:1035:U:O2' | 2.28 | 0.41 |
| 25:DA:1142:U:H5'' | 25:DA:1142(A):A:H5' | 2.02 | 0.41 |
| 39:DR:88:ILE:CD1 | 39:DR:91:ARG:HG2 | 2.50 | 0.41 |
| 39:DR:90:GLN:HG3 | 39:DR:91:ARG:N | 2.35 | 0.41 |
| 1:CA:1157:A:H62 | 1:CA:1178:G:N2 | 2.18 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 25:DA:2469:A:N1 | 25:DA:2470:G:C4 | 2.88 | 0.41 |
| 10:AM:49:VAL:HG21 | 14:AQ:41:ARG:HB2 | 1.99 | 0.41 |
| 35:DO:60:MET:HG3 | 35:DO:60:MET:O | 2.21 | 0.41 |
| 1:CA:1126:U:H1' | 1:CA:1127:G:P | 2.61 | 0.41 |
| 50:D4:24:THR:HB | 50:D4:25:TYR:H | 1.68 | 0.41 |
| 2:CE:188:ALA:O | 2:CE:203:GLY:O | 2.39 | 0.41 |
| 25:DA:1652:A:N6 | 37:D0:11:ASN:HD21 | 1.95 | 0.41 |
| 1:CA:561:U:HO2' | 1:CA:562:C:P | 2.44 | 0.41 |
| 25:BA:2799:A:N7 | 25:BA:2801:A:N6 | 2.68 | 0.41 |
| 2:AE:219:VAL:HA | 2:AE:222:ILE:CD1 | 2.51 | 0.41 |
| 25:DA:196:A:O2' | 25:DA:805:G:O6 | 2.29 | 0.41 |
| 33:BM:131:GLN:NE2 | 33:BM:132:ALA:N | 2.63 | 0.41 |
| 6:CI:61:LEU:HD23 | 6:CI:63:TYR:HH | 1.82 | 0.41 |
| 19:AV:65:ASN:ND2 | 19:AV:65:ASN:H | 2.06 | 0.41 |
| 29:DF:7:TYR:CE2 | 29:DF:16:GLY:HA3 | 2.56 | 0.41 |
| 1:AA:1227:A:OP2 | 13:AP:96:LEU:HD21 | 2.20 | 0.41 |
| 35:BO:112:LEU:HA | 35:BO:112:LEU:HD23 | 1.86 | 0.41 |
| 25:DA:2552:U:C2 | 25:DA:2554:U:H5' | 2.56 | 0.41 |
| 1:CA:1326:C:H2' | 1:CA:1327:C:C6 | 2.56 | 0.41 |
| 25:BA:2690:C:H6 | 25:BA:2690:C:OP2 | 2.03 | 0.41 |
| 25:BA:2109:U:C4 | 25:BA:2110:G:O6 | 2.74 | 0.41 |
| 23:CD:31:G:C2 | 23:CD:32:G:C5 | 3.08 | 0.41 |
| 32:DK:104:GLN:CG | 32:DK:105:HIS:CD2 | 3.03 | 0.41 |
| 43:DT:12:VAL:HG22 | 43:DT:17:ALA:HB2 | 2.02 | 0.41 |
| 5:AH:99:GLY:O | 5:AH:117:ASP:HA | 2.20 | 0.41 |
| 1:AA:1336:C:C4' | 1:AA:1336:C:OP1 | 2.66 | 0.41 |
| 39:DR:64:ARG:CB | 39:DR:73:GLU:HG3 | 2.47 | 0.41 |
| 25:DA:1288:U:C2 | 25:DA:1327:C:C2 | 3.08 | 0.41 |
| 1:AA:1256:A:O4' | 1:AA:1258:G:C2 | 2.74 | 0.41 |
| 37:B0:87:TYR:CE1 | 37:B0:117:VAL:HG12 | 2.55 | 0.41 |
| 25:BA:1449(A):G:O2' | 25:BA:1450:C:H5' | 2.21 | 0.41 |
| 1:AA:735:C:O2' | 1:AA:736:C:H5' | 2.20 | 0.41 |
| 25:DA:628:G:H5'' | 54:D8:18:ALA:HB2 | 2.03 | 0.41 |
| 1:CA:92:G:H2' | 1:CA:93:U:O4' | 2.21 | 0.41 |
| 1:CA:1374:A:C2' | 1:CA:1375:A:H5' | 2.50 | 0.41 |
| 1:CA:1121:U:O2' | 1:CA:1122:U:H5' | 2.20 | 0.41 |
| 8:CK:134:ILE:O | 8:CK:135:CYS:HB3 | 2.20 | 0.41 |
| 25:BA:2663:G:C2 | 25:BA:2664:G:H1' | 2.56 | 0.41 |
| 4:CG:189:PRO:HB2 | 4:CG:194:LEU:HD21 | 2.02 | 0.41 |
| 25:BA:1092:C:H42 | 25:BA:1099:G:H1 | 1.67 | 0.41 |
| 25:BA:856:C:H2' | 25:BA:857:C:C6 | 2.49 | 0.41 |
| 29:BF:10:PRO:HG2 | 29:BF:124:LEU:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:866:A:C2 | 25:DA:867:C:C4 | 3.09 | 0.41 |
| 1:AA:323:U:H5' | 20:AW:23:ARG:HB2 | 2.03 | 0.41 |
| 25:BA:814:C:O2' | 25:BA:1225:C:N3 | 2.49 | 0.41 |
| 10:CM:28:ARG:NH2 | 10:CM:34:VAL:HB | 2.35 | 0.41 |
| 5:CH:118:ILE:HD12 | 5:CH:118:ILE:HA | 1.92 | 0.41 |
| 29:DF:129:PHE:HA | 29:DF:142:TRP:NE1 | 2.35 | 0.41 |
| 14:CQ:15:LYS:HZ3 | 14:CQ:15:LYS:HB3 | 1.85 | 0.41 |
| 1:CA:9:G:H5' | 5:CH:122:GLU:OE2 | 2.21 | 0.41 |
| 25:DA:250:G:P | 54:D8:13:ARG:HH21 | 2.44 | 0.41 |
| 26:DB:99:A:C5 | 26:DB:100:G:C8 | 3.09 | 0.41 |
| 1:CA:671:G:C4 | 1:CA:672:U:C6 | 3.09 | 0.41 |
| 25:BA:1913:A:H4' | 25:BA:1914:C:H5'' | 2.02 | 0.41 |
| 25:DA:842:G:H2' | 25:DA:843:G:O4' | 2.19 | 0.41 |
| 26:DB:21:G:H2' | 26:DB:22:U:O4' | 2.21 | 0.41 |
| 1:CA:476:G:O2' | 1:CA:477:G:H5' | 2.19 | 0.41 |
| 49:BX:22:ALA:C | 49:BX:24:LYS:N | 2.73 | 0.41 |
| 40:D1:39:LEU:HA | 40:D1:39:LEU:HD23 | 1.89 | 0.41 |
| 17:AT:100:LYS:O | 17:AT:101:ARG:NE | 2.53 | 0.41 |
| 25:BA:1750:G:C2' | 25:BA:1751:C:H5' | 2.50 | 0.41 |
| 1:CA:393:A:C4 | 1:CA:394:G:C8 | 3.08 | 0.41 |
| 1:AA:453:A:C5 | 1:AA:454:C:C5 | 3.08 | 0.41 |
| 25:DA:1945:G:H2' | 25:DA:1946:U:H6 | 1.85 | 0.41 |
| 27:BD:223:GLY:HA3 | 27:BD:231:HIS:CE1 | 2.55 | 0.41 |
| 25:BA:36:G:C5 | 25:BA:37:C:C5 | 3.09 | 0.41 |
| 2:AE:167:PRO:HG3 | 2:AE:188:ALA:HB2 | 2.01 | 0.41 |
| 25:BA:2642:G:N2 | 25:BA:2773:C:C2 | 2.89 | 0.41 |
| 36:BP:87:LYS:O | 36:BP:89:ASN:N | 2.51 | 0.41 |
| 25:BA:2409:G:H2' | 25:BA:2410:G:O4' | 2.21 | 0.41 |
| 25:DA:46:C:H42 | 25:DA:179:G:H1 | 1.68 | 0.41 |
| 35:DO:93:GLY:O | 35:DO:123:LEU:HB2 | 2.20 | 0.41 |
| 5:AH:154:GLY:O | 5:AH:155:GLU:CB | 2.67 | 0.41 |
| 36:DP:32:TYR:CD1 | 36:DP:114:ALA:HB3 | 2.55 | 0.41 |
| 11:CN:13:GLN:HG3 | 11:CN:14:VAL:N | 2.35 | 0.41 |
| 3:AF:47:LEU:HD12 | 3:AF:47:LEU:HA | 1.78 | 0.41 |
| 13:AP:34:LEU:HA | 13:AP:34:LEU:HD22 | 1.82 | 0.41 |
| 48:BW:61:LEU:HD23 | 48:BW:61:LEU:HA | 1.78 | 0.41 |
| 25:DA:679:C:H2' | 25:DA:680:G:C8 | 2.55 | 0.41 |
| 25:BA:1057:A:C8 | 25:BA:1086:A:H2' | 2.56 | 0.41 |
| 25:BA:1813:G:H4' | 27:BD:44:ASN:O | 2.21 | 0.41 |
| 39:DR:45:PHE:CE1 | 39:DR:74:ARG:HD2 | 2.56 | 0.41 |
| 4:AG:14:ARG:HD3 | 4:AG:14:ARG:HA | 1.80 | 0.41 |
| 23:CC:23:G:C4 | 23:CC:24:C:C5 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 44:BU:79:CYS:O | 44:BU:81:LYS:HD2 | 2.20 | 0.41 |
| 10:CM:54:PHE:CE2 | 10:CM:55:LYS:CD | 3.01 | 0.41 |
| 25:DA:2579:C:H2' | 25:DA:2580:U:O4' | 2.20 | 0.41 |
| 2:CE:73:THR:O | 2:CE:74:LYS:C | 2.58 | 0.41 |
| 43:DT:43:VAL:HG11 | 43:DT:81:VAL:HG11 | 2.02 | 0.41 |
| 45:BV:5:LEU:HB3 | 45:BV:59:LEU:HA | 2.02 | 0.41 |
| 48:DW:15:LYS:HD3 | 48:DW:67:LYS:NZ | 2.36 | 0.41 |
| 34:DN:103:ALA:O | 34:DN:106:LEU:HB2 | 2.20 | 0.41 |
| 25:DA:1533:C:H3' | 25:DA:1534:G:O4' | 2.21 | 0.41 |
| 40:B1:88:ILE:HG22 | 40:B1:90:VAL:H | 1.85 | 0.41 |
| 40:B1:92:ARG:NE | 41:B2:11:GLN:H | 2.19 | 0.41 |
| 9:CL:89:ASN:N | 9:CL:89:ASN:HD22 | 2.18 | 0.41 |
| 4:AG:19:LEU:CD2 | 4:AG:21:LEU:HD12 | 2.50 | 0.41 |
| 2:AE:7:VAL:CG2 | 2:AE:8:LYS:HE2 | 2.50 | 0.41 |
| 25:BA:784:A:C8 | 25:BA:792:G:C5 | 3.09 | 0.41 |
| 25:BA:2161:C:C2' | 25:BA:2162:G:H5' | 2.50 | 0.41 |
| 5:CH:92:LYS:HG2 | 5:CH:93:PRO:HD2 | 2.02 | 0.41 |
| 26:DB:90:C:H6 | 26:DB:90:C:H5'' | 1.85 | 0.41 |
| 43:DT:44:GLU:HG2 | 43:DT:49:VAL:O | 2.20 | 0.41 |
| 25:DA:1421:G:C2 | 25:DA:1422:G:N7 | 2.89 | 0.41 |
| 38:DQ:35:ILE:HD11 | 38:DQ:101:LEU:CD2 | 2.41 | 0.41 |
| 25:BA:1471:A:C2 | 25:BA:1472:A:C4 | 3.09 | 0.41 |
| 19:CV:31:ILE:HG21 | 19:CV:33:THR:HG22 | 2.03 | 0.41 |
| 7:AJ:78:ARG:HH11 | 7:AJ:80:VAL:HG22 | 1.85 | 0.41 |
| 2:AE:165:VAL:CG2 | 2:AE:166:ASP:N | 2.82 | 0.41 |
| 9:AL:85:LEU:O | 9:AL:88:TYR:O | 2.38 | 0.41 |
| 25:DA:2602:A:H4' | 25:DA:2603:G:C5' | 2.49 | 0.41 |
| 12:AO:113:ARG:NH2 | 12:AO:120:TYR:CE1 | 2.88 | 0.41 |
| 49:BX:32:GLN:HE21 | 49:BX:32:GLN:HA | 1.86 | 0.41 |
| 22:AB:50:A:H1' | 22:AB:54:G:N2 | 2.36 | 0.41 |
| 32:DK:78:THR:HB | 32:DK:104:GLN:NE2 | 2.30 | 0.41 |
| 47:DZ:65:SER:OG | 47:DZ:66:HIS:CD2 | 2.66 | 0.41 |
| 1:CA:940:C:H2' | 1:CA:941:G:H8 | 1.85 | 0.41 |
| 46:B3:42:GLY:C | 46:B3:57:PHE:CD1 | 2.92 | 0.41 |
| 36:BP:17:LEU:HD22 | 36:BP:17:LEU:HA | 1.85 | 0.41 |
| 1:AA:877:C:H5'' | 8:AK:88:LYS:HD3 | 2.03 | 0.41 |
| 1:CA:740:U:OP2 | 15:CR:2:PRO:HA | 2.21 | 0.41 |
| 22:AB:23:A:HO2' | 22:AB:24:C:P | 2.39 | 0.41 |
| 22:CB:31:C:N3 | 22:CB:32:C:C5 | 2.88 | 0.41 |
| 8:AK:129:VAL:HG23 | 8:AK:130:GLY:N | 2.33 | 0.41 |
| 25:DA:1810:A:H2' | 25:DA:1811:G:H5' | 2.01 | 0.41 |
| 25:BA:301:G:C2 | 25:BA:302:C:N3 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:BA:412:A:N6 | 25:BA:2412:A:O4' | 2.54 | 0.41 |
| 25:BA:445:C:OP1 | 40:B1:2:PRO:HA | 2.21 | 0.41 |
| 16:AS:74:LEU:HD23 | 16:AS:74:LEU:HA | 1.94 | 0.41 |
| 25:DA:2138:C:C2 | 25:DA:2139:C:C5 | 3.08 | 0.41 |
| 25:DA:946:G:O2' | 25:DA:947:G:H5' | 2.21 | 0.41 |
| 1:AA:988:G:C2 | 1:AA:1218:C:C2 | 3.08 | 0.41 |
| 25:BA:1856:G:C2' | 25:BA:1857:G:H5' | 2.50 | 0.41 |
| 16:AS:12:LYS:HB3 | 16:AS:12:LYS:HE2 | 1.74 | 0.41 |
| 1:AA:108:G:C2 | 1:AA:109:A:C2 | 3.08 | 0.41 |
| 23:CC:54:G:O2' | 23:CC:55:U:H5' | 2.21 | 0.41 |
| 1:CA:1480:G:H2' | 1:CA:1481:U:C6 | 2.56 | 0.41 |
| 1:AA:937:A:C4 | 1:AA:938:A:C8 | 3.08 | 0.41 |
| 31:DH:35:VAL:HG12 | 31:DH:35:VAL:O | 2.21 | 0.41 |
| 1:CA:436:C:H2' | 1:CA:437:U:H6 | 1.84 | 0.41 |
| 25:DA:1870:C:N4 | 25:DA:1871:A:C6 | 2.89 | 0.41 |
| 23:AC:54:G:O2' | 23:AC:55:U:H5' | 2.21 | 0.41 |
| 1:CA:101:A:C2' | 1:CA:102:G:H5' | 2.50 | 0.41 |
| 1:CA:89:U:C4' | 1:CA:90:C:OP1 | 2.68 | 0.41 |
| 1:AA:1157:A:O2' | 1:AA:1158:C:C2 | 2.62 | 0.41 |
| 54:D8:50:LEU:N | 54:D8:50:LEU:CD1 | 2.79 | 0.41 |
| 23:AC:77:A:H5' | 23:AC:77:A:H8 | 1.85 | 0.41 |
| 23:AC:76:C:C5' | 23:AC:77:A:OP2 | 2.50 | 0.41 |
| 43:DT:40:LYS:HG3 | 43:DT:51:VAL:HG11 | 2.03 | 0.41 |
| 45:BV:59:LEU:O | 45:BV:60:GLU:C | 2.59 | 0.41 |
| 44:DU:98:VAL:CG1 | 44:DU:99:CYS:H | 2.29 | 0.41 |
| 31:BH:30:LYS:HG3 | 31:BH:79:VAL:O | 2.21 | 0.41 |
| 25:DA:527:C:OP2 | 25:DA:2779:U:C5 | 2.60 | 0.41 |
| 26:DB:46:A:H2' | 26:DB:47:C:H6 | 1.86 | 0.41 |
| 20:AW:72:LEU:HD21 | 20:AW:77:ALA:N | 2.36 | 0.41 |
| 2:AE:8:LYS:HG2 | 2:AE:11:LEU:H | 1.85 | 0.41 |
| 25:DA:2157:G:O2' | 25:DA:2158:A:O4' | 2.27 | 0.41 |
| 25:DA:2173:A:H5' | 25:DA:2174:C:OP2 | 2.20 | 0.41 |
| 1:CA:1297:C:OP2 | 1:CA:1297:C:H6 | 2.04 | 0.41 |
| 25:BA:2163:C:C5 | 25:BA:2164:C:C5 | 3.08 | 0.41 |
| 15:AR:56:LEU:HD12 | 15:AR:56:LEU:O | 2.20 | 0.41 |
| 34:DN:22:ILE:HG22 | 34:DN:23:ARG:N | 2.36 | 0.41 |
| 16:CS:8:ARG:HD2 | 16:CS:17:TYR:HE2 | 1.85 | 0.41 |
| 26:DB:90:C:O5' | 36:DP:17:LEU:O | 2.38 | 0.41 |
| 1:AA:397:A:N6 | 1:AA:548:G:N7 | 2.69 | 0.41 |
| 35:DO:47:ASP:O | 35:DO:48:PRO:C | 2.59 | 0.41 |
| 25:BA:1535:U:N3 | 25:BA:1537:C:O4' | 2.52 | 0.41 |
| 1:CA:389:A:H2' | 1:CA:389:A:N3 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:2387:U:H5' | 25:DA:2388:A:OP2 | 2.20 | 0.41 |
| 1:CA:1069:C:HO2' | 1:CA:1192:C:H1' | 1.86 | 0.41 |
| 1:CA:1192:C:N4 | 1:CA:1193:G:C5 | 2.89 | 0.41 |
| 4:AG:155:LEU:O | 4:AG:156:GLU:C | 2.59 | 0.41 |
| 1:CA:1089:G:C6 | 1:CA:1090:U:C4 | 3.08 | 0.41 |
| 2:AE:72:GLY:CA | 2:AE:165:VAL:HG22 | 2.50 | 0.41 |
| 25:BA:847:U:H5' | 25:BA:848:G:OP2 | 2.21 | 0.41 |
| 1:AA:1309:G:C5 | 1:AA:1329:A:C2 | 3.09 | 0.41 |
| 1:AA:186(F):C:H2' | 1:AA:187:C:O4' | 2.21 | 0.41 |
| 27:DD:132:PRO:HD3 | 27:DD:190:TYR:CZ | 2.55 | 0.41 |
| 1:CA:1347:G:C5 | 9:CL:107:ARG:NH2 | 2.89 | 0.41 |
| 25:DA:204:A:H5' | 25:DA:206:U:H1' | 2.02 | 0.41 |
| 23:AD:13:C:C2' | 23:AD:14:A:OP1 | 2.68 | 0.41 |
| 25:DA:511:U:H4' | 25:DA:1235:G:H4' | 2.02 | 0.41 |
| 25:DA:12:U:O2 | 25:DA:12:U:C2' | 2.64 | 0.41 |
| 1:CA:862:C:C2 | 1:CA:863:U:C6 | 3.08 | 0.41 |
| 1:AA:103:C:C2 | 1:AA:104:G:C8 | 3.09 | 0.41 |
| 25:BA:404:C:C2' | 25:BA:405:U:OP2 | 2.68 | 0.41 |
| 1:AA:428:G:C5 | 1:AA:430:A:C6 | 3.08 | 0.41 |
| 2:AE:224:GLN:HB2 | 2:AE:229:VAL:HG23 | 2.02 | 0.41 |
| 1:AA:674:G:H2' | 1:AA:675:A:H8 | 1.84 | 0.41 |
| 25:BA:1446:C:H2' | 25:BA:1447:G:O5' | 2.20 | 0.41 |
| 39:BR:93:ARG:NH1 | 39:BR:93:ARG:HG3 | 2.32 | 0.41 |
| 25:DA:988:A:C2' | 25:DA:989:G:O5' | 2.69 | 0.41 |
| 25:DA:988:A:H3' | 49:DX:11:SER:HG | 1.84 | 0.41 |
| 3:CF:27:LYS:HB3 | 3:CF:27:LYS:HZ3 | 1.84 | 0.41 |
| 25:DA:565:C:H4' | 25:DA:1253:A:C6 | 2.55 | 0.41 |
| 5:CH:107:ARG:HG2 | 5:CH:108:ALA:H | 1.83 | 0.41 |
| 16:CS:81:ARG:O | 16:CS:81:ARG:HG3 | 2.20 | 0.41 |
| 23:AD:11:A:N1 | 23:AD:26:C:C2 | 2.89 | 0.41 |
| 44:DU:46:LYS:O | 44:DU:47:LYS:C | 2.58 | 0.41 |
| 31:BH:102:ALA:HB2 | 31:BH:116:GLU:HB2 | 2.03 | 0.41 |
| 50:D4:38:LYS:C | 50:D4:40:HIS:N | 2.74 | 0.41 |
| 25:DA:278:A:O2' | 25:DA:279:C:P | 2.78 | 0.41 |
| 31:DH:94:TYR:CZ | 31:DH:107:VAL:O | 2.74 | 0.41 |
| 5:CH:33:VAL:HG12 | 5:CH:34:VAL:N | 2.35 | 0.41 |
| 29:BF:191:ARG:HH11 | 29:BF:191:ARG:HB3 | 1.86 | 0.41 |
| 3:AF:34:LEU:HD21 | 3:AF:38:ARG:NH1 | 2.33 | 0.41 |
| 25:BA:638:G:H2' | 25:BA:639:U:O4' | 2.19 | 0.41 |
| 1:CA:34:C:O2' | 1:CA:35:G:H5' | 2.20 | 0.41 |
| 30:BG:26:GLN:HG3 | 30:BG:30:GLU:OE2 | 2.20 | 0.41 |
| 1:AA:258:G:H2' | 1:AA:259:G:C8 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:BA:2607:G:H2' | 25:BA:2608:G:O4' | 2.21 | 0.41 |
| 29:DF:72:ARG:HH11 | 29:DF:72:ARG:HB3 | 1.86 | 0.41 |
| 25:BA:910:A:C5 | 36:BP:13:GLN:HG3 | 2.56 | 0.41 |
| 25:BA:2492:U:H2' | 25:BA:2493:U:H6 | 1.85 | 0.41 |
| 43:BT:26:TYR:O | 43:BT:81:VAL:HG12 | 2.21 | 0.41 |
| 29:DF:206:ILE:HG13 | 29:DF:206:ILE:O | 2.19 | 0.41 |
| 8:AK:94:TYR:HD1 | 8:AK:132:GLU:HA | 1.86 | 0.41 |
| 25:DA:991:C:O2 | 25:DA:1164:G:C2 | 2.74 | 0.41 |
| 27:BD:269:PHE:N | 27:BD:269:PHE:CD2 | 2.89 | 0.41 |
| 41:D2:62:LEU:HB2 | 41:D2:93:GLU:O | 2.21 | 0.41 |
| 46:B3:32:ARG:HB3 | 46:B3:32:ARG:HE | 1.67 | 0.41 |
| 25:DA:405:U:C2' | 25:DA:405:U:O2 | 2.68 | 0.41 |
| 25:DA:2464:C:H2' | 25:DA:2465:C:O4' | 2.20 | 0.41 |
| 1:CA:1294:G:O2' | 1:CA:1295:G:H5' | 2.21 | 0.41 |
| 30:BG:44:GLY:O | 30:BG:47:LYS:HE2 | 2.21 | 0.41 |
| 25:BA:809:G:O4' | 25:BA:1254:A:H1' | 2.21 | 0.41 |
| 25:DA:1932:A:H2' | 25:DA:1933:G:O4' | 2.21 | 0.41 |
| 1:CA:1076:C:C2 | 1:CA:1082:G:N2 | 2.89 | 0.41 |
| 25:DA:1424:G:H2' | 25:DA:1425:G:O4' | 2.21 | 0.41 |
| 39:BR:6:LEU:HA | 39:BR:9:LEU:HB2 | 2.01 | 0.41 |
| 25:BA:1195:G:N3 | 25:BA:1227:A:H2 | 2.18 | 0.41 |
| 2:AE:177:ALA:HB1 | 2:AE:182:ILE:HB | 2.02 | 0.41 |
| 20:CW:94:ALA:O | 20:CW:95:ALA:HB2 | 2.20 | 0.41 |
| 25:BA:2059:A:O2' | 29:BF:69:HIS:HD2 | 2.03 | 0.41 |
| 1:AA:781:A:H4' | 1:AA:1522:U:O2' | 2.20 | 0.41 |
| 25:DA:1198:U:H2' | 25:DA:1199:U:C6 | 2.55 | 0.41 |
| 28:DE:181:LEU:HD11 | 39:DR:7:ILE:HD12 | 2.01 | 0.41 |
| 25:BA:466:A:N3 | 25:BA:683:C:H1' | 2.36 | 0.41 |
| 25:BA:2082:A:H2' | 25:BA:2083:G:O4' | 2.21 | 0.41 |
| 31:BH:13:LYS:HA | 31:BH:13:LYS:HE2 | 2.03 | 0.41 |
| 25:DA:944:G:H2' | 25:DA:944:G:N3 | 2.36 | 0.41 |
| 1:AA:1381:U:H2' | 1:AA:1381:U:O2 | 2.21 | 0.41 |
| 18:CU:25:THR:O | 18:CU:25:THR:HG22 | 2.20 | 0.41 |
| 37:D0:29:LEU:HA | 37:D0:29:LEU:HD12 | 1.93 | 0.41 |
| 37:B0:92:GLY:N | 37:B0:94:TYR:CE2 | 2.89 | 0.41 |
| 25:BA:2166:G:C2' | 25:BA:2167:U:OP1 | 2.69 | 0.41 |
| 25:DA:681:G:H2' | 25:DA:682:G:O4' | 2.20 | 0.41 |
| 30:BG:70:VAL:HA | 30:BG:90:LEU:HD12 | 2.02 | 0.41 |
| 25:BA:2467:C:N4 | 25:BA:2468:G:C6 | 2.89 | 0.41 |
| 1:AA:1162:C:C2 | 1:AA:1175:G:N2 | 2.89 | 0.41 |
| 27:BD:35:LYS:HG2 | 27:BD:64:ILE:CA | 2.50 | 0.41 |
| 16:AS:25:ARG:HG2 | 16:AS:25:ARG:H | 1.61 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:588:U:H1' | 29:DF:90:PHE:HB3 | 2.03 | 0.41 |
| 1:AA:1124:G:O2' | 10:AM:38:ILE:HD13 | 2.21 | 0.41 |
| 25:DA:674:G:O2' | 29:DF:67:GLN:OE1 | 2.27 | 0.41 |
| 26:BB:42:C:H4' | 30:BG:67:LYS:CD | 2.51 | 0.41 |
| 27:DD:26:LYS:N | 27:DD:26:LYS:HE3 | 2.36 | 0.41 |
| 1:CA:980:C:C5 | 1:CA:981:U:C2 | 3.09 | 0.41 |
| 1:AA:1305:G:OP1 | 21:AX:2:GLY:HA3 | 2.21 | 0.41 |
| 25:DA:2415:G:C5 | 25:DA:2416:C:C4 | 3.09 | 0.41 |
| 52:B6:40:CYS:CA | 52:B6:46:HIS:HA | 2.40 | 0.41 |
| 1:CA:1060:C:C2 | 1:CA:1198:G:C2 | 3.09 | 0.41 |
| 36:BP:34:LEU:HD23 | 36:BP:104:PHE:CD1 | 2.56 | 0.41 |
| 25:DA:1140:C:C4' | 25:DA:1143:A:N7 | 2.84 | 0.41 |
| 1:CA:328:C:C2' | 1:CA:329:A:OP2 | 2.68 | 0.41 |
| 45:BV:61:LEU:HA | 45:BV:62:PRO:HD3 | 1.95 | 0.41 |
| 1:CA:1234:C:C2' | 1:CA:1235:U:H5' | 2.50 | 0.41 |
| 1:CA:630:G:H5' | 1:CA:631:G:OP2 | 2.21 | 0.41 |
| 1:CA:1128:C:C4 | 1:CA:1139:G:N1 | 2.89 | 0.41 |
| 11:CN:29:ILE:HG22 | 11:CN:44:SER:CB | 2.37 | 0.41 |
| 10:CM:78:ASN:HB3 | 10:CM:80:LYS:HB3 | 2.03 | 0.41 |
| 32:BK:99:GLU:O | 32:BK:100:ALA:C | 2.59 | 0.41 |
| 25:DA:888:C:C4' | 25:DA:889:C:OP2 | 2.69 | 0.41 |
| 1:AA:1303:C:N4 | 1:AA:1304:G:C6 | 2.89 | 0.41 |
| 2:AE:5:ILE:CG2 | 2:AE:221:LEU:HD23 | 2.50 | 0.41 |
| 33:BM:23:LEU:C | 33:BM:23:LEU:HD12 | 2.41 | 0.41 |
| 24:C1:13:U:O2 | 24:C1:13:U:C2' | 2.52 | 0.41 |
| 31:BH:152:ARG:C | 31:BH:153:LYS:HD2 | 2.41 | 0.41 |
| 31:BH:153:LYS:HG3 | 31:BH:161:GLY:CA | 2.50 | 0.41 |
| 25:DA:2410:G:N3 | 25:DA:2411:A:H1' | 2.35 | 0.41 |
| 25:DA:654(A):A:N1 | 25:DA:654(T):A:N1 | 2.69 | 0.41 |
| 3:CF:134:ILE:CG2 | 3:CF:168:ALA:HB3 | 2.41 | 0.41 |
| 18:AU:76:LEU:HA | 18:AU:76:LEU:HD22 | 1.87 | 0.41 |
| 25:DA:1483:G:C6 | 25:DA:1507:A:C2 | 3.09 | 0.41 |
| 25:BA:1265:A:OP1 | 25:BA:1265:A:H8 | 2.04 | 0.41 |
| 33:BM:57:ALA:O | 33:BM:58:ASP:OD1 | 2.39 | 0.41 |
| 36:DP:1:MET:HB3 | 36:DP:69:PHE:HE1 | 1.85 | 0.41 |
| 25:DA:322:A:H5' | 25:DA:340:A:C1' | 2.47 | 0.41 |
| 1:CA:828:A:H61 | 1:CA:858:G:C2' | 2.34 | 0.41 |
| 28:BE:92:THR:H | 28:BE:95:ILE:HD11 | 1.86 | 0.41 |
| 25:BA:1889:A:N1 | 25:BA:2234:G:H1' | 2.36 | 0.41 |
| 28:DE:11:MET:HG3 | 28:DE:24:THR:CA | 2.50 | 0.41 |
| 20:CW:53:LEU:HD21 | 20:CW:92:LEU:HD11 | 2.02 | 0.41 |
| 1:CA:932:C:H2' | 1:CA:932:C:O2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|---------------------|-------------|----------|
| 32:BK:21:VAL:HG22 | 32:BK:22:LYS:H | 1.85 | 0.41 |
| 31:DH:120:GLY:O | 31:DH:121:ILE:HD13 | 2.21 | 0.41 |
| 25:BA:1449:A:C5' | 25:BA:1449(A):G:OP2 | 2.68 | 0.41 |
| 43:DT:57:LEU:N | 43:DT:57:LEU:CD2 | 2.81 | 0.41 |
| 23:AC:48:U:H1' | 23:AC:49:C:OP2 | 2.21 | 0.41 |
| 23:AD:29:C:O2' | 23:AD:30:G:H5' | 2.21 | 0.41 |
| 25:DA:1190:G:H2' | 25:DA:1191:G:C8 | 2.51 | 0.41 |
| 25:DA:817:C:O2' | 25:DA:839:U:H5'' | 2.21 | 0.41 |
| 25:DA:898:C:H3' | 25:DA:899:A:H5'' | 2.03 | 0.41 |
| 1:AA:1180:A:H8 | 1:AA:1180:A:O5' | 2.03 | 0.41 |
| 25:DA:771:G:OP1 | 53:D7:10:ARG:HD3 | 2.21 | 0.41 |
| 25:BA:1952:A:C6 | 34:BN:22:ILE:HD11 | 2.56 | 0.41 |
| 2:CE:179:LYS:HA | 8:CK:72:PRO:HG3 | 2.03 | 0.41 |
| 26:BB:81:G:H2' | 26:BB:82:G:C5' | 2.50 | 0.41 |
| 25:BA:943:U:OP2 | 35:BO:36:LYS:CG | 2.68 | 0.41 |
| 2:AE:130:ARG:HA | 2:AE:131:PRO:HD3 | 1.91 | 0.41 |
| 1:AA:184:G:H2' | 1:AA:185:A:C8 | 2.56 | 0.41 |
| 25:BA:1914:C:O5' | 25:BA:1914:C:O2 | 2.39 | 0.41 |
| 41:B2:18:LEU:HD22 | 41:B2:19:LYS:N | 2.35 | 0.41 |
| 1:CA:161:A:N6 | 1:CA:162:A:C6 | 2.88 | 0.41 |
| 31:DH:35:VAL:HG11 | 31:DH:71:LEU:HG | 2.02 | 0.41 |
| 7:AJ:54:THR:OG1 | 7:AJ:56:GLN:HG2 | 2.21 | 0.41 |
| 1:AA:61:G:H2' | 1:AA:62:U:O4' | 2.21 | 0.41 |
| 25:DA:1401:G:H2' | 25:DA:1402:C:O4' | 2.21 | 0.41 |
| 25:DA:1130:U:C2 | 25:DA:2025:C:H5'' | 2.56 | 0.41 |
| 1:CA:675:A:H1' | 11:CN:116:HIS:CG | 2.55 | 0.41 |
| 1:CA:1258:G:O2' | 1:CA:1259:C:H5' | 2.21 | 0.41 |
| 25:BA:738:G:C6 | 25:BA:739:G:C2 | 3.09 | 0.41 |
| 13:AP:86:CYS:HB2 | 19:AV:73:GLU:HB3 | 2.03 | 0.41 |
| 8:AK:56:LYS:HA | 8:AK:57:PRO:HD2 | 1.95 | 0.41 |
| 30:DG:103:LEU:O | 30:DG:106:LEU:HB3 | 2.21 | 0.41 |
| 1:CA:1394:A:H4' | 1:CA:1395:C:OP2 | 2.20 | 0.41 |
| 44:BU:54:LYS:O | 44:BU:55:TYR:HB2 | 2.21 | 0.41 |
| 16:CS:82:GLN:HG2 | 16:CS:82:GLN:H | 1.54 | 0.41 |
| 25:BA:1056:G:C2 | 25:BA:1103:A:N6 | 2.68 | 0.41 |
| 35:BO:62:LEU:O | 35:BO:62:LEU:HD23 | 2.21 | 0.41 |
| 25:DA:2393:A:H2' | 25:DA:2394:C:O4' | 2.20 | 0.41 |
| 38:DQ:106:ARG:HA | 38:DQ:110:LEU:CG | 2.51 | 0.41 |
| 38:DQ:104:GLY:C | 38:DQ:106:ARG:H | 2.24 | 0.41 |
| 38:DQ:107:GLU:H | 38:DQ:110:LEU:HG | 1.86 | 0.41 |
| 25:DA:1225:C:O2' | 41:D2:85:LYS:HB2 | 2.21 | 0.41 |
| 27:BD:34:VAL:HG21 | 27:BD:103:ARG:HA | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 27:BD:64:ILE:HG21 | 27:BD:64:ILE:HD13 | 1.75 | 0.41 |
| 1:CA:1022:G:C6 | 1:CA:1023:G:C5 | 3.09 | 0.41 |
| 25:BA:2415:G:C4' | 35:BO:66:GLY:HA3 | 2.47 | 0.41 |
| 1:AA:1131:G:C2' | 1:AA:1132:C:H5' | 2.51 | 0.41 |
| 23:AD:5:G:N2 | 23:AD:70:C:C4 | 2.78 | 0.41 |
| 44:BU:81:LYS:HB3 | 44:BU:82:PRO:O | 2.21 | 0.41 |
| 27:DD:83:GLU:HB2 | 27:DD:92:ILE:HG13 | 2.03 | 0.41 |
| 1:AA:1330:U:O4 | 1:AA:1331:G:C2 | 2.74 | 0.41 |
| 25:DA:2415:G:C4' | 35:DO:66:GLY:HA3 | 2.48 | 0.41 |
| 1:CA:1052:U:C5' | 1:CA:1053:G:OP2 | 2.69 | 0.41 |
| 1:CA:962:C:H2' | 1:CA:963:G:O4' | 2.21 | 0.41 |
| 36:BP:85:LYS:HG2 | 36:BP:86:GLY:H | 1.86 | 0.41 |
| 29:BF:197:ASP:OD2 | 29:BF:197:ASP:N | 2.52 | 0.41 |
| 29:BF:101:LEU:HA | 29:BF:101:LEU:HD12 | 1.81 | 0.41 |
| 1:AA:1004:A:C5 | 1:AA:1025:U:H1' | 2.55 | 0.41 |
| 24:C1:19:U:H2' | 24:C1:20:U:H6 | 1.86 | 0.41 |
| 1:CA:515:G:H2' | 1:CA:516:U:O4' | 2.21 | 0.41 |
| 19:AV:40:ILE:O | 19:AV:41:VAL:CG2 | 2.69 | 0.41 |
| 19:AV:41:VAL:O | 50:B4:63:TYR:CE1 | 2.74 | 0.41 |
| 43:DT:51:VAL:O | 43:DT:51:VAL:HG12 | 2.20 | 0.41 |
| 25:BA:442:G:N3 | 29:BF:48:THR:HG23 | 2.35 | 0.41 |
| 1:AA:55:A:C6 | 32:DK:89:TYR:CD1 | 3.09 | 0.41 |
| 25:DA:1012:U:N3 | 33:DM:25:ARG:HD3 | 2.36 | 0.41 |
| 39:DR:90:GLN:NE2 | 39:DR:90:GLN:HA | 2.25 | 0.41 |
| 51:D5:56:LYS:HA | 51:D5:56:LYS:HD2 | 1.67 | 0.41 |
| 25:BA:882:G:H1 | 25:BA:894:C:N4 | 2.19 | 0.41 |
| 29:DF:29:ASN:HA | 29:DF:30:PRO:HD3 | 1.90 | 0.41 |
| 29:DF:25:PRO:C | 29:DF:27:GLU:N | 2.74 | 0.41 |
| 1:CA:992:U:C2' | 1:CA:993:G:OP2 | 2.69 | 0.41 |
| 23:CD:15:G:C2' | 23:CD:15:G:N3 | 2.83 | 0.41 |
| 1:CA:1132:C:H2' | 1:CA:1133:G:O4' | 2.20 | 0.41 |
| 17:AT:68:ARG:O | 17:AT:68:ARG:HG3 | 2.19 | 0.41 |
| 26:DB:37:C:C5 | 26:DB:38:C:C5 | 3.09 | 0.41 |
| 1:CA:265:G:H5' | 17:CT:64:PRO:O | 2.20 | 0.41 |
| 25:BA:2554:U:H2' | 25:BA:2555:U:C6 | 2.55 | 0.41 |
| 25:DA:309:G:O3' | 44:DU:18:GLY:HA3 | 2.21 | 0.41 |
| 1:CA:345:C:O2 | 1:CA:346:G:N2 | 2.54 | 0.41 |
| 44:BU:52:SER:CB | 44:BU:53:PRO:HD3 | 2.51 | 0.41 |
| 32:BK:77:LEU:CD1 | 32:BK:140:LEU:HB2 | 2.51 | 0.41 |
| 25:BA:997:G:OP1 | 40:B1:93:LYS:HD2 | 2.21 | 0.41 |
| 1:AA:1301:U:C4 | 1:AA:1303:C:N1 | 2.89 | 0.41 |
| 25:DA:71:A:H5'' | 25:DA:73:A:C8 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 9:CL:47:LEU:C | 9:CL:49:PRO:HD2 | 2.41 | 0.41 |
| 5:CH:79:GLU:HB3 | 5:CH:92:LYS:HG3 | 2.02 | 0.41 |
| 25:DA:857:C:C6 | 25:DA:858:U:H5 | 2.39 | 0.41 |
| 26:DB:89(A):A:N7 | 26:DB:90:C:H1' | 2.35 | 0.41 |
| 25:DA:2873:A:H2' | 25:DA:2873:A:N3 | 2.36 | 0.41 |
| 19:CV:16:LEU:O | 19:CV:20:LEU:HD23 | 2.21 | 0.41 |
| 25:BA:2135:A:C2' | 25:BA:2136:C:O5' | 2.68 | 0.41 |
| 25:BA:1331:A:HO2' | 25:BA:1332:G:H8 | 1.67 | 0.41 |
| 13:CP:3:ARG:HB2 | 50:D4:34:GLU:CD | 2.41 | 0.41 |
| 2:CE:71:VAL:HB | 2:CE:164:VAL:HG13 | 2.03 | 0.41 |
| 16:CS:3:LYS:HG3 | 16:CS:24:ALA:HB2 | 2.03 | 0.41 |
| 35:DO:101:VAL:HG12 | 35:DO:102:ARG:N | 2.36 | 0.41 |
| 23:CD:5:G:N2 | 23:CD:70:C:C2 | 2.89 | 0.41 |
| 46:D3:19:LYS:HG3 | 46:D3:41:ARG:HH12 | 1.86 | 0.41 |
| 45:BV:164:ALA:C | 45:BV:165:VAL:CG1 | 2.76 | 0.41 |
| 1:CA:1068:G:N7 | 1:CA:1094:G:N7 | 2.68 | 0.41 |
| 12:CO:60:LEU:CD2 | 12:CO:66:VAL:HG22 | 2.51 | 0.41 |
| 5:CH:70:PRO:HB3 | 5:CH:144:THR:CG2 | 2.46 | 0.41 |
| 4:AG:119:GLN:HG3 | 4:AG:123:HIS:CD2 | 2.56 | 0.41 |
| 54:B8:58:ILE:HA | 54:B8:61:LEU:HG | 2.03 | 0.41 |
| 35:BO:49:ARG:HD2 | 54:B8:58:ILE:CG2 | 2.51 | 0.41 |
| 25:BA:141:A:H1' | 25:BA:1408:C:O4' | 2.20 | 0.41 |
| 1:AA:545:C:O2' | 1:AA:549:C:H5'' | 2.21 | 0.41 |
| 2:AE:210:SER:O | 2:AE:214:ILE:HG13 | 2.20 | 0.41 |
| 25:DA:1651:G:OP1 | 37:D0:40:LYS:HE2 | 2.21 | 0.41 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:C2 | 2.38 | 0.41 |
| 36:DP:7:MET:HB3 | 36:DP:10:ARG:NH1 | 2.36 | 0.41 |
| 3:AF:150:LYS:HE3 | 3:AF:152:ILE:CD1 | 2.51 | 0.41 |
| 1:AA:46:G:H2' | 1:AA:366:C:H5 | 1.85 | 0.41 |
| 45:DV:59:LEU:O | 45:DV:60:GLU:CB | 2.68 | 0.41 |
| 30:BG:115:ARG:HG2 | 30:BG:115:ARG:H | 1.67 | 0.41 |
| 1:CA:407:G:H2' | 1:CA:408:A:H8 | 1.83 | 0.41 |
| 45:BV:121:HIS:C | 45:BV:123:ASP:H | 2.24 | 0.41 |
| 1:AA:198:G:O6 | 1:AA:220:G:C6 | 2.74 | 0.41 |
| 23:AD:21:U:H3' | 23:AD:22:A:H5' | 2.02 | 0.41 |
| 25:BA:559:G:N2 | 40:B1:49:HIS:CD2 | 2.82 | 0.41 |
| 19:AV:32:LYS:HA | 19:AV:50:ALA:HB3 | 2.03 | 0.41 |
| 31:BH:115:VAL:HG11 | 31:BH:148:ILE:CG1 | 2.49 | 0.41 |
| 1:CA:859:A:H2' | 1:CA:860:A:O4' | 2.21 | 0.41 |
| 25:BA:1048:A:N3 | 25:BA:1048:A:H2' | 2.36 | 0.41 |
| 36:DP:68:ILE:HD13 | 36:DP:103:MET:CB | 2.47 | 0.41 |
| 32:DK:97:ILE:CD1 | 32:DK:140:LEU:HD22 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 31:DH:20:ALA:O | 31:DH:22:GLY:N | 2.49 | 0.41 |
| 25:BA:2864:G:OP1 | 39:BR:119:LYS:HD2 | 2.21 | 0.41 |
| 25:BA:2591:C:OP1 | 27:BD:239:ARG:HG3 | 2.20 | 0.41 |
| 1:CA:464:G:C6 | 1:CA:466:C:H5' | 2.56 | 0.41 |
| 1:CA:1379:G:C2' | 1:CA:1380:U:H5' | 2.51 | 0.41 |
| 1:CA:932:C:N4 | 7:CJ:3:ARG:NH2 | 2.69 | 0.41 |
| 1:CA:1378:C:C5 | 1:CA:1379:G:C4 | 3.02 | 0.41 |
| 24:A1:14:U:HO2' | 24:A1:15:U:C4' | 2.34 | 0.41 |
| 25:BA:1652:A:H2' | 25:BA:1653:G:H5' | 2.03 | 0.41 |
| 53:B7:47:ARG:HB2 | 53:B7:48:LYS:H | 1.64 | 0.41 |
| 25:DA:1599:C:C2 | 25:DA:1600:C:C5 | 3.09 | 0.41 |
| 1:CA:1206:G:O6 | 1:CA:1207:G:C6 | 2.73 | 0.41 |
| 25:DA:2819:G:H2' | 25:DA:2821:A:N7 | 2.35 | 0.41 |
| 25:DA:986:C:H2' | 25:DA:987:G:C5' | 2.49 | 0.41 |
| 45:DV:117:LEU:HD13 | 45:DV:117:LEU:HA | 1.78 | 0.41 |
| 16:AS:50:LYS:HD3 | 16:AS:50:LYS:C | 2.40 | 0.41 |
| 38:BQ:111:GLU:CA | 38:BQ:111:GLU:OE1 | 2.66 | 0.41 |
| 1:AA:8:A:H5' | 5:AH:101:ILE:CG2 | 2.49 | 0.41 |
| 1:AA:148:G:H2' | 1:AA:149:A:H8 | 1.85 | 0.41 |
| 25:DA:2745:C:O2' | 31:DH:142:GLY:HA3 | 2.21 | 0.41 |
| 30:DG:11:TYR:CE2 | 30:DG:16:ARG:HD2 | 2.56 | 0.41 |
| 25:DA:2517:C:N3 | 25:DA:2542:A:N6 | 2.69 | 0.41 |
| 32:BK:135:GLU:CD | 32:BK:135:GLU:N | 2.74 | 0.41 |
| 1:AA:136:C:N4 | 1:AA:227:G:H1 | 2.18 | 0.41 |
| 12:CO:35:GLY:HA3 | 12:CO:58:VAL:CG1 | 2.50 | 0.41 |
| 25:BA:1586:A:N3 | 25:BA:1586:A:O4' | 2.53 | 0.41 |
| 22:AB:45:U:C6 | 22:AB:45:U:C3' | 3.03 | 0.41 |
| 25:DA:868:U:N3 | 25:DA:869:G:N7 | 2.69 | 0.41 |
| 22:CB:31:C:C4 | 22:CB:32:C:H5 | 2.39 | 0.41 |
| 25:DA:1859:A:C2 | 25:DA:1884:A:H1' | 2.56 | 0.41 |
| 25:DA:5:A:C2 | 25:DA:2899:G:C2 | 3.09 | 0.41 |
| 25:BA:975:G:H1' | 25:BA:990:A:C2 | 2.55 | 0.41 |
| 25:BA:981:A:H1' | 25:BA:2037:G:O4' | 2.21 | 0.41 |
| 44:DU:89:PHE:HD1 | 44:DU:90:LEU:CD2 | 2.34 | 0.41 |
| 1:CA:577:G:H2' | 1:CA:578:C:C6 | 2.56 | 0.41 |
| 6:AI:61:LEU:HD23 | 6:AI:63:TYR:OH | 2.21 | 0.41 |
| 1:CA:1413:A:C2 | 1:CA:1488:G:C2 | 3.09 | 0.41 |
| 30:DG:70:VAL:HA | 30:DG:90:LEU:HD12 | 2.02 | 0.41 |
| 1:CA:1349:A:C2' | 1:CA:1350:A:O5' | 2.69 | 0.41 |
| 25:DA:2698:U:H2' | 25:DA:2699:C:H6 | 1.85 | 0.41 |
| 18:AU:88:LYS:HB3 | 18:AU:88:LYS:HZ3 | 1.85 | 0.41 |
| 1:CA:1106:G:C4 | 1:CA:1107:C:C5 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 1:CA:373:A:H2' | 1:CA:374:A:H8 | 1.86 | 0.41 |
| 25:DA:2103:C:O2' | 25:DA:2104:G:H5' | 2.21 | 0.41 |
| 25:DA:1686:C:C2 | 25:DA:1703:G:N2 | 2.89 | 0.41 |
| 25:BA:728:G:H4' | 27:BD:13:ARG:HD3 | 2.03 | 0.41 |
| 25:DA:2593:U:C2 | 25:DA:2594:C:C5 | 3.09 | 0.41 |
| 25:BA:2839:G:H2' | 25:BA:2840:C:C6 | 2.56 | 0.41 |
| 8:CK:95:VAL:HG22 | 8:CK:131:GLY:O | 2.20 | 0.41 |
| 25:BA:2815:C:H2' | 25:BA:2816:C:C6 | 2.54 | 0.41 |
| 35:BO:96:THR:C | 35:BO:98:GLU:N | 2.74 | 0.41 |
| 3:AF:69:HIS:HA | 3:AF:104:GLN:O | 2.20 | 0.41 |
| 27:DD:9:TYR:HD2 | 27:DD:10:THR:HG23 | 1.86 | 0.41 |
| 13:CP:73:GLU:OE2 | 50:D4:52:THR:HG21 | 2.21 | 0.41 |
| 4:CG:111:ALA:HB2 | 4:CG:120:LEU:HD12 | 2.03 | 0.41 |
| 25:BA:1578:U:O2 | 25:BA:1578:U:H2' | 2.21 | 0.41 |
| 3:CF:52:LEU:N | 3:CF:52:LEU:HD23 | 2.36 | 0.41 |
| 25:DA:2093:G:O5' | 32:DK:24:GLY:HA3 | 2.21 | 0.41 |
| 25:BA:2598:A:C2' | 25:BA:2599:G:O5' | 2.69 | 0.41 |
| 9:CL:11:LYS:HG2 | 9:CL:11:LYS:O | 2.21 | 0.41 |
| 1:AA:775:G:C2' | 1:AA:776:G:H5' | 2.51 | 0.41 |
| 35:DO:125:VAL:HG13 | 35:DO:144:GLU:HB3 | 2.01 | 0.41 |
| 1:CA:864:A:C2 | 1:CA:917:G:N3 | 2.89 | 0.41 |
| 1:CA:1483:A:H8 | 1:CA:1483:A:O5' | 2.02 | 0.41 |
| 25:BA:1824:G:N3 | 27:BD:254:THR:OG1 | 2.54 | 0.41 |
| 36:DP:42:ILE:N | 36:DP:42:ILE:HD12 | 2.36 | 0.41 |
| 18:CU:84:LYS:HE2 | 18:CU:84:LYS:CA | 2.50 | 0.41 |
| 3:AF:43:LEU:O | 3:AF:47:LEU:HB2 | 2.20 | 0.41 |
| 25:DA:1223:C:C2' | 25:DA:1224:G:H5' | 2.50 | 0.41 |
| 1:CA:1423:G:H2' | 1:CA:1424:C:C6 | 2.56 | 0.41 |
| 25:BA:1637:A:H4' | 25:BA:2711:A:O2' | 2.21 | 0.41 |
| 25:BA:2805:G:H5'' | 25:BA:2807:G:OP2 | 2.21 | 0.41 |
| 25:BA:830:G:H4' | 25:BA:831:G:OP2 | 2.21 | 0.41 |
| 34:BN:34:THR:HG22 | 34:BN:37:ASP:OD2 | 2.20 | 0.41 |
| 41:B2:53:GLU:O | 41:B2:53:GLU:HG2 | 2.21 | 0.41 |
| 25:DA:1029:A:H8 | 25:DA:1029:A:O5' | 2.03 | 0.41 |
| 1:AA:1290:G:N3 | 1:AA:1290:G:H2' | 2.36 | 0.41 |
| 7:CJ:60:LYS:HA | 7:CJ:60:LYS:HD2 | 1.90 | 0.41 |
| 25:DA:1113:U:H2' | 25:DA:1114:G:C8 | 2.56 | 0.41 |
| 1:CA:227:G:H2' | 1:CA:228:A:O4' | 2.21 | 0.41 |
| 25:DA:775:G:C4 | 25:DA:794:G:C8 | 3.09 | 0.41 |
| 1:AA:1242:C:O2' | 1:AA:1243:C:H5' | 2.21 | 0.41 |
| 25:DA:2525:G:N2 | 25:DA:2539:C:C2 | 2.89 | 0.41 |
| 25:BA:468:G:C6 | 25:BA:469:G:C4 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|---------------------|-------------|----------|
| 8:CK:33:GLU:OE1 | 8:CK:50:ARG:HD2 | 2.20 | 0.41 |
| 1:CA:1417:G:C6 | 1:CA:1482:G:C6 | 3.09 | 0.41 |
| 40:D1:24:TYR:O | 40:D1:29:SER:HB3 | 2.20 | 0.41 |
| 32:BK:84:GLY:N | 32:BK:89:TYR:CE1 | 2.89 | 0.41 |
| 23:CD:29:C:H2' | 23:CD:30:G:C8 | 2.55 | 0.41 |
| 10:AM:80:LYS:HD3 | 10:AM:80:LYS:O | 2.21 | 0.41 |
| 39:BR:13:ARG:HG2 | 39:BR:13:ARG:H | 1.73 | 0.41 |
| 44:BU:27:VAL:O | 44:BU:27:VAL:CG2 | 2.69 | 0.41 |
| 31:BH:149:ARG:HG2 | 31:BH:149:ARG:O | 2.21 | 0.41 |
| 45:BV:104:PHE:CE1 | 45:BV:119:GLU:HA | 2.55 | 0.41 |
| 25:BA:690:G:H2' | 25:BA:691:C:C6 | 2.56 | 0.41 |
| 25:DA:773:U:H5' | 27:DD:47:GLY:HA2 | 2.03 | 0.41 |
| 17:CT:86:GLU:O | 17:CT:90:ILE:HG12 | 2.21 | 0.41 |
| 27:BD:58:HIS:HD2 | 27:BD:59:LYS:O | 2.04 | 0.41 |
| 25:BA:1091:G:N2 | 25:BA:1101:U:H1' | 2.36 | 0.41 |
| 25:BA:1102:C:H2' | 25:BA:1103:A:C8 | 2.52 | 0.41 |
| 1:AA:1157:A:N6 | 1:AA:1178:G:N2 | 2.68 | 0.41 |
| 38:BQ:87:PHE:CE1 | 38:BQ:102:ALA:HB2 | 2.56 | 0.41 |
| 33:DM:38:HIS:CE1 | 33:DM:39:ARG:CG | 3.04 | 0.41 |
| 27:BD:101:GLU:HG3 | 27:BD:102:LYS:N | 2.36 | 0.41 |
| 28:DE:28:ALA:O | 28:DE:93:VAL:HG22 | 2.21 | 0.41 |
| 25:DA:820:A:H2' | 25:DA:821:A:O4' | 2.20 | 0.41 |
| 27:DD:28:GLU:CB | 27:DD:29:PRO:CD | 2.98 | 0.41 |
| 1:AA:1004:A:C4' | 1:AA:1025:U:H3 | 2.33 | 0.41 |
| 29:DF:18:ARG:CG | 29:DF:19:GLU:N | 2.84 | 0.41 |
| 9:CL:81:ILE:O | 9:CL:81:ILE:HG22 | 2.22 | 0.41 |
| 26:DB:42:C:H4' | 30:DG:67:LYS:CD | 2.49 | 0.41 |
| 42:BS:88:ARG:HD3 | 42:BS:94:ASP:OD1 | 2.21 | 0.41 |
| 1:CA:345:C:O2' | 1:CA:346:G:P | 2.74 | 0.41 |
| 29:BF:9:ILE:CD1 | 29:BF:125:LEU:HG | 2.38 | 0.41 |
| 31:BH:4:ILE:CG1 | 31:BH:6:ARG:CZ | 2.93 | 0.41 |
| 25:DA:2134:A:H2' | 25:DA:2134:A:N3 | 2.36 | 0.41 |
| 26:BB:31:C:O2' | 26:BB:32:C:H5' | 2.21 | 0.41 |
| 25:BA:2125:G:C2 | 25:BA:2172:U:OP1 | 2.73 | 0.41 |
| 12:CO:47:LYS:O | 12:CO:49:ASN:N | 2.54 | 0.41 |
| 1:CA:625:G:H4' | 16:CS:16:HIS:CD2 | 2.56 | 0.41 |
| 33:BM:23:LEU:HD12 | 33:BM:23:LEU:O | 2.21 | 0.41 |
| 25:BA:2712:U:O2' | 25:BA:2712(A):A:OP2 | 2.34 | 0.41 |
| 25:BA:2473:U:O2 | 25:BA:2473:U:H2' | 2.21 | 0.41 |
| 25:BA:2472:G:C4 | 25:BA:2475:C:N4 | 2.89 | 0.41 |
| 27:DD:172:TYR:CD1 | 27:DD:186:HIS:HA | 2.56 | 0.41 |
| 50:B4:55:ARG:NH1 | 50:B4:56:VAL:HG23 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 28:DE:57:LYS:NZ | 28:DE:72:VAL:HG13 | 2.35 | 0.41 |
| 1:AA:1223:C:H3' | 1:AA:1224:G:H5'' | 2.02 | 0.41 |
| 25:DA:862:G:H2' | 25:DA:863:A:O4' | 2.21 | 0.41 |
| 14:AQ:26:ARG:HD3 | 14:AQ:43:CYS:HB3 | 2.03 | 0.41 |
| 1:CA:1091:U:C2 | 1:CA:1093:A:OP2 | 2.74 | 0.41 |
| 12:AO:6:THR:OG1 | 12:AO:9:GLN:HG3 | 2.20 | 0.41 |
| 25:BA:529:A:C8 | 25:BA:530:G:O6 | 2.74 | 0.41 |
| 45:DV:24:LEU:HA | 45:DV:25:PRO:HD3 | 1.93 | 0.41 |
| 25:BA:654(B):C:H2' | 25:BA:654(C):G:C8 | 2.56 | 0.41 |
| 25:BA:304:G:C2 | 25:BA:314:A:N3 | 2.89 | 0.41 |
| 25:DA:2529:G:H5'' | 25:DA:2530:A:H5'' | 2.03 | 0.41 |
| 25:BA:1049:C:C4 | 25:BA:1050:A:C2 | 3.09 | 0.41 |
| 1:AA:198:G:C5 | 1:AA:220:G:C2 | 3.09 | 0.41 |
| 23:CD:31:G:C4 | 23:CD:32:G:C8 | 3.09 | 0.41 |
| 31:BH:77:LYS:O | 31:BH:77:LYS:HG2 | 2.21 | 0.41 |
| 35:BO:19:VAL:HG23 | 35:BO:27:HIS:CG | 2.55 | 0.41 |
| 1:CA:66:G:H4' | 1:CA:173:U:C5 | 2.55 | 0.41 |
| 25:BA:2313:C:H2' | 25:BA:2314:C:H6 | 1.85 | 0.41 |
| 25:BA:1447:G:O2' | 25:BA:1448:G:H5' | 2.21 | 0.41 |
| 25:DA:2364:C:H2' | 25:DA:2365:G:C5' | 2.51 | 0.41 |
| 37:B0:44:LEU:HA | 37:B0:44:LEU:HD23 | 1.89 | 0.41 |
| 10:CM:99:LYS:HD3 | 10:CM:100:THR:N | 2.35 | 0.41 |
| 1:AA:373:A:N6 | 1:AA:391:G:C2 | 2.89 | 0.41 |
| 25:BA:856:C:O2' | 25:BA:857:C:O5' | 2.39 | 0.41 |
| 25:DA:668:G:C2' | 25:DA:669:G:OP1 | 2.68 | 0.41 |
| 35:DO:71:VAL:HG13 | 35:DO:72:PRO:CD | 2.51 | 0.41 |
| 25:DA:2526:G:C2 | 25:DA:2538:C:O2 | 2.74 | 0.41 |
| 4:CG:126:ILE:HG23 | 4:CG:147:ALA:O | 2.21 | 0.41 |
| 1:AA:859:A:H2' | 1:AA:860:A:O4' | 2.20 | 0.41 |
| 23:CC:38:A:O2' | 23:CC:39:A:H5' | 2.21 | 0.41 |
| 25:BA:649:G:C5 | 25:BA:650:C:C4 | 3.09 | 0.41 |
| 7:AJ:17:VAL:HB | 7:AJ:44:TYR:CZ | 2.56 | 0.41 |
| 3:AF:84:ILE:O | 3:AF:84:ILE:HG12 | 2.21 | 0.41 |
| 1:CA:1438:G:H2' | 1:CA:1439:C:H6 | 1.84 | 0.41 |
| 20:CW:72:LEU:HD11 | 20:CW:80:ARG:NH1 | 2.36 | 0.41 |
| 25:DA:61:G:C8 | 48:DW:47:ASN:HB3 | 2.56 | 0.41 |
| 25:DA:1488:G:C6 | 25:DA:1489:U:N3 | 2.89 | 0.41 |
| 1:CA:1272:G:H2' | 1:CA:1273:G:O4' | 2.21 | 0.41 |
| 29:DF:128:ALA:O | 29:DF:129:PHE:C | 2.59 | 0.41 |
| 31:BH:84:SER:O | 31:BH:85:LYS:HB2 | 2.20 | 0.41 |
| 1:CA:1205:U:H1' | 3:CF:195:VAL:HG23 | 2.03 | 0.41 |
| 25:BA:743:G:C2' | 25:BA:744:G:H5' | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:CA:359:U:H2' | 1:CA:360:A:C8 | 2.56 | 0.41 |
| 25:BA:2301:C:C6 | 25:BA:2301:C:C3' | 3.04 | 0.41 |
| 31:BH:167:GLU:HA | 31:BH:168:PRO:HD3 | 1.72 | 0.41 |
| 32:DK:11:ASN:O | 32:DK:12:LEU:HD12 | 2.21 | 0.41 |
| 25:BA:2598:A:H2' | 25:BA:2599:G:O5' | 2.21 | 0.41 |
| 45:BV:52:SER:O | 45:BV:52:SER:OG | 2.30 | 0.41 |
| 8:CK:119:LEU:HD13 | 8:CK:123:GLU:O | 2.21 | 0.41 |
| 25:DA:1438:U:O2' | 25:DA:1439:A:H5' | 2.21 | 0.41 |
| 25:DA:1831:G:H2' | 25:DA:1832:C:C6 | 2.55 | 0.41 |
| 25:BA:1458:C:H4' | 25:BA:1459:G:C5' | 2.50 | 0.41 |
| 25:BA:809:G:H2' | 25:BA:810:U:O5' | 2.20 | 0.41 |
| 39:BR:37:GLY:O | 39:BR:38:ASN:HB3 | 2.21 | 0.41 |
| 32:DK:110:ASP:OD2 | 32:DK:130:TYR:HE1 | 2.04 | 0.41 |
| 1:CA:1164:G:N1 | 1:CA:1173:G:C6 | 2.89 | 0.41 |
| 44:BU:30:VAL:HG22 | 44:BU:37:VAL:HG12 | 2.03 | 0.41 |
| 6:CI:7:ASN:HB3 | 18:CU:76:LEU:HD21 | 2.03 | 0.41 |
| 25:DA:370:G:H4' | 25:DA:371:A:OP2 | 2.21 | 0.41 |
| 20:AW:58:LYS:O | 20:AW:62:LEU:HD12 | 2.21 | 0.41 |
| 50:B4:43:TYR:O | 50:B4:43:TYR:CG | 2.73 | 0.41 |
| 17:AT:78:GLU:O | 17:AT:78:GLU:HG2 | 2.20 | 0.41 |
| 42:DS:40:ASN:O | 42:DS:40:ASN:ND2 | 2.52 | 0.41 |
| 2:AE:114:ARG:HE | 2:AE:118:LEU:HD11 | 1.84 | 0.41 |
| 28:DE:46:ALA:CB | 28:DE:82:ARG:CB | 2.76 | 0.40 |
| 25:BA:1084:A:C6 | 25:BA:1085:A:N6 | 2.89 | 0.40 |
| 35:DO:62:LEU:O | 35:DO:62:LEU:HD23 | 2.21 | 0.40 |
| 38:DQ:106:ARG:H | 38:DQ:106:ARG:HG3 | 1.30 | 0.40 |
| 23:AC:19:G:C2 | 23:AC:59:A:C5 | 3.09 | 0.40 |
| 1:CA:1002:G:C2 | 1:CA:1003:G:C4 | 3.09 | 0.40 |
| 1:AA:1053:G:C5 | 1:AA:1199:U:C5 | 3.09 | 0.40 |
| 33:BM:114:ARG:O | 33:BM:115:ARG:CB | 2.69 | 0.40 |
| 28:DE:8:LYS:C | 28:DE:9:VAL:HG13 | 2.41 | 0.40 |
| 25:DA:2401:U:O2 | 25:DA:2402:C:C5 | 2.73 | 0.40 |
| 22:CB:15:A:OP2 | 22:CB:16:U:H5 | 2.03 | 0.40 |
| 29:BF:101:LEU:HD12 | 29:BF:102:PRO:CD | 2.51 | 0.40 |
| 19:AV:41:VAL:HG21 | 19:AV:67:VAL:HG22 | 2.01 | 0.40 |
| 36:BP:103:MET:CE | 36:BP:125:LEU:HD13 | 2.51 | 0.40 |
| 1:AA:1443:G:H3' | 1:AA:1446:A:C5' | 2.51 | 0.40 |
| 25:BA:747:U:P | 51:B5:3:LYS:HG2 | 2.61 | 0.40 |
| 29:DF:116:ASP:OD1 | 29:DF:119:ARG:NH2 | 2.49 | 0.40 |
| 1:AA:838:G:N2 | 1:AA:848:C:N3 | 2.55 | 0.40 |
| 23:CD:54:G:C4 | 23:CD:55:U:C5 | 3.08 | 0.40 |
| 1:CA:1126:U:C1' | 1:CA:1127:G:P | 3.08 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 25:DA:1300:U:H4' | 25:DA:1301:A:OP2 | 2.20 | 0.40 |
| 35:BO:60:MET:HG3 | 35:BO:60:MET:O | 2.21 | 0.40 |
| 27:BD:25:THR:HG23 | 27:BD:26:LYS:HD2 | 2.02 | 0.40 |
| 30:DG:142:PRO:HG2 | 30:DG:143:GLU:CD | 2.41 | 0.40 |
| 1:AA:1251:A:H1' | 1:AA:1369:C:O2' | 2.21 | 0.40 |
| 25:BA:654:A:C2' | 25:BA:654:A:N3 | 2.79 | 0.40 |
| 25:DA:2262:U:O2' | 25:DA:2263:C:H5' | 2.21 | 0.40 |
| 45:BV:112:ARG:C | 45:BV:114:GLY:HA2 | 2.40 | 0.40 |
| 25:DA:2335:A:O2' | 25:DA:2336:A:O5' | 2.35 | 0.40 |
| 25:DA:84:A:OP2 | 44:DU:8:LYS:HD3 | 2.21 | 0.40 |
| 23:AC:2:G:C4 | 23:AC:3:C:C5 | 3.09 | 0.40 |
| 25:DA:2805:G:H2' | 25:DA:2807:G:H8 | 1.85 | 0.40 |
| 30:BG:111:LEU:O | 30:BG:114:ILE:HG12 | 2.21 | 0.40 |
| 1:AA:1347:G:OP2 | 9:AL:107:ARG:HG2 | 2.21 | 0.40 |
| 7:CJ:79:ARG:HA | 7:CJ:83:ALA:O | 2.21 | 0.40 |
| 26:BB:99:A:C6 | 26:BB:100:G:C5 | 3.09 | 0.40 |
| 28:DE:58:ARG:O | 28:DE:60:ASN:OD1 | 2.38 | 0.40 |
| 14:CQ:22:THR:OG1 | 14:CQ:33:VAL:CG1 | 2.68 | 0.40 |
| 18:CU:71:LYS:O | 18:CU:75:ILE:HG13 | 2.21 | 0.40 |
| 1:CA:1348:U:H4' | 9:CL:120:ARG:HG3 | 2.03 | 0.40 |
| 8:CK:21:LYS:HG2 | 8:CK:23:SER:O | 2.22 | 0.40 |
| 5:AH:9:LYS:HE3 | 5:AH:9:LYS:HB2 | 1.88 | 0.40 |
| 18:AU:22:VAL:O | 18:AU:22:VAL:HG13 | 2.22 | 0.40 |
| 22:AB:42:U:H5' | 22:AB:43:A:P | 2.60 | 0.40 |
| 25:DA:839:U:H1' | 25:DA:1191:G:H1' | 2.03 | 0.40 |
| 25:BA:2098:U:N3 | 25:BA:2099:U:C5 | 2.89 | 0.40 |
| 30:DG:81:LYS:HA | 30:DG:81:LYS:HD3 | 1.90 | 0.40 |
| 25:BA:991:C:C2 | 25:BA:992:C:C5 | 3.09 | 0.40 |
| 25:BA:814:C:C2' | 25:BA:815:C:H5' | 2.51 | 0.40 |
| 25:BA:1831:G:H2' | 25:BA:1832:C:C6 | 2.57 | 0.40 |
| 25:DA:1545(A):A:H2' | 25:DA:1546:C:O5' | 2.21 | 0.40 |
| 25:DA:619:G:H5'' | 25:DA:620:G:OP2 | 2.21 | 0.40 |
| 25:DA:620:G:H8 | 25:DA:622:G:O6 | 2.03 | 0.40 |
| 25:BA:464:U:H4' | 53:B7:5:TRP:CZ3 | 2.56 | 0.40 |
| 3:CF:154:SER:O | 3:CF:196:LEU:HD13 | 2.21 | 0.40 |
| 4:AG:88:VAL:HG12 | 4:AG:88:VAL:O | 2.21 | 0.40 |
| 1:CA:655:A:C2 | 1:CA:754:C:N4 | 2.90 | 0.40 |
| 25:DA:1450:C:C2 | 25:DA:1451:C:C5 | 3.09 | 0.40 |
| 3:CF:123:GLN:HB3 | 3:CF:128:PHE:HB2 | 2.03 | 0.40 |
| 3:CF:190:ARG:N | 3:CF:190:ARG:HD2 | 2.35 | 0.40 |
| 5:CH:43:LEU:HB2 | 5:CH:136:MET:SD | 2.60 | 0.40 |
| 25:DA:1973:G:H2' | 25:DA:1974:C:H6 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 34:DN:98:VAL:HG13 | 34:DN:117:LEU:HB3 | 2.03 | 0.40 |
| 25:BA:818:G:H5' | 25:BA:839:U:OP1 | 2.21 | 0.40 |
| 25:DA:616:A:C8 | 29:DF:176:LEU:HD11 | 2.56 | 0.40 |
| 25:BA:1532:C:H42 | 25:BA:1539:G:H1 | 1.68 | 0.40 |
| 25:DA:1131:G:C2 | 25:DA:1132:A:C4 | 3.09 | 0.40 |
| 28:DE:105:THR:HA | 28:DE:166:THR:HA | 2.03 | 0.40 |
| 23:CC:12:G:H1' | 25:DA:1923:U:O2' | 2.21 | 0.40 |
| 25:DA:2016:U:H2' | 25:DA:2017:U:H6 | 1.86 | 0.40 |
| 48:BW:59:ARG:O | 48:BW:63:VAL:HG23 | 2.21 | 0.40 |
| 41:D2:62:LEU:HD22 | 41:D2:95:LEU:N | 2.36 | 0.40 |
| 46:B3:31:VAL:HG11 | 46:B3:67:VAL:CG2 | 2.51 | 0.40 |
| 25:BA:459:U:H2' | 25:BA:460:A:C8 | 2.56 | 0.40 |
| 1:CA:444:C:H2' | 1:CA:445:G:C8 | 2.56 | 0.40 |
| 25:DA:611:C:C2' | 25:DA:612:G:H5' | 2.51 | 0.40 |
| 25:DA:1817:G:H2' | 25:DA:1818:U:H5' | 2.02 | 0.40 |
| 4:CG:88:VAL:HG13 | 5:CH:97:GLY:CA | 2.51 | 0.40 |
| 1:CA:934:C:C4 | 1:CA:1345:U:C5 | 3.09 | 0.40 |
| 25:BA:776:G:H4' | 25:BA:777:A:O5' | 2.22 | 0.40 |
| 25:DA:1742:C:H5' | 25:DA:1743:G:OP2 | 2.21 | 0.40 |
| 44:BU:102:CYS:SG | 44:BU:103:GLY:N | 2.90 | 0.40 |
| 17:CT:100:LYS:HA | 17:CT:100:LYS:HD2 | 1.78 | 0.40 |
| 50:D4:8:LYS:HA | 50:D4:8:LYS:HD2 | 1.72 | 0.40 |
| 30:DG:52:ILE:HD13 | 30:DG:52:ILE:HA | 1.79 | 0.40 |
| 1:CA:559:A:N3 | 1:CA:559:A:H2' | 2.36 | 0.40 |
| 47:BZ:81:LYS:HA | 47:BZ:81:LYS:HD2 | 1.89 | 0.40 |
| 1:AA:335:C:O2' | 1:AA:1433:A:N3 | 2.45 | 0.40 |
| 16:AS:82:GLN:H | 16:AS:82:GLN:HG2 | 1.62 | 0.40 |
| 25:DA:2581:G:N3 | 25:DA:2581:G:H2' | 2.36 | 0.40 |
| 25:BA:979:G:H3' | 25:BA:980:A:H5'' | 2.03 | 0.40 |
| 25:DA:1491:G:O2' | 25:DA:1492:G:H5' | 2.20 | 0.40 |
| 25:DA:2241:A:H2' | 25:DA:2242:G:C8 | 2.56 | 0.40 |
| 25:DA:213:A:H2' | 25:DA:214:G:O4' | 2.21 | 0.40 |
| 27:DD:35:LYS:HB3 | 27:DD:64:ILE:H | 1.86 | 0.40 |
| 38:DQ:83:LYS:C | 38:DQ:109:GLY:HA3 | 2.42 | 0.40 |
| 40:D1:100:VAL:C | 40:D1:101:ARG:HG2 | 2.40 | 0.40 |
| 27:BD:44:ASN:HB3 | 27:BD:48:ARG:C | 2.41 | 0.40 |
| 28:BE:31:CYS:HB3 | 28:BE:49:LEU:HG | 2.04 | 0.40 |
| 23:AC:17:C:O2 | 23:AC:17:C:O2' | 2.39 | 0.40 |
| 9:AL:5:TYR:CG | 9:AL:6:GLY:N | 2.89 | 0.40 |
| 1:CA:1227:A:H3' | 1:CA:1227:A:C8 | 2.56 | 0.40 |
| 4:CG:13:ARG:O | 4:CG:15:GLU:N | 2.52 | 0.40 |
| 11:AN:73:MET:HA | 11:AN:77:MET:H | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 25:DA:1059:G:O6 | 25:DA:1080:A:C6 | 2.75 | 0.40 |
| 25:BA:889:C:O2 | 25:BA:889:C:O5' | 2.39 | 0.40 |
| 25:BA:893:C:C4 | 25:BA:894:C:N4 | 2.90 | 0.40 |
| 48:DW:10:LEU:HA | 48:DW:10:LEU:HD12 | 1.76 | 0.40 |
| 13:CP:22:ILE:HB | 13:CP:25:ILE:HG13 | 2.02 | 0.40 |
| 25:DA:2751:G:C2 | 31:DH:2:SER:N | 2.88 | 0.40 |
| 25:BA:1142(A):A:C5 | 25:BA:1144:G:C5 | 3.09 | 0.40 |
| 25:DA:329:G:C4' | 25:DA:330:A:OP2 | 2.69 | 0.40 |
| 1:AA:872:A:C2 | 1:AA:874:G:C6 | 3.09 | 0.40 |
| 1:AA:1301:U:O2 | 1:AA:1301:U:C2' | 2.69 | 0.40 |
| 25:DA:2162:G:O2' | 25:DA:2173:A:OP2 | 2.39 | 0.40 |
| 25:BA:2124:G:C2' | 25:BA:2125:G:H5' | 2.51 | 0.40 |
| 25:DA:139:G:N3 | 25:DA:141:A:N1 | 2.69 | 0.40 |
| 25:BA:2032:G:O2' | 28:BE:145:LYS:HE3 | 2.22 | 0.40 |
| 21:AX:25:LYS:O | 21:AX:26:LYS:HB3 | 2.21 | 0.40 |
| 44:BU:6:HIS:ND1 | 44:BU:7:VAL:HG13 | 2.37 | 0.40 |
| 25:DA:2263:C:O2' | 25:DA:2264:C:H5' | 2.22 | 0.40 |
| 1:CA:1190:G:OP1 | 3:CF:4:LYS:HA | 2.22 | 0.40 |
| 27:BD:18:VAL:HG12 | 27:BD:19:ALA:N | 2.37 | 0.40 |
| 25:BA:2474:C:H3' | 25:BA:2475:C:H6 | 1.85 | 0.40 |
| 25:BA:1210:A:C8 | 25:BA:1210:A:H5' | 2.43 | 0.40 |
| 1:AA:457:C:N3 | 1:AA:476:G:C2 | 2.89 | 0.40 |
| 2:CE:178:ARG:HA | 2:CE:178:ARG:HD3 | 1.90 | 0.40 |
| 45:DV:60:GLU:O | 45:DV:61:LEU:O | 2.39 | 0.40 |
| 25:BA:1163:G:C2 | 25:BA:1164:G:C8 | 3.10 | 0.40 |
| 50:B4:14:ILE:HG23 | 50:B4:15:ILE:N | 2.36 | 0.40 |
| 49:BX:32:GLN:NE2 | 49:BX:32:GLN:HA | 2.36 | 0.40 |
| 31:BH:137:ASP:O | 31:BH:138:LYS:CB | 2.68 | 0.40 |
| 37:B0:75:LEU:HA | 37:B0:78:LYS:HB3 | 2.03 | 0.40 |
| 28:DE:60:ASN:HD22 | 28:DE:61:ARG:H | 1.69 | 0.40 |
| 19:CV:14:HIS:HD2 | 19:CV:15:LEU:H | 1.68 | 0.40 |
| 1:AA:1510:U:H1' | 1:AA:1526:G:N2 | 2.36 | 0.40 |
| 1:CA:719:C:H42 | 18:CU:71:LYS:HE2 | 1.85 | 0.40 |
| 1:AA:723:U:C5' | 1:AA:724:G:OP2 | 2.70 | 0.40 |
| 25:BA:2199:A:OP2 | 25:BA:2205:C:H5 | 2.04 | 0.40 |
| 1:AA:943:U:H2' | 1:AA:944:G:H5' | 2.04 | 0.40 |
| 2:AE:102:LEU:HB3 | 2:AE:180:LEU:CD1 | 2.52 | 0.40 |
| 4:CG:190:ASP:O | 4:CG:194:LEU:HD22 | 2.21 | 0.40 |
| 18:AU:25:THR:C | 18:AU:26:LEU:HD23 | 2.41 | 0.40 |
| 32:BK:79:ILE:O | 32:BK:142:VAL:HA | 2.20 | 0.40 |
| 14:AQ:2:ALA:HB1 | 14:AQ:6:LEU:HD12 | 2.02 | 0.40 |
| 23:CD:24:C:H2' | 23:CD:25:U:H6 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 42:BS:57:ASN:HA | 42:BS:57:ASN:HD22 | 1.57 | 0.40 |
| 29:BF:117:ARG:HD3 | 29:BF:117:ARG:HA | 1.50 | 0.40 |
| 10:CM:24:VAL:HG12 | 10:CM:25:GLU:N | 2.36 | 0.40 |
| 12:AO:89:ARG:NH1 | 12:AO:89:ARG:CG | 2.82 | 0.40 |
| 1:CA:1105:A:H2' | 1:CA:1106:G:C8 | 2.56 | 0.40 |
| 32:BK:133:HIS:HB2 | 32:BK:134:PRO:HD2 | 2.03 | 0.40 |
| 25:BA:2768:C:C2 | 25:BA:2769:C:C6 | 3.09 | 0.40 |
| 46:D3:50:ASN:C | 46:D3:62:LEU:HD12 | 2.42 | 0.40 |
| 25:DA:2461:C:H2' | 25:DA:2462:U:H6 | 1.84 | 0.40 |
| 37:D0:84:ALA:N | 37:D0:85:PRO:HD2 | 2.36 | 0.40 |
| 25:BA:1364:G:N7 | 47:BZ:2:SER:HB3 | 2.36 | 0.40 |
| 28:BE:1:MET:HB3 | 28:BE:200:GLU:CD | 2.41 | 0.40 |
| 25:DA:221:A:C4 | 25:DA:266:G:N7 | 2.89 | 0.40 |
| 25:BA:355:G:O2' | 25:BA:356:G:H5' | 2.21 | 0.40 |
| 38:DQ:49:VAL:CG2 | 38:DQ:80:LEU:HD12 | 2.51 | 0.40 |
| 36:BP:137:TYR:C | 36:BP:139:GLU:N | 2.74 | 0.40 |
| 1:AA:9:G:C2 | 1:AA:26:A:N1 | 2.89 | 0.40 |
| 1:CA:852:G:C6 | 1:CA:853:G:N7 | 2.89 | 0.40 |
| 49:BX:59:VAL:HG22 | 49:BX:60:GLU:N | 2.37 | 0.40 |
| 29:BF:24:LEU:HA | 29:BF:25:PRO:HD2 | 1.89 | 0.40 |
| 25:BA:477:A:C6 | 25:BA:478:A:C6 | 3.09 | 0.40 |
| 11:CN:33:THR:HG22 | 11:CN:39:PRO:HA | 2.03 | 0.40 |
| 11:AN:85:ARG:HH11 | 11:AN:85:ARG:HG3 | 1.87 | 0.40 |
| 25:DA:2107:C:H2' | 25:DA:2108:C:O4' | 2.22 | 0.40 |
| 25:BA:117:G:C6 | 25:BA:119:A:C6 | 3.09 | 0.40 |
| 29:BF:165:ARG:NH1 | 29:BF:165:ARG:HG3 | 2.36 | 0.40 |
| 47:BZ:21:ARG:HD3 | 47:BZ:35:THR:CG2 | 2.52 | 0.40 |
| 42:DS:57:ASN:O | 42:DS:61:ASN:HB2 | 2.22 | 0.40 |
| 13:CP:32:GLU:O | 13:CP:35:GLU:HB3 | 2.20 | 0.40 |
| 25:DA:1321:A:H2' | 25:DA:1322:A:O4' | 2.22 | 0.40 |
| 26:BB:18:G:H1 | 26:BB:65:C:H42 | 1.70 | 0.40 |
| 1:CA:1429:C:H2' | 1:CA:1430:C:C6 | 2.56 | 0.40 |
| 25:BA:452:G:C4 | 25:BA:458:G:C6 | 3.09 | 0.40 |
| 25:BA:365:C:H2' | 25:BA:366:C:O4' | 2.21 | 0.40 |
| 25:BA:284:U:H2' | 25:BA:285:C:C6 | 2.56 | 0.40 |
| 43:BT:3:THR:O | 43:BT:6:ASP:HB2 | 2.21 | 0.40 |
| 5:AH:151:LEU:HD11 | 8:AK:77:GLU:OE2 | 2.20 | 0.40 |
| 1:AA:144:G:C5 | 1:AA:179:A:C2 | 3.09 | 0.40 |
| 39:DR:113:LYS:HD2 | 39:DR:113:LYS:HA | 1.78 | 0.40 |
| 38:BQ:20:ARG:HE | 38:BQ:20:ARG:HB3 | 1.57 | 0.40 |
| 44:BU:86:ARG:HA | 44:BU:86:ARG:HD2 | 1.87 | 0.40 |
| 15:AR:48:LYS:HA | 15:AR:48:LYS:HD2 | 1.90 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 3:CF:79:ARG:HG2 | 3:CF:79:ARG:H | 1.70 | 0.40 |
| 1:AA:493:G:O5' | 1:AA:493:G:H8 | 2.04 | 0.40 |
| 25:DA:1908:C:O5' | 25:DA:1908:C:H6 | 2.04 | 0.40 |
| 1:CA:966:G:O2' | 9:CL:127:LYS:O | 2.39 | 0.40 |
| 29:DF:140:LEU:HD22 | 29:DF:170:LEU:HD21 | 2.04 | 0.40 |
| 25:BA:1438:U:O2' | 25:BA:1439:A:H5' | 2.20 | 0.40 |
| 25:BA:11:G:C2' | 25:BA:12:U:H5' | 2.51 | 0.40 |
| 25:BA:1077:A:N3 | 25:BA:1078:U:H5'' | 2.36 | 0.40 |
| 38:DQ:41:ASP:C | 38:DQ:41:ASP:OD1 | 2.58 | 0.40 |
| 27:BD:43:ARG:HB2 | 27:BD:54:ARG:HB2 | 2.02 | 0.40 |
| 27:BD:35:LYS:HZ3 | 27:BD:104:TYR:CB | 2.32 | 0.40 |
| 39:DR:19:LEU:HD22 | 39:DR:86:ILE:CG2 | 2.50 | 0.40 |
| 1:CA:1354:C:O2' | 1:CA:1355:G:H5' | 2.22 | 0.40 |
| 4:CG:59:ARG:NH2 | 4:CG:66:ARG:NH1 | 2.69 | 0.40 |
| 51:D5:40:LYS:HE3 | 51:D5:40:LYS:HB2 | 1.90 | 0.40 |
| 1:CA:1176:A:N6 | 1:CA:1177:G:C5 | 2.86 | 0.40 |
| 25:BA:1728:G:C3' | 25:BA:1729:A:H5'' | 2.44 | 0.40 |
| 48:DW:15:LYS:HD3 | 48:DW:67:LYS:HZ1 | 1.85 | 0.40 |
| 25:DA:2469:A:C8 | 25:DA:2482:G:C4 | 3.09 | 0.40 |
| 33:BM:28:THR:HA | 33:BM:106:MET:CE | 2.51 | 0.40 |
| 25:BA:1012:U:O4 | 33:BM:25:ARG:HA | 2.21 | 0.40 |
| 9:CL:5:TYR:CD2 | 9:CL:17:VAL:O | 2.74 | 0.40 |
| 36:DP:77:LYS:HD3 | 36:DP:81:VAL:HG21 | 2.04 | 0.40 |
| 25:DA:2309:A:H2' | 25:DA:2310:A:O4' | 2.22 | 0.40 |
| 25:DA:309:G:O3' | 44:DU:18:GLY:CA | 2.69 | 0.40 |
| 25:DA:2115:G:H2' | 25:DA:2116:G:C8 | 2.56 | 0.40 |
| 25:DA:2127:G:C2 | 25:DA:2173:A:C8 | 3.09 | 0.40 |
| 25:BA:2572:A:H2' | 28:BE:144:ARG:HG3 | 2.04 | 0.40 |
| 25:BA:1533:C:N4 | 25:BA:1538:G:H1 | 2.17 | 0.40 |
| 16:CS:3:LYS:N | 16:CS:22:THR:O | 2.47 | 0.40 |
| 25:BA:1654:A:OP2 | 37:B0:2:ARG:HD3 | 2.21 | 0.40 |
| 25:BA:2472:G:H22 | 25:BA:2477:C:H5'' | 1.86 | 0.40 |
| 25:BA:671:C:H2' | 25:BA:672:C:C6 | 2.57 | 0.40 |
| 25:BA:529:A:C8 | 25:BA:530:G:C6 | 3.07 | 0.40 |
| 25:DA:684:G:C2 | 25:DA:774:A:C2 | 3.10 | 0.40 |
| 45:DV:58:VAL:CG1 | 45:DV:60:GLU:HB3 | 2.52 | 0.40 |
| 25:BA:2689:U:H5' | 25:BA:2689:U:C6 | 2.56 | 0.40 |
| 1:AA:464:G:N2 | 1:AA:468:A:H62 | 2.20 | 0.40 |
| 23:CC:35:C:C2 | 23:CC:36:A:C8 | 3.09 | 0.40 |
| 25:DA:319:C:H2' | 25:DA:320:A:O4' | 2.22 | 0.40 |
| 23:CD:42:C:C5 | 23:CD:43:G:N7 | 2.90 | 0.40 |
| 23:CD:21:U:H3' | 23:CD:22:A:C5' | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|---------------------|-------------|----------|
| 5:AH:96:PRO:HA | 5:AH:117:ASP:OD1 | 2.22 | 0.40 |
| 26:DB:55:U:O2' | 30:DG:29:TRP:HD1 | 2.03 | 0.40 |
| 1:AA:1256:A:C2 | 1:AA:1277:C:C4 | 3.08 | 0.40 |
| 4:AG:25:ARG:CZ | 4:AG:30:LYS:HG3 | 2.51 | 0.40 |
| 10:AM:81:THR:O | 10:AM:84:GLN:HB2 | 2.22 | 0.40 |
| 27:BD:131:LEU:HB2 | 27:BD:136:ILE:HD11 | 2.03 | 0.40 |
| 11:AN:12:ARG:HG2 | 11:AN:13:GLN:H | 1.87 | 0.40 |
| 25:BA:2729:G:H1' | 28:BE:187:ALA:HB2 | 2.03 | 0.40 |
| 1:CA:57:G:C5 | 1:CA:58:C:C5 | 3.09 | 0.40 |
| 31:BH:89:ILE:O | 31:BH:89:ILE:CG1 | 2.66 | 0.40 |
| 44:DU:90:LEU:HD23 | 44:DU:90:LEU:N | 2.35 | 0.40 |
| 25:BA:287:C:O2' | 25:BA:288:C:H5' | 2.21 | 0.40 |
| 48:BW:24:LEU:O | 48:BW:28:LYS:HG2 | 2.22 | 0.40 |
| 1:AA:1190:G:OP2 | 3:AF:5:ILE:HG23 | 2.21 | 0.40 |
| 25:BA:270(Z):U:O3' | 25:BA:271(A):C:H6 | 2.05 | 0.40 |
| 25:DA:1476:C:O2' | 25:DA:1477:A:H5' | 2.22 | 0.40 |
| 25:DA:2817:G:OP1 | 37:D0:99:LYS:NZ | 2.55 | 0.40 |
| 52:B6:36:LEU:HD23 | 52:B6:36:LEU:H | 1.86 | 0.40 |
| 1:CA:1449:C:H2' | 1:CA:1450:U:OP1 | 2.21 | 0.40 |
| 1:CA:1212:U:HO2' | 1:CA:1213:A:H8 | 1.70 | 0.40 |
| 25:DA:631:A:C6 | 25:DA:632:A:C2 | 3.09 | 0.40 |
| 25:BA:1444:G:H5'' | 25:BA:1444(A):A:OP1 | 2.21 | 0.40 |
| 1:AA:260:G:H2' | 1:AA:261:U:C6 | 2.57 | 0.40 |
| 1:AA:109:A:C6 | 1:AA:326:G:C6 | 3.10 | 0.40 |
| 25:DA:2815:C:O2' | 51:D5:43:HIS:CD2 | 2.75 | 0.40 |
| 25:DA:68:G:H2' | 25:DA:69:C:C6 | 2.57 | 0.40 |
| 30:DG:56:ALA:HA | 30:DG:59:GLU:HB3 | 2.04 | 0.40 |
| 48:DW:68:ARG:HG3 | 48:DW:68:ARG:NH1 | 2.36 | 0.40 |
| 30:DG:150:ASP:CG | 30:DG:151:ALA:N | 2.75 | 0.40 |
| 50:D4:14:ILE:HA | 50:D4:30:GLU:HB3 | 2.04 | 0.40 |
| 35:DO:30:THR:O | 35:DO:31:ALA:HB3 | 2.21 | 0.40 |
| 19:AV:13:ASP:O | 19:AV:16:LEU:N | 2.55 | 0.40 |
| 30:BG:125:PHE:CZ | 30:BG:170:ARG:HA | 2.56 | 0.40 |
| 9:AL:3:GLN:OE1 | 9:AL:20:ARG:NH1 | 2.54 | 0.40 |
| 15:CR:4:THR:OG1 | 15:CR:7:GLU:HB2 | 2.21 | 0.40 |
| 8:AK:118:VAL:O | 8:AK:119:LEU:HD23 | 2.21 | 0.40 |
| 4:CG:76:ARG:NH2 | 4:CG:80:GLU:OE1 | 2.50 | 0.40 |
| 25:BA:2246:G:H2' | 25:BA:2247:A:C8 | 2.56 | 0.40 |
| 25:BA:868:U:C4 | 25:BA:869:G:N7 | 2.90 | 0.40 |
| 25:BA:779:U:OP1 | 27:BD:49:ILE:HG13 | 2.21 | 0.40 |
| 27:DD:45:ASN:OD1 | 27:DD:45:ASN:C | 2.60 | 0.40 |
| 32:BK:47:LEU:O | 32:BK:47:LEU:HD12 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 47:DZ:50:ARG:HE | 47:DZ:50:ARG:HB2 | 1.61 | 0.40 |
| 25:BA:1894:C:O2' | 25:BA:1895:C:H5' | 2.21 | 0.40 |
| 1:AA:15:G:H4' | 5:AH:24:ARG:NH1 | 2.36 | 0.40 |
| 1:AA:424:G:C2 | 1:AA:425:G:C8 | 3.09 | 0.40 |
| 1:CA:147:G:O2' | 1:CA:148:G:H5' | 2.22 | 0.40 |
| 30:BG:73:ALA:CB | 30:BG:82:LEU:HD11 | 2.51 | 0.40 |
| 25:BA:1063:G:H22 | 25:BA:1076:C:H1' | 1.86 | 0.40 |
| 25:BA:1085:A:N3 | 25:BA:1086:A:C5 | 2.89 | 0.40 |
| 54:D8:29:LYS:HB2 | 54:D8:44:LYS:HB3 | 2.03 | 0.40 |
| 54:D8:30:ARG:O | 54:D8:31:HIS:CB | 2.70 | 0.40 |
| 38:BQ:106:ARG:O | 38:BQ:107:GLU:HB3 | 2.21 | 0.40 |
| 25:DA:993:G:C5 | 25:DA:994:C:C5 | 3.10 | 0.40 |
| 28:BE:35:GLN:CB | 28:BE:48:GLN:HB2 | 2.51 | 0.40 |
| 28:BE:51:PHE:CE1 | 28:BE:52:LEU:CD2 | 2.98 | 0.40 |
| 23:CC:62:C:N3 | 23:CC:63:C:C5 | 2.90 | 0.40 |
| 1:CA:977:A:H8 | 1:CA:982:U:O4 | 2.05 | 0.40 |
| 1:AA:1305:G:C8 | 1:AA:1305:G:OP2 | 2.75 | 0.40 |
| 25:BA:2370:G:C6 | 25:BA:2371:G:C6 | 3.09 | 0.40 |
| 4:CG:31:CYS:O | 4:CG:32:ALA:CB | 2.66 | 0.40 |
| 1:AA:1004:A:C1' | 1:AA:1036:G:N1 | 2.63 | 0.40 |
| 22:CB:37:G:H2' | 22:CB:38:G:H8 | 1.85 | 0.40 |
| 25:DA:1087:G:H2' | 25:DA:1089:G:O4' | 2.21 | 0.40 |
| 1:AA:55:A:H2 | 32:DK:82:ARG:HG2 | 1.86 | 0.40 |
| 1:AA:56:U:H2' | 1:AA:57:G:C8 | 2.56 | 0.40 |
| 35:BO:64:LYS:CG | 54:B8:25:MET:SD | 3.09 | 0.40 |
| 4:CG:108:LEU:HD13 | 4:CG:174:LEU:HD13 | 2.03 | 0.40 |
| 1:AA:1061:G:OP2 | 3:AF:2:GLY:O | 2.40 | 0.40 |
| 9:AL:111:ARG:O | 9:AL:111:ARG:HG3 | 2.20 | 0.40 |
| 1:CA:1305:G:N2 | 1:CA:1331:G:O2' | 2.54 | 0.40 |
| 23:CD:15:G:C2 | 23:CD:49:C:O2 | 2.73 | 0.40 |
| 31:BH:62:LYS:HB2 | 31:BH:62:LYS:HE2 | 1.88 | 0.40 |
| 1:CA:1278:U:H5'' | 1:CA:1279:A:O4' | 2.21 | 0.40 |
| 26:DB:43:C:C4' | 30:DG:66:GLN:NE2 | 2.84 | 0.40 |
| 30:DG:94:LEU:HD23 | 30:DG:94:LEU:H | 1.87 | 0.40 |
| 1:CA:1446:A:C6 | 39:DR:118:ARG:NH1 | 2.90 | 0.40 |
| 32:BK:101:LEU:HD22 | 32:BK:109:ILE:CG2 | 2.51 | 0.40 |
| 32:BK:104:GLN:O | 32:BK:105:HIS:HB2 | 2.19 | 0.40 |
| 2:AE:8:LYS:N | 2:AE:8:LYS:CD | 2.84 | 0.40 |
| 26:DB:9:G:C2 | 26:DB:112:G:C4 | 3.10 | 0.40 |
| 2:AE:206:ASP:O | 2:AE:207:ALA:HB3 | 2.22 | 0.40 |
| 1:CA:1436:U:H2' | 1:CA:1437:C:C6 | 2.57 | 0.40 |
| 25:BA:2801:A:OP1 | 25:BA:2895:U:O2' | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 19:CV:11:VAL:CG2 | 19:CV:16:LEU:HD11 | 2.51 | 0.40 |
| 27:BD:26:LYS:CD | 27:BD:26:LYS:H | 2.35 | 0.40 |
| 1:CA:376:G:N3 | 1:CA:389:A:C2 | 2.90 | 0.40 |
| 37:B0:1:MET:HE3 | 37:B0:1:MET:HB2 | 1.99 | 0.40 |
| 28:DE:70:ALA:O | 28:DE:72:VAL:HG23 | 2.21 | 0.40 |
| 31:BH:50:VAL:O | 31:BH:50:VAL:CG2 | 2.70 | 0.40 |
| 50:D4:58:ARG:HH21 | 50:D4:58:ARG:HG3 | 1.87 | 0.40 |
| 22:AB:18:G:H1' | 22:AB:19:G:P | 2.62 | 0.40 |
| 26:BB:40:U:C2' | 26:BB:41:U:OP1 | 2.69 | 0.40 |
| 1:AA:1394:A:C5 | 1:AA:1501:C:H4' | 2.56 | 0.40 |
| 54:D8:39:LYS:C | 54:D8:41:ILE:N | 2.70 | 0.40 |
| 25:BA:314:A:O2' | 25:BA:315:G:H5' | 2.21 | 0.40 |
| 1:CA:410:G:C2 | 1:CA:429:U:C2 | 3.09 | 0.40 |
| 2:CE:6:THR:O | 2:CE:7:VAL:HB | 2.21 | 0.40 |
| 22:CB:44:G:C6 | 22:CB:45:U:N3 | 2.89 | 0.40 |
| 45:BV:111:VAL:HG21 | 45:BV:146:ILE:HG13 | 2.03 | 0.40 |
| 1:CA:1218:C:H2' | 1:CA:1219:U:C6 | 2.57 | 0.40 |
| 46:B3:75:LEU:HA | 46:B3:75:LEU:HD23 | 1.90 | 0.40 |
| 37:D0:104:ARG:HB2 | 37:D0:107:ASP:OD2 | 2.20 | 0.40 |
| 31:DH:68:THR:HG22 | 31:DH:72:ILE:HD11 | 2.02 | 0.40 |
| 10:AM:30:SER:HG | 10:AM:84:GLN:HE21 | 1.58 | 0.40 |
| 1:AA:816:A:OP1 | 1:AA:1526:G:O2' | 2.29 | 0.40 |
| 25:BA:2756:U:H1' | 25:BA:2757:A:H5'' | 2.02 | 0.40 |
| 25:DA:1000:A:N1 | 25:DA:1155:A:C4 | 2.89 | 0.40 |
| 1:AA:114:U:H2' | 1:AA:115:G:C8 | 2.56 | 0.40 |
| 22:CB:2:C:H2' | 22:CB:3:C:O4' | 2.21 | 0.40 |
| 3:AF:181:ASN:HD21 | 3:AF:204:LEU:HB2 | 1.83 | 0.40 |
| 1:CA:468:A:C8 | 1:CA:474:G:C8 | 3.09 | 0.40 |
| 1:CA:474:G:C2 | 1:CA:475:G:C4 | 3.10 | 0.40 |
| 25:BA:1581:G:C6 | 25:BA:1582:C:C4 | 3.10 | 0.40 |
| 25:BA:821:A:C5' | 25:BA:822:U:H6 | 2.35 | 0.40 |
| 10:AM:100:THR:O | 10:AM:101:VAL:HG23 | 2.22 | 0.40 |
| 32:BK:81:VAL:HG21 | 32:BK:88:ILE:CD1 | 2.50 | 0.40 |
| 6:AI:97:PHE:CD2 | 18:AU:31:LEU:HD21 | 2.54 | 0.40 |
| 2:CE:55:PHE:HD1 | 2:CE:55:PHE:HA | 1.76 | 0.40 |
| 53:D7:42:LEU:HA | 53:D7:42:LEU:HD23 | 1.84 | 0.40 |
| 25:BA:269:U:C5 | 25:BA:270(Z):U:C6 | 3.09 | 0.40 |
| 24:C1:16:A:H2' | 24:C1:17:U:O4' | 2.21 | 0.40 |
| 45:DV:23:LYS:HE2 | 45:DV:40:ASP:OD2 | 2.22 | 0.40 |
| 37:D0:82:GLU:C | 37:D0:85:PRO:HD2 | 2.41 | 0.40 |
| 25:DA:751:A:C6 | 25:DA:789:A:C5 | 3.09 | 0.40 |
| 3:CF:120:VAL:HG12 | 3:CF:121:ALA:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 1:AA:812:C:H2' | 1:AA:812:C:H6 | 1.63 | 0.40 |
| 27:DD:96:HIS:ND1 | 27:DD:102:LYS:HD3 | 2.37 | 0.40 |
| 23:AC:25:U:H2' | 23:AC:26:C:O4' | 2.21 | 0.40 |
| 25:BA:2364:C:C2' | 25:BA:2365:G:H5' | 2.51 | 0.40 |
| 1:CA:879:C:H5 | 12:CO:6:THR:HG21 | 1.87 | 0.40 |
| 25:DA:1105:U:O2' | 25:DA:1106:G:H5' | 2.21 | 0.40 |
| 25:DA:1131:G:O6 | 25:DA:2040:C:H1' | 2.22 | 0.40 |
| 1:AA:578:C:C2' | 1:AA:579:G:O5' | 2.69 | 0.40 |
| 46:B3:31:VAL:HG23 | 46:B3:32:ARG:N | 2.37 | 0.40 |
| 7:AJ:69:VAL:HG12 | 7:AJ:69:VAL:O | 2.21 | 0.40 |
| 25:DA:809:G:O4' | 25:DA:1254:A:H1' | 2.21 | 0.40 |
| 30:BG:145:THR:HG22 | 50:B4:28:LYS:NZ | 2.36 | 0.40 |
| 25:DA:1945:G:C4 | 25:DA:1946:U:C5 | 3.10 | 0.40 |
| 25:DA:2489:G:O2' | 25:DA:2490:G:H5' | 2.20 | 0.40 |
| 25:DA:1967:C:H2' | 25:DA:1968:G:O5' | 2.22 | 0.40 |
| 25:DA:2070:G:C2 | 25:DA:2442:C:C2 | 3.09 | 0.40 |
| 25:DA:1508:A:H4' | 25:DA:1510:A:C2 | 2.57 | 0.40 |
| 23:AD:75:C:H2' | 23:AD:76:C:O4' | 2.21 | 0.40 |
| 4:CG:50:ARG:HA | 4:CG:51:PRO:HD3 | 1.80 | 0.40 |
| 25:BA:1642:G:O2' | 25:BA:1643:G:H5' | 2.20 | 0.40 |
| 37:D0:101:ALA:HB1 | 51:D5:41:PRO:HG3 | 2.03 | 0.40 |
| 25:DA:270(T):G:C6 | 25:DA:270(U):C:C4 | 3.09 | 0.40 |
| 4:CG:132:ARG:HG3 | 4:CG:133:VAL:N | 2.36 | 0.40 |
| 7:AJ:29:LYS:HA | 7:AJ:29:LYS:HE2 | 2.02 | 0.40 |
| 34:BN:73:ASP:C | 34:BN:73:ASP:OD1 | 2.59 | 0.40 |
| 39:BR:113:LYS:HD2 | 39:BR:113:LYS:HA | 1.87 | 0.40 |
| 1:AA:815:A:O2' | 1:AA:1527:C:H1' | 2.21 | 0.40 |
| 45:DV:155:LEU:HA | 45:DV:155:LEU:HD23 | 1.76 | 0.40 |
| 32:BK:94:ALA:HB2 | 32:BK:116:LEU:HB2 | 2.04 | 0.40 |
| 54:D8:30:ARG:C | 54:D8:32:LEU:H | 2.24 | 0.40 |
| 27:BD:181:GLU:HB2 | 27:BD:273:ARG:HB2 | 2.02 | 0.40 |
| 25:DA:835:A:OP1 | 54:D8:52:LYS:HG3 | 2.21 | 0.40 |
| 36:DP:54:MET:HG2 | 36:DP:117:ALA:HB1 | 2.03 | 0.40 |
| 27:DD:44:ASN:HB3 | 27:DD:49:ILE:CA | 2.29 | 0.40 |
| 40:D1:92:ARG:HG3 | 40:D1:94:ASN:N | 2.31 | 0.40 |
| 28:BE:61:ARG:C | 28:BE:63:LEU:N | 2.73 | 0.40 |
| 1:CA:1007:C:C4 | 1:CA:1008:C:C5 | 3.10 | 0.40 |
| 25:BA:2298:A:N6 | 25:BA:2318:G:H1' | 2.37 | 0.40 |
| 33:BM:114:ARG:O | 33:BM:116:LEU:N | 2.55 | 0.40 |
| 33:BM:43:THR:H | 33:BM:48:MET:CE | 2.34 | 0.40 |
| 23:AD:6:G:O2' | 23:AD:7:G:H5' | 2.22 | 0.40 |
| 1:CA:1320:C:C2 | 19:CV:72:GLY:HA3 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 25:BA:608:A:C4 | 25:BA:621:A:C6 | 3.10 | 0.40 |
| 36:BP:29:PHE:HB3 | 36:BP:65:PHE:CE1 | 2.57 | 0.40 |
| 2:CE:169:LYS:O | 2:CE:169:LYS:HD3 | 2.21 | 0.40 |
| 40:B1:50:ARG:HG2 | 40:B1:53:ARG:HH22 | 1.86 | 0.40 |
| 39:DR:92:GLY:HA2 | 39:DR:116:ALA:CA | 2.49 | 0.40 |
| 25:DA:1902:C:OP1 | 27:DD:242:ARG:HD3 | 2.21 | 0.40 |
| 25:DA:2271:G:H2' | 25:DA:2272:U:H6 | 1.87 | 0.40 |
| 10:AM:50:ILE:HD13 | 10:AM:60:ARG:HD3 | 2.03 | 0.40 |
| 25:DA:2712:U:H1' | 25:DA:2712(A):A:C8 | 2.57 | 0.40 |
| 54:B8:36:LYS:HD3 | 54:B8:40:GLU:OE2 | 2.21 | 0.40 |
| 25:BA:2213:U:H6 | 25:BA:2213:U:O5' | 2.04 | 0.40 |
| 25:DA:1299:G:H5'' | 25:DA:1300:U:H5'' | 2.02 | 0.40 |
| 25:BA:1558:A:O2' | 25:BA:1559:G:OP2 | 2.40 | 0.40 |
| 1:AA:687:A:H2' | 1:AA:701:C:N4 | 2.37 | 0.40 |
| 42:BS:9:TYR:N | 42:BS:102:HIS:CD2 | 2.80 | 0.40 |
| 53:B7:8:ASN:ND2 | 53:B7:11:LYS:HB3 | 2.36 | 0.40 |
| 25:DA:1359:A:N7 | 25:DA:1372:U:O4 | 2.55 | 0.40 |
| 19:CV:40:ILE:HG22 | 19:CV:67:VAL:HA | 2.02 | 0.40 |
| 33:BM:17:ASP:O | 33:BM:18:ALA:HB3 | 2.22 | 0.40 |
| 45:DV:131:ARG:CD | 45:DV:131:ARG:H | 2.35 | 0.40 |
| 25:BA:1534:G:O2' | 25:BA:1535:U:H4' | 2.22 | 0.40 |
| 31:BH:152:ARG:HH21 | 31:BH:153:LYS:HE2 | 1.85 | 0.40 |
| 35:DO:102:ARG:HH21 | 35:DO:102:ARG:HG3 | 1.87 | 0.40 |
| 35:DO:128:HIS:CE1 | 35:DO:148:LEU:HD21 | 2.57 | 0.40 |
| 25:DA:910:A:N3 | 25:DA:2264:C:O2' | 2.49 | 0.40 |
| 1:CA:1116:C:O2' | 9:CL:108:VAL:HG11 | 2.22 | 0.40 |
| 2:CE:85:ALA:CB | 2:CE:92:TYR:HD1 | 2.32 | 0.40 |
| 40:B1:79:PHE:CE2 | 40:B1:83:LEU:CD2 | 3.01 | 0.40 |
| 25:BA:2335:A:C8 | 25:BA:2337:G:C6 | 3.10 | 0.40 |
| 29:BF:63:LYS:HE2 | 29:BF:67:GLN:HB2 | 2.04 | 0.40 |
| 3:CF:47:LEU:HD13 | 3:CF:47:LEU:O | 2.21 | 0.40 |
| 1:AA:1372:U:C2' | 1:AA:1373:G:O5' | 2.70 | 0.40 |
| 25:BA:2734:A:C8 | 25:BA:2734:A:C5' | 3.02 | 0.40 |
| 1:CA:1399:C:H4' | 1:CA:1400:C:O5' | 2.21 | 0.40 |
| 5:CH:151:LEU:HD11 | 8:CK:77:GLU:OE2 | 2.20 | 0.40 |
| 12:CO:32:PHE:HD1 | 12:CO:86:ARG:HA | 1.87 | 0.40 |
| 3:AF:58:GLU:O | 3:AF:59:ARG:HG3 | 2.21 | 0.40 |
| 2:AE:111:ARG:HH11 | 2:AE:111:ARG:HA | 1.86 | 0.40 |
| 25:DA:686:G:H1 | 53:D7:16:HIS:CD2 | 2.37 | 0.40 |
| 25:DA:1150:C:H2' | 25:DA:1151:G:O4' | 2.21 | 0.40 |
| 39:BR:111:ARG:O | 39:BR:112:ARG:CG | 2.69 | 0.40 |
| 25:DA:2:G:H1 | 25:DA:2901:C:N4 | 2.12 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:DA:959:A:N1 | 25:DA:960:A:C2 | 2.89 | 0.40 |
| 28:DE:30:PRO:HB2 | 28:DE:90:THR:HG23 | 2.04 | 0.40 |
| 52:B6:11:LEU:CD2 | 52:B6:26:ASN:HB3 | 2.52 | 0.40 |
| 52:B6:11:LEU:HD23 | 52:B6:26:ASN:HB3 | 2.04 | 0.40 |
| 38:DQ:62:LYS:HB3 | 38:DQ:97:ARG:CD | 2.49 | 0.40 |
| 23:CD:37:U:C5 | 23:CD:38:A:N7 | 2.90 | 0.40 |
| 11:CN:58:PRO:HG3 | 11:CN:89:ALA:O | 2.20 | 0.40 |
| 1:CA:1045:C:H2' | 1:CA:1046:A:C4' | 2.52 | 0.40 |
| 4:AG:3:ARG:H | 4:AG:3:ARG:HG3 | 1.58 | 0.40 |
| 25:BA:988:A:O4' | 25:BA:1155:A:H2 | 2.03 | 0.40 |
| 25:BA:988:A:H8 | 25:BA:988:A:O5' | 2.04 | 0.40 |
| 38:BQ:38:GLN:CG | 38:BQ:47:THR:HG21 | 2.51 | 0.40 |
| 1:AA:1405:G:H2' | 1:AA:1406:U:O5' | 2.22 | 0.40 |
| 4:AG:146:ILE:CD1 | 4:AG:146:ILE:N | 2.84 | 0.40 |
| 1:CA:810:C:C2' | 1:CA:811:C:H5' | 2.51 | 0.40 |
| 25:DA:637:A:OP1 | 35:DO:133:SER:HB3 | 2.21 | 0.40 |
| 7:AJ:31:MET:CE | 7:AJ:36:LYS:HZ2 | 2.35 | 0.40 |
| 25:BA:1043:C:C2' | 25:BA:1044:G:H5' | 2.51 | 0.40 |
| 35:BO:91:PHE:HZ | 35:BO:103:ALA:CB | 2.33 | 0.40 |
| 4:CG:60:GLU:OE2 | 4:CG:199:ASN:N | 2.53 | 0.40 |
| 25:DA:2103:C:H2' | 25:DA:2104:G:H8 | 1.83 | 0.40 |
| 1:AA:1429:C:H2' | 1:AA:1430:C:C6 | 2.56 | 0.40 |
| 1:CA:1292:U:H2' | 1:CA:1293:G:C8 | 2.57 | 0.40 |
| 25:DA:1889:A:H2' | 25:DA:1890:A:O4' | 2.22 | 0.40 |
| 25:BA:2855:C:H2' | 25:BA:2856:C:C6 | 2.55 | 0.40 |
| 1:CA:949:A:C2 | 1:CA:1233:G:N3 | 2.89 | 0.40 |
| 45:DV:6:LYS:H | 45:DV:6:LYS:HG3 | 1.65 | 0.40 |
| 27:BD:161:THR:O | 27:BD:162:SER:HB3 | 2.22 | 0.40 |
| 43:BT:92:LEU:HD23 | 43:BT:92:LEU:HA | 1.84 | 0.40 |
| 25:BA:1758:G:H4' | 25:BA:1759:A:OP2 | 2.20 | 0.40 |
| 7:AJ:56:GLN:H | 7:AJ:56:GLN:HG2 | 1.65 | 0.40 |
| 25:DA:2695:C:H2' | 25:DA:2696:U:H6 | 1.85 | 0.40 |
| 3:AF:108:ASN:HB3 | 3:AF:111:LEU:HB2 | 2.04 | 0.40 |
| 4:AG:144:ASP:O | 4:AG:184:LYS:HA | 2.22 | 0.40 |
| 25:BA:2841:C:C2 | 25:BA:2877:G:N2 | 2.90 | 0.40 |
| 25:BA:1726:G:H2' | 25:BA:1727:U:O4' | 2.21 | 0.40 |
| 25:BA:2559:C:H2' | 25:BA:2560:C:H6 | 1.86 | 0.40 |
| 25:DA:506:G:H5'' | 25:DA:509:C:H1' | 2.04 | 0.40 |
| 1:CA:836:G:C6 | 1:CA:851:G:C6 | 3.10 | 0.40 |
| 42:DS:37:ARG:HG2 | 42:DS:38:TYR:CE2 | 2.57 | 0.40 |
| 25:DA:1903:G:OP1 | 27:DD:241:PRO:HB2 | 2.21 | 0.40 |
| 38:BQ:99:LYS:O | 38:BQ:103:GLU:HG3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 25:DA:826:U:H2' | 25:DA:828:U:O4' | 2.22 | 0.40 |
| 25:BA:1018:C:H2' | 25:BA:1018:C:O2 | 2.21 | 0.40 |

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

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------------|-------------|----------|
| 1:AA:85:U:O2' | 31:DH:100:GLY:O[3_555] | 1.90 | 0.30 |
| 1:CA:86:U:O2' | 25:DA:276:A:OP2[3_545] | 2.02 | 0.18 |
| 6:AI:15:ASP:OD2 | 4:CG:27:TYR:OH[4_555] | 2.17 | 0.03 |

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | AE | 235/256 (92%) | 190 (81%) | 45 (19%) | 0 | 100 | 100 |
| 2 | CE | 235/256 (92%) | 190 (81%) | 41 (17%) | 4 (2%) | 14 | 54 |
| 3 | AF | 203/239 (85%) | 179 (88%) | 24 (12%) | 0 | 100 | 100 |
| 3 | CF | 204/239 (85%) | 179 (88%) | 23 (11%) | 2 (1%) | 22 | 70 |
| 4 | AG | 206/208 (99%) | 179 (87%) | 24 (12%) | 3 (2%) | 15 | 58 |
| 4 | CG | 206/208 (99%) | 179 (87%) | 25 (12%) | 2 (1%) | 22 | 70 |
| 5 | AH | 149/162 (92%) | 137 (92%) | 10 (7%) | 2 (1%) | 18 | 62 |
| 5 | CH | 149/162 (92%) | 139 (93%) | 10 (7%) | 0 | 100 | 100 |
| 6 | AI | 99/101 (98%) | 92 (93%) | 7 (7%) | 0 | 100 | 100 |
| 6 | CI | 99/101 (98%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |
| 7 | AJ | 153/156 (98%) | 142 (93%) | 11 (7%) | 0 | 100 | 100 |
| 7 | CJ | 153/156 (98%) | 143 (94%) | 10 (6%) | 0 | 100 | 100 |
| 8 | AK | 136/138 (99%) | 123 (90%) | 12 (9%) | 1 (1%) | 30 | 78 |
| 8 | CK | 136/138 (99%) | 123 (90%) | 13 (10%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9 | AL | 125/128 (98%) | 110 (88%) | 15 (12%) | 0 | 100 | 100 |
| 9 | CL | 125/128 (98%) | 114 (91%) | 11 (9%) | 0 | 100 | 100 |
| 10 | AM | 97/105 (92%) | 86 (89%) | 11 (11%) | 0 | 100 | 100 |
| 10 | CM | 97/105 (92%) | 84 (87%) | 9 (9%) | 4 (4%) | 4 | 24 |
| 11 | AN | 117/129 (91%) | 102 (87%) | 14 (12%) | 1 (1%) | 25 | 73 |
| 11 | CN | 117/129 (91%) | 104 (89%) | 13 (11%) | 0 | 100 | 100 |
| 12 | AO | 123/132 (93%) | 105 (85%) | 16 (13%) | 2 (2%) | 14 | 56 |
| 12 | CO | 123/132 (93%) | 105 (85%) | 15 (12%) | 3 (2%) | 9 | 42 |
| 13 | AP | 114/126 (90%) | 89 (78%) | 23 (20%) | 2 (2%) | 13 | 53 |
| 13 | CP | 115/126 (91%) | 96 (84%) | 17 (15%) | 2 (2%) | 14 | 54 |
| 14 | AQ | 58/61 (95%) | 49 (84%) | 9 (16%) | 0 | 100 | 100 |
| 14 | CQ | 58/61 (95%) | 49 (84%) | 8 (14%) | 1 (2%) | 14 | 54 |
| 15 | AR | 86/89 (97%) | 74 (86%) | 11 (13%) | 1 (1%) | 19 | 64 |
| 15 | CR | 86/89 (97%) | 76 (88%) | 10 (12%) | 0 | 100 | 100 |
| 16 | AS | 82/88 (93%) | 71 (87%) | 8 (10%) | 3 (4%) | 5 | 28 |
| 16 | CS | 82/88 (93%) | 75 (92%) | 7 (8%) | 0 | 100 | 100 |
| 17 | AT | 98/105 (93%) | 91 (93%) | 7 (7%) | 0 | 100 | 100 |
| 17 | CT | 98/105 (93%) | 91 (93%) | 7 (7%) | 0 | 100 | 100 |
| 18 | AU | 70/88 (80%) | 64 (91%) | 5 (7%) | 1 (1%) | 16 | 60 |
| 18 | CU | 70/88 (80%) | 61 (87%) | 9 (13%) | 0 | 100 | 100 |
| 19 | AV | 76/93 (82%) | 68 (90%) | 6 (8%) | 2 (3%) | 8 | 39 |
| 19 | CV | 76/93 (82%) | 60 (79%) | 12 (16%) | 4 (5%) | 3 | 18 |
| 20 | AW | 97/106 (92%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 20 | CW | 97/106 (92%) | 80 (82%) | 16 (16%) | 1 (1%) | 22 | 70 |
| 21 | AX | 23/27 (85%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 21 | CX | 23/27 (85%) | 21 (91%) | 2 (9%) | 0 | 100 | 100 |
| 27 | BD | 270/276 (98%) | 243 (90%) | 22 (8%) | 5 (2%) | 12 | 51 |
| 27 | DD | 270/276 (98%) | 248 (92%) | 15 (6%) | 7 (3%) | 8 | 39 |
| 28 | BE | 203/206 (98%) | 149 (73%) | 30 (15%) | 24 (12%) | 1 | 2 |
| 28 | DE | 203/206 (98%) | 144 (71%) | 41 (20%) | 18 (9%) | 1 | 5 |
| 29 | BF | 200/210 (95%) | 179 (90%) | 21 (10%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 29 | DF | 206/210 (98%) | 168 (82%) | 30 (15%) | 8 (4%) | 5 | 26 |
| 30 | BG | 179/182 (98%) | 154 (86%) | 20 (11%) | 5 (3%) | 8 | 37 |
| 30 | DG | 179/182 (98%) | 150 (84%) | 28 (16%) | 1 (1%) | 33 | 81 |
| 31 | BH | 168/180 (93%) | 133 (79%) | 28 (17%) | 7 (4%) | 4 | 24 |
| 31 | DH | 168/180 (93%) | 125 (74%) | 35 (21%) | 8 (5%) | 4 | 20 |
| 32 | BK | 144/148 (97%) | 102 (71%) | 32 (22%) | 10 (7%) | 2 | 9 |
| 32 | DK | 144/148 (97%) | 113 (78%) | 28 (19%) | 3 (2%) | 11 | 47 |
| 33 | BM | 136/140 (97%) | 113 (83%) | 16 (12%) | 7 (5%) | 3 | 18 |
| 33 | DM | 136/140 (97%) | 119 (88%) | 15 (11%) | 2 (2%) | 15 | 58 |
| 34 | BN | 120/122 (98%) | 111 (92%) | 9 (8%) | 0 | 100 | 100 |
| 34 | DN | 120/122 (98%) | 113 (94%) | 6 (5%) | 1 (1%) | 27 | 76 |
| 35 | BO | 148/150 (99%) | 107 (72%) | 27 (18%) | 14 (10%) | 1 | 4 |
| 35 | DO | 148/150 (99%) | 102 (69%) | 24 (16%) | 22 (15%) | 0 | 1 |
| 36 | BP | 139/141 (99%) | 109 (78%) | 27 (19%) | 3 (2%) | 10 | 45 |
| 36 | DP | 139/141 (99%) | 93 (67%) | 30 (22%) | 16 (12%) | 1 | 3 |
| 37 | B0 | 116/118 (98%) | 101 (87%) | 13 (11%) | 2 (2%) | 14 | 54 |
| 37 | D0 | 115/118 (98%) | 109 (95%) | 6 (5%) | 0 | 100 | 100 |
| 38 | BQ | 109/112 (97%) | 86 (79%) | 20 (18%) | 3 (3%) | 8 | 37 |
| 38 | DQ | 109/112 (97%) | 87 (80%) | 19 (17%) | 3 (3%) | 8 | 37 |
| 39 | BR | 135/146 (92%) | 114 (84%) | 21 (16%) | 0 | 100 | 100 |
| 39 | DR | 135/146 (92%) | 119 (88%) | 14 (10%) | 2 (2%) | 15 | 58 |
| 40 | B1 | 115/118 (98%) | 103 (90%) | 11 (10%) | 1 (1%) | 25 | 73 |
| 40 | D1 | 115/118 (98%) | 101 (88%) | 14 (12%) | 0 | 100 | 100 |
| 41 | B2 | 99/101 (98%) | 92 (93%) | 5 (5%) | 2 (2%) | 11 | 48 |
| 41 | D2 | 99/101 (98%) | 78 (79%) | 14 (14%) | 7 (7%) | 2 | 9 |
| 42 | BS | 111/113 (98%) | 97 (87%) | 10 (9%) | 4 (4%) | 5 | 29 |
| 42 | DS | 111/113 (98%) | 103 (93%) | 8 (7%) | 0 | 100 | 100 |
| 43 | BT | 90/96 (94%) | 84 (93%) | 4 (4%) | 2 (2%) | 10 | 45 |
| 43 | DT | 90/96 (94%) | 78 (87%) | 10 (11%) | 2 (2%) | 10 | 45 |
| 44 | BU | 100/110 (91%) | 80 (80%) | 15 (15%) | 5 (5%) | 3 | 19 |
| 44 | DU | 100/110 (91%) | 70 (70%) | 24 (24%) | 6 (6%) | 2 | 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 45 | BV | 173/206 (84%) | 129 (75%) | 37 (21%) | 7 (4%) | 5 | 25 |
| 45 | DV | 177/206 (86%) | 132 (75%) | 35 (20%) | 10 (6%) | 3 | 16 |
| 46 | B3 | 74/85 (87%) | 67 (90%) | 5 (7%) | 2 (3%) | 8 | 38 |
| 46 | D3 | 75/85 (88%) | 69 (92%) | 6 (8%) | 0 | 100 | 100 |
| 47 | BZ | 95/98 (97%) | 85 (90%) | 7 (7%) | 3 (3%) | 6 | 33 |
| 47 | DZ | 95/98 (97%) | 84 (88%) | 10 (10%) | 1 (1%) | 21 | 67 |
| 48 | BW | 64/72 (89%) | 58 (91%) | 4 (6%) | 2 (3%) | 7 | 34 |
| 48 | DW | 67/72 (93%) | 60 (90%) | 6 (9%) | 1 (2%) | 15 | 58 |
| 49 | BX | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 49 | DX | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 50 | B4 | 64/71 (90%) | 41 (64%) | 21 (33%) | 2 (3%) | 7 | 34 |
| 50 | D4 | 61/71 (86%) | 32 (52%) | 28 (46%) | 1 (2%) | 14 | 56 |
| 51 | B5 | 57/60 (95%) | 49 (86%) | 7 (12%) | 1 (2%) | 13 | 53 |
| 51 | D5 | 56/60 (93%) | 48 (86%) | 7 (12%) | 1 (2%) | 13 | 53 |
| 52 | B6 | 43/54 (80%) | 27 (63%) | 14 (33%) | 2 (5%) | 4 | 21 |
| 52 | D6 | 43/54 (80%) | 29 (67%) | 10 (23%) | 4 (9%) | 1 | 5 |
| 53 | B7 | 47/49 (96%) | 44 (94%) | 3 (6%) | 0 | 100 | 100 |
| 53 | D7 | 47/49 (96%) | 45 (96%) | 2 (4%) | 0 | 100 | 100 |
| 54 | B8 | 59/65 (91%) | 47 (80%) | 7 (12%) | 5 (8%) | 1 | 6 |
| 54 | D8 | 59/65 (91%) | 40 (68%) | 12 (20%) | 7 (12%) | 1 | 2 |
| All | All | 11335/12052 (94%) | 9588 (85%) | 1457 (13%) | 290 (3%) | 8 | 39 |

All (290) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AG | 13 | ARG |
| 4 | AG | 14 | ARG |
| 11 | AN | 82 | VAL |
| 16 | AS | 17 | TYR |
| 18 | AU | 22 | VAL |
| 27 | BD | 237 | GLU |
| 27 | BD | 271 | ILE |
| 28 | BE | 15 | PHE |
| 28 | BE | 48 | GLN |
| 28 | BE | 49 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BE | 54 | GLN |
| 28 | BE | 75 | VAL |
| 28 | BE | 83 | ASP |
| 30 | BG | 78 | SER |
| 30 | BG | 79 | ASN |
| 31 | BH | 165 | ALA |
| 31 | BH | 168 | PRO |
| 32 | BK | 15 | VAL |
| 32 | BK | 105 | HIS |
| 33 | BM | 22 | THR |
| 33 | BM | 46 | VAL |
| 33 | BM | 47 | ALA |
| 35 | BO | 10 | PRO |
| 35 | BO | 16 | ARG |
| 35 | BO | 56 | SER |
| 35 | BO | 57 | THR |
| 35 | BO | 58 | THR |
| 42 | BS | 92 | ARG |
| 42 | BS | 95 | ILE |
| 43 | BT | 68 | ARG |
| 45 | BV | 165 | VAL |
| 45 | BV | 171 | ILE |
| 50 | B4 | 50 | VAL |
| 51 | B5 | 4 | HIS |
| 52 | B6 | 45 | LYS |
| 54 | B8 | 32 | LEU |
| 3 | CF | 64 | VAL |
| 4 | CG | 14 | ARG |
| 10 | CM | 58 | ASP |
| 19 | CV | 31 | ILE |
| 27 | DD | 237 | GLU |
| 28 | DE | 9 | VAL |
| 28 | DE | 25 | VAL |
| 28 | DE | 37 | ARG |
| 28 | DE | 45 | THR |
| 28 | DE | 51 | PHE |
| 28 | DE | 54 | GLN |
| 28 | DE | 80 | GLU |
| 28 | DE | 81 | ILE |
| 29 | DF | 68 | LYS |
| 29 | DF | 89 | VAL |
| 31 | DH | 151 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | DH | 153 | LYS |
| 31 | DH | 155 | SER |
| 33 | DM | 46 | VAL |
| 35 | DO | 10 | PRO |
| 35 | DO | 16 | ARG |
| 35 | DO | 21 | ARG |
| 35 | DO | 35 | HIS |
| 35 | DO | 36 | LYS |
| 35 | DO | 46 | LYS |
| 35 | DO | 56 | SER |
| 35 | DO | 57 | THR |
| 35 | DO | 58 | THR |
| 36 | DP | 25 | ASP |
| 36 | DP | 60 | ARG |
| 36 | DP | 63 | LYS |
| 36 | DP | 67 | ARG |
| 36 | DP | 89 | ASN |
| 38 | DQ | 87 | PHE |
| 38 | DQ | 88 | ASP |
| 39 | DR | 55 | ASN |
| 41 | D2 | 71 | LEU |
| 41 | D2 | 79 | VAL |
| 41 | D2 | 83 | ARG |
| 41 | D2 | 84 | LYS |
| 45 | DV | 53 | ILE |
| 45 | DV | 146 | ILE |
| 45 | DV | 171 | ILE |
| 50 | D4 | 5 | ILE |
| 51 | D5 | 4 | HIS |
| 52 | D6 | 44 | ARG |
| 52 | D6 | 48 | VAL |
| 52 | D6 | 49 | HIS |
| 54 | D8 | 32 | LEU |
| 54 | D8 | 35 | GLN |
| 54 | D8 | 51 | ALA |
| 8 | AK | 86 | ILE |
| 13 | AP | 113 | PRO |
| 13 | AP | 116 | THR |
| 16 | AS | 15 | PRO |
| 27 | BD | 28 | GLU |
| 28 | BE | 37 | ARG |
| 28 | BE | 47 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BE | 57 | LYS |
| 28 | BE | 58 | ARG |
| 28 | BE | 78 | LEU |
| 28 | BE | 81 | ILE |
| 28 | BE | 82 | ARG |
| 30 | BG | 82 | LEU |
| 32 | BK | 100 | ALA |
| 32 | BK | 106 | GLY |
| 32 | BK | 144 | VAL |
| 33 | BM | 9 | VAL |
| 33 | BM | 97 | ARG |
| 35 | BO | 12 | ALA |
| 35 | BO | 65 | ARG |
| 35 | BO | 66 | GLY |
| 35 | BO | 67 | MET |
| 36 | BP | 66 | ILE |
| 38 | BQ | 89 | ARG |
| 40 | B1 | 93 | LYS |
| 43 | BT | 67 | GLY |
| 45 | BV | 53 | ILE |
| 48 | BW | 16 | LEU |
| 50 | B4 | 5 | ILE |
| 52 | B6 | 46 | HIS |
| 54 | B8 | 34 | TRP |
| 54 | B8 | 35 | GLN |
| 54 | B8 | 37 | SER |
| 2 | CE | 7 | VAL |
| 2 | CE | 74 | LYS |
| 10 | CM | 57 | LYS |
| 12 | CO | 26 | ALA |
| 19 | CV | 9 | VAL |
| 19 | CV | 67 | VAL |
| 19 | CV | 68 | GLY |
| 28 | DE | 34 | VAL |
| 28 | DE | 131 | ALA |
| 29 | DF | 87 | GLY |
| 29 | DF | 91 | GLY |
| 31 | DH | 169 | VAL |
| 32 | DK | 143 | SER |
| 32 | DK | 144 | VAL |
| 35 | DO | 11 | GLY |
| 35 | DO | 12 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DO | 38 | GLN |
| 35 | DO | 50 | ARG |
| 35 | DO | 65 | ARG |
| 35 | DO | 66 | GLY |
| 35 | DO | 67 | MET |
| 36 | DP | 7 | MET |
| 36 | DP | 19 | GLY |
| 36 | DP | 27 | VAL |
| 36 | DP | 28 | ALA |
| 36 | DP | 29 | PHE |
| 36 | DP | 66 | ILE |
| 36 | DP | 79 | LEU |
| 36 | DP | 88 | GLY |
| 38 | DQ | 89 | ARG |
| 39 | DR | 57 | PHE |
| 41 | D2 | 45 | THR |
| 44 | DU | 77 | PRO |
| 45 | DV | 142 | SER |
| 45 | DV | 145 | GLU |
| 45 | DV | 165 | VAL |
| 54 | D8 | 48 | PHE |
| 54 | D8 | 49 | VAL |
| 12 | AO | 18 | VAL |
| 12 | AO | 48 | PRO |
| 28 | BE | 17 | ASP |
| 28 | BE | 42 | ASP |
| 28 | BE | 52 | LEU |
| 28 | BE | 79 | ARG |
| 31 | BH | 84 | SER |
| 31 | BH | 154 | PRO |
| 32 | BK | 11 | ASN |
| 32 | BK | 101 | LEU |
| 32 | BK | 145 | VAL |
| 35 | BO | 6 | LEU |
| 38 | BQ | 86 | ALA |
| 41 | B2 | 45 | THR |
| 42 | BS | 94 | ASP |
| 44 | BU | 39 | VAL |
| 45 | BV | 7 | ALA |
| 45 | BV | 141 | VAL |
| 46 | B3 | 83 | PRO |
| 46 | B3 | 84 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | BZ | 82 | LEU |
| 47 | BZ | 92 | LYS |
| 54 | B8 | 11 | LYS |
| 2 | CE | 153 | ARG |
| 28 | DE | 53 | PRO |
| 28 | DE | 82 | ARG |
| 29 | DF | 84 | VAL |
| 35 | DO | 6 | LEU |
| 41 | D2 | 85 | LYS |
| 45 | DV | 116 | VAL |
| 52 | D6 | 45 | LYS |
| 54 | D8 | 50 | LEU |
| 16 | AS | 16 | HIS |
| 28 | BE | 4 | ILE |
| 28 | BE | 14 | ILE |
| 28 | BE | 39 | PRO |
| 28 | BE | 53 | PRO |
| 31 | BH | 83 | TYR |
| 32 | BK | 39 | ALA |
| 38 | BQ | 85 | VAL |
| 44 | BU | 42 | VAL |
| 44 | BU | 49 | VAL |
| 44 | BU | 77 | PRO |
| 10 | CM | 32 | ALA |
| 14 | CQ | 14 | PRO |
| 20 | CW | 95 | ALA |
| 27 | DD | 26 | LYS |
| 27 | DD | 28 | GLU |
| 29 | DF | 92 | PRO |
| 31 | DH | 152 | ARG |
| 31 | DH | 154 | PRO |
| 41 | D2 | 49 | THR |
| 44 | DU | 49 | VAL |
| 45 | DV | 161 | VAL |
| 4 | AG | 156 | GLU |
| 15 | AR | 87 | ILE |
| 27 | BD | 240 | ALA |
| 33 | BM | 128 | HIS |
| 35 | BO | 7 | ARG |
| 35 | BO | 11 | GLY |
| 35 | BO | 62 | LEU |
| 47 | BZ | 88 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | CG | 151 | LYS |
| 10 | CM | 86 | MET |
| 12 | CO | 79 | GLU |
| 27 | DD | 29 | PRO |
| 27 | DD | 239 | ARG |
| 28 | DE | 26 | ILE |
| 28 | DE | 52 | LEU |
| 28 | DE | 83 | ASP |
| 29 | DF | 128 | ALA |
| 29 | DF | 132 | VAL |
| 33 | DM | 128 | HIS |
| 34 | DN | 48 | PRO |
| 35 | DO | 23 | PRO |
| 35 | DO | 48 | PRO |
| 35 | DO | 62 | LEU |
| 36 | DP | 21 | THR |
| 36 | DP | 90 | VAL |
| 28 | BE | 62 | PRO |
| 28 | BE | 118 | LYS |
| 30 | BG | 81 | LYS |
| 33 | BM | 115 | ARG |
| 37 | B0 | 11 | ASN |
| 37 | B0 | 71 | GLN |
| 48 | BW | 15 | LYS |
| 27 | DD | 240 | ALA |
| 28 | DE | 61 | ARG |
| 30 | DG | 5 | VAL |
| 43 | DT | 68 | ARG |
| 44 | DU | 85 | VAL |
| 19 | AV | 9 | VAL |
| 19 | AV | 41 | VAL |
| 28 | BE | 72 | VAL |
| 30 | BG | 5 | VAL |
| 32 | BK | 133 | HIS |
| 35 | BO | 95 | VAL |
| 12 | CO | 47 | LYS |
| 28 | DE | 134 | ILE |
| 43 | DT | 51 | VAL |
| 48 | DW | 17 | SER |
| 44 | BU | 3 | VAL |
| 45 | BV | 161 | VAL |
| 2 | CE | 39 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CF | 66 | VAL |
| 27 | DD | 3 | VAL |
| 28 | DE | 62 | PRO |
| 35 | DO | 34 | GLY |
| 44 | DU | 42 | VAL |
| 54 | D8 | 53 | PRO |
| 5 | AH | 70 | PRO |
| 5 | AH | 115 | VAL |
| 31 | BH | 167 | GLU |
| 45 | BV | 166 | SER |
| 13 | CP | 117 | VAL |
| 31 | DH | 49 | VAL |
| 31 | DH | 167 | GLU |
| 32 | DK | 145 | VAL |
| 35 | DO | 7 | ARG |
| 36 | DP | 61 | GLY |
| 45 | DV | 141 | VAL |
| 47 | DZ | 30 | VAL |
| 36 | BP | 27 | VAL |
| 41 | B2 | 49 | THR |
| 44 | DU | 3 | VAL |
| 27 | BD | 35 | LYS |
| 31 | BH | 10 | PRO |
| 36 | BP | 90 | VAL |
| 42 | BS | 59 | VAL |
| 13 | CP | 84 | ILE |
| 44 | DU | 96 | ILE |
| 45 | DV | 61 | LEU |

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 | AE | 205/220 (93%) | 155 (76%) | 50 (24%) | 1 | 5 |
| 2 | CE | 205/220 (93%) | 159 (78%) | 46 (22%) | 1 | 7 |
| 3 | AF | 159/188 (85%) | 120 (76%) | 39 (24%) | 1 | 5 |
| 3 | CF | 160/188 (85%) | 124 (78%) | 36 (22%) | 1 | 7 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4 | AG | 180/180 (100%) | 144 (80%) | 36 (20%) | 2 | 10 |
| 4 | CG | 180/180 (100%) | 140 (78%) | 40 (22%) | 1 | 7 |
| 5 | AH | 116/123 (94%) | 88 (76%) | 28 (24%) | 1 | 5 |
| 5 | CH | 116/123 (94%) | 89 (77%) | 27 (23%) | 1 | 6 |
| 6 | AI | 90/90 (100%) | 76 (84%) | 14 (16%) | 4 | 18 |
| 6 | CI | 90/90 (100%) | 74 (82%) | 16 (18%) | 2 | 14 |
| 7 | AJ | 126/127 (99%) | 104 (82%) | 22 (18%) | 3 | 14 |
| 7 | CJ | 126/127 (99%) | 89 (71%) | 37 (29%) | 0 | 2 |
| 8 | AK | 119/119 (100%) | 100 (84%) | 19 (16%) | 3 | 17 |
| 8 | CK | 119/119 (100%) | 94 (79%) | 25 (21%) | 1 | 8 |
| 9 | AL | 98/99 (99%) | 70 (71%) | 28 (29%) | 0 | 3 |
| 9 | CL | 98/99 (99%) | 69 (70%) | 29 (30%) | 0 | 2 |
| 10 | AM | 89/92 (97%) | 66 (74%) | 23 (26%) | 1 | 4 |
| 10 | CM | 89/92 (97%) | 60 (67%) | 29 (33%) | 0 | 2 |
| 11 | AN | 90/99 (91%) | 74 (82%) | 16 (18%) | 2 | 14 |
| 11 | CN | 90/99 (91%) | 73 (81%) | 17 (19%) | 2 | 12 |
| 12 | AO | 104/109 (95%) | 88 (85%) | 16 (15%) | 4 | 19 |
| 12 | CO | 104/109 (95%) | 80 (77%) | 24 (23%) | 1 | 6 |
| 13 | AP | 94/101 (93%) | 71 (76%) | 23 (24%) | 1 | 5 |
| 13 | CP | 94/101 (93%) | 75 (80%) | 19 (20%) | 2 | 10 |
| 14 | AQ | 49/50 (98%) | 33 (67%) | 16 (33%) | 0 | 2 |
| 14 | CQ | 49/50 (98%) | 39 (80%) | 10 (20%) | 2 | 9 |
| 15 | AR | 79/80 (99%) | 68 (86%) | 11 (14%) | 5 | 23 |
| 15 | CR | 79/80 (99%) | 66 (84%) | 13 (16%) | 3 | 16 |
| 16 | AS | 72/74 (97%) | 53 (74%) | 19 (26%) | 1 | 4 |
| 16 | CS | 72/74 (97%) | 62 (86%) | 10 (14%) | 5 | 23 |
| 17 | AT | 95/97 (98%) | 82 (86%) | 13 (14%) | 5 | 24 |
| 17 | CT | 95/97 (98%) | 89 (94%) | 6 (6%) | 25 | 66 |
| 18 | AU | 63/77 (82%) | 50 (79%) | 13 (21%) | 2 | 9 |
| 18 | CU | 63/77 (82%) | 48 (76%) | 15 (24%) | 1 | 5 |
| 19 | AV | 67/80 (84%) | 47 (70%) | 20 (30%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 19 | CV | 67/80 (84%) | 53 (79%) | 14 (21%) | 1 | 8 |
| 20 | AW | 76/82 (93%) | 60 (79%) | 16 (21%) | 1 | 8 |
| 20 | CW | 76/82 (93%) | 55 (72%) | 21 (28%) | 0 | 3 |
| 21 | AX | 20/22 (91%) | 17 (85%) | 3 (15%) | 4 | 20 |
| 21 | CX | 20/22 (91%) | 20 (100%) | 0 | 100 | 100 |
| 27 | BD | 214/218 (98%) | 172 (80%) | 42 (20%) | 2 | 11 |
| 27 | DD | 214/218 (98%) | 162 (76%) | 52 (24%) | 1 | 5 |
| 28 | BE | 165/166 (99%) | 114 (69%) | 51 (31%) | 0 | 2 |
| 28 | DE | 165/166 (99%) | 121 (73%) | 44 (27%) | 1 | 4 |
| 29 | BF | 161/166 (97%) | 129 (80%) | 32 (20%) | 2 | 10 |
| 29 | DF | 165/166 (99%) | 122 (74%) | 43 (26%) | 1 | 4 |
| 30 | BG | 155/156 (99%) | 115 (74%) | 40 (26%) | 1 | 4 |
| 30 | DG | 155/156 (99%) | 113 (73%) | 42 (27%) | 1 | 3 |
| 31 | BH | 142/148 (96%) | 107 (75%) | 35 (25%) | 1 | 4 |
| 31 | DH | 142/148 (96%) | 110 (78%) | 32 (22%) | 1 | 7 |
| 32 | BK | 122/124 (98%) | 91 (75%) | 31 (25%) | 1 | 4 |
| 32 | DK | 122/124 (98%) | 84 (69%) | 38 (31%) | 0 | 2 |
| 33 | BM | 117/119 (98%) | 87 (74%) | 30 (26%) | 1 | 4 |
| 33 | DM | 117/119 (98%) | 96 (82%) | 21 (18%) | 2 | 13 |
| 34 | BN | 100/100 (100%) | 83 (83%) | 17 (17%) | 3 | 15 |
| 34 | DN | 100/100 (100%) | 78 (78%) | 22 (22%) | 1 | 7 |
| 35 | BO | 116/116 (100%) | 78 (67%) | 38 (33%) | 0 | 2 |
| 35 | DO | 116/116 (100%) | 72 (62%) | 44 (38%) | 0 | 1 |
| 36 | BP | 111/111 (100%) | 84 (76%) | 27 (24%) | 1 | 5 |
| 36 | DP | 111/111 (100%) | 85 (77%) | 26 (23%) | 1 | 5 |
| 37 | B0 | 101/101 (100%) | 78 (77%) | 23 (23%) | 1 | 6 |
| 37 | D0 | 100/101 (99%) | 80 (80%) | 20 (20%) | 2 | 10 |
| 38 | BQ | 87/88 (99%) | 65 (75%) | 22 (25%) | 1 | 4 |
| 38 | DQ | 87/88 (99%) | 53 (61%) | 34 (39%) | 0 | 1 |
| 39 | BR | 120/127 (94%) | 92 (77%) | 28 (23%) | 1 | 6 |
| 39 | DR | 120/127 (94%) | 84 (70%) | 36 (30%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-------------|----|
| 40 | B1 | 93/94 (99%) | 76 (82%) | 17 (18%) | 2 | 13 |
| 40 | D1 | 93/94 (99%) | 80 (86%) | 13 (14%) | 5 | 23 |
| 41 | B2 | 82/82 (100%) | 61 (74%) | 21 (26%) | 1 | 4 |
| 41 | D2 | 82/82 (100%) | 50 (61%) | 32 (39%) | 0 | 1 |
| 42 | BS | 92/92 (100%) | 72 (78%) | 20 (22%) | 1 | 8 |
| 42 | DS | 92/92 (100%) | 65 (71%) | 27 (29%) | 0 | 2 |
| 43 | BT | 74/78 (95%) | 61 (82%) | 13 (18%) | 3 | 14 |
| 43 | DT | 74/78 (95%) | 57 (77%) | 17 (23%) | 1 | 6 |
| 44 | BU | 85/91 (93%) | 65 (76%) | 20 (24%) | 1 | 5 |
| 44 | DU | 85/91 (93%) | 51 (60%) | 34 (40%) | 0 | 0 |
| 45 | BV | 154/179 (86%) | 116 (75%) | 38 (25%) | 1 | 4 |
| 45 | DV | 158/179 (88%) | 124 (78%) | 34 (22%) | 1 | 8 |
| 46 | B3 | 61/67 (91%) | 54 (88%) | 7 (12%) | 8 | 32 |
| 46 | D3 | 62/67 (92%) | 47 (76%) | 15 (24%) | 1 | 5 |
| 47 | BZ | 82/83 (99%) | 64 (78%) | 18 (22%) | 1 | 7 |
| 47 | DZ | 82/83 (99%) | 64 (78%) | 18 (22%) | 1 | 7 |
| 48 | BW | 62/67 (92%) | 42 (68%) | 20 (32%) | 0 | 2 |
| 48 | DW | 64/67 (96%) | 50 (78%) | 14 (22%) | 1 | 7 |
| 49 | BX | 51/52 (98%) | 41 (80%) | 10 (20%) | 2 | 11 |
| 49 | DX | 51/52 (98%) | 42 (82%) | 9 (18%) | 3 | 14 |
| 50 | B4 | 59/63 (94%) | 41 (70%) | 18 (30%) | 0 | 2 |
| 50 | D4 | 57/63 (90%) | 38 (67%) | 19 (33%) | 0 | 2 |
| 51 | B5 | 51/52 (98%) | 35 (69%) | 16 (31%) | 0 | 2 |
| 51 | D5 | 51/52 (98%) | 37 (72%) | 14 (28%) | 0 | 3 |
| 52 | B6 | 44/52 (85%) | 27 (61%) | 17 (39%) | 0 | 1 |
| 52 | D6 | 44/52 (85%) | 31 (70%) | 13 (30%) | 0 | 2 |
| 53 | B7 | 42/42 (100%) | 34 (81%) | 8 (19%) | 2 | 12 |
| 53 | D7 | 42/42 (100%) | 32 (76%) | 10 (24%) | 1 | 5 |
| 54 | B8 | 51/55 (93%) | 40 (78%) | 11 (22%) | 1 | 8 |
| 54 | D8 | 51/55 (93%) | 41 (80%) | 10 (20%) | 2 | 11 |
| All | All | 9579/9996 (96%) | 7317 (76%) | 2262 (24%) | 1 | 5 |

All (2262) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AE | 4 | GLU |
| 2 | AE | 8 | LYS |
| 2 | AE | 9 | GLU |
| 2 | AE | 12 | GLU |
| 2 | AE | 15 | VAL |
| 2 | AE | 16 | HIS |
| 2 | AE | 17 | PHE |
| 2 | AE | 20 | GLU |
| 2 | AE | 21 | ARG |
| 2 | AE | 22 | LYS |
| 2 | AE | 24 | TRP |
| 2 | AE | 32 | ILE |
| 2 | AE | 64 | ARG |
| 2 | AE | 67 | THR |
| 2 | AE | 68 | ILE |
| 2 | AE | 71 | VAL |
| 2 | AE | 75 | LYS |
| 2 | AE | 78 | GLN |
| 2 | AE | 82 | ARG |
| 2 | AE | 96 | ARG |
| 2 | AE | 107 | THR |
| 2 | AE | 111 | ARG |
| 2 | AE | 112 | VAL |
| 2 | AE | 119 | GLU |
| 2 | AE | 121 | LEU |
| 2 | AE | 144 | ARG |
| 2 | AE | 145 | LEU |
| 2 | AE | 154 | LEU |
| 2 | AE | 156 | LYS |
| 2 | AE | 163 | PHE |
| 2 | AE | 164 | VAL |
| 2 | AE | 169 | LYS |
| 2 | AE | 172 | ILE |
| 2 | AE | 174 | VAL |
| 2 | AE | 176 | GLU |
| 2 | AE | 178 | ARG |
| 2 | AE | 179 | LYS |
| 2 | AE | 185 | ILE |
| 2 | AE | 187 | LEU |
| 2 | AE | 190 | THR |
| 2 | AE | 191 | ASP |
| 2 | AE | 196 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AE | 200 | ILE |
| 2 | AE | 204 | ASN |
| 2 | AE | 211 | ILE |
| 2 | AE | 214 | ILE |
| 2 | AE | 215 | LEU |
| 2 | AE | 222 | ILE |
| 2 | AE | 223 | ILE |
| 2 | AE | 240 | GLN |
| 3 | AF | 3 | ASN |
| 3 | AF | 5 | ILE |
| 3 | AF | 6 | HIS |
| 3 | AF | 14 | ILE |
| 3 | AF | 15 | THR |
| 3 | AF | 20 | SER |
| 3 | AF | 21 | ARG |
| 3 | AF | 26 | LYS |
| 3 | AF | 27 | LYS |
| 3 | AF | 29 | TYR |
| 3 | AF | 32 | LEU |
| 3 | AF | 36 | ASP |
| 3 | AF | 38 | ARG |
| 3 | AF | 40 | ARG |
| 3 | AF | 47 | LEU |
| 3 | AF | 49 | SER |
| 3 | AF | 52 | LEU |
| 3 | AF | 62 | ASP |
| 3 | AF | 63 | ASN |
| 3 | AF | 64 | VAL |
| 3 | AF | 79 | ARG |
| 3 | AF | 85 | ARG |
| 3 | AF | 104 | GLN |
| 3 | AF | 111 | LEU |
| 3 | AF | 125 | GLU |
| 3 | AF | 126 | ARG |
| 3 | AF | 128 | PHE |
| 3 | AF | 132 | ARG |
| 3 | AF | 136 | GLN |
| 3 | AF | 138 | VAL |
| 3 | AF | 152 | ILE |
| 3 | AF | 154 | SER |
| 3 | AF | 161 | GLU |
| 3 | AF | 165 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AF | 167 | TRP |
| 3 | AF | 188 | LEU |
| 3 | AF | 192 | THR |
| 3 | AF | 196 | LEU |
| 3 | AF | 202 | ILE |
| 4 | AG | 3 | ARG |
| 4 | AG | 10 | ARG |
| 4 | AG | 11 | LEU |
| 4 | AG | 12 | CYS |
| 4 | AG | 13 | ARG |
| 4 | AG | 14 | ARG |
| 4 | AG | 15 | GLU |
| 4 | AG | 19 | LEU |
| 4 | AG | 26 | CYS |
| 4 | AG | 30 | LYS |
| 4 | AG | 33 | MET |
| 4 | AG | 35 | ARG |
| 4 | AG | 52 | SER |
| 4 | AG | 58 | LEU |
| 4 | AG | 65 | ARG |
| 4 | AG | 84 | LYS |
| 4 | AG | 86 | LYS |
| 4 | AG | 96 | LEU |
| 4 | AG | 110 | PHE |
| 4 | AG | 114 | ARG |
| 4 | AG | 122 | ARG |
| 4 | AG | 127 | THR |
| 4 | AG | 132 | ARG |
| 4 | AG | 134 | ASP |
| 4 | AG | 135 | LEU |
| 4 | AG | 139 | ARG |
| 4 | AG | 154 | ASN |
| 4 | AG | 155 | LEU |
| 4 | AG | 181 | MET |
| 4 | AG | 188 | LEU |
| 4 | AG | 190 | ASP |
| 4 | AG | 192 | GLU |
| 4 | AG | 193 | ASP |
| 4 | AG | 194 | LEU |
| 4 | AG | 200 | GLU |
| 4 | AG | 201 | GLN |
| 5 | AH | 5 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AH | 10 | MET |
| 5 | AH | 11 | ILE |
| 5 | AH | 12 | LEU |
| 5 | AH | 16 | THR |
| 5 | AH | 20 | GLN |
| 5 | AH | 31 | LEU |
| 5 | AH | 33 | VAL |
| 5 | AH | 41 | VAL |
| 5 | AH | 43 | LEU |
| 5 | AH | 56 | GLN |
| 5 | AH | 57 | LYS |
| 5 | AH | 60 | TYR |
| 5 | AH | 64 | ARG |
| 5 | AH | 72 | GLN |
| 5 | AH | 73 | ASN |
| 5 | AH | 79 | GLU |
| 5 | AH | 81 | GLU |
| 5 | AH | 83 | GLU |
| 5 | AH | 87 | SER |
| 5 | AH | 91 | LEU |
| 5 | AH | 116 | THR |
| 5 | AH | 121 | LYS |
| 5 | AH | 126 | ARG |
| 5 | AH | 131 | ILE |
| 5 | AH | 147 | ASP |
| 5 | AH | 153 | LYS |
| 5 | AH | 155 | GLU |
| 6 | AI | 16 | GLN |
| 6 | AI | 19 | LEU |
| 6 | AI | 21 | LEU |
| 6 | AI | 23 | LYS |
| 6 | AI | 24 | GLU |
| 6 | AI | 25 | ILE |
| 6 | AI | 40 | VAL |
| 6 | AI | 55 | ASP |
| 6 | AI | 64 | GLN |
| 6 | AI | 71 | ARG |
| 6 | AI | 73 | ASN |
| 6 | AI | 75 | LEU |
| 6 | AI | 93 | SER |
| 6 | AI | 98 | LEU |
| 7 | AJ | 8 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AJ | 12 | LEU |
| 7 | AJ | 24 | THR |
| 7 | AJ | 27 | ILE |
| 7 | AJ | 33 | ASP |
| 7 | AJ | 35 | LYS |
| 7 | AJ | 38 | LEU |
| 7 | AJ | 49 | ILE |
| 7 | AJ | 56 | GLN |
| 7 | AJ | 63 | LYS |
| 7 | AJ | 78 | ARG |
| 7 | AJ | 80 | VAL |
| 7 | AJ | 89 | MET |
| 7 | AJ | 90 | GLU |
| 7 | AJ | 92 | SER |
| 7 | AJ | 104 | LEU |
| 7 | AJ | 113 | GLU |
| 7 | AJ | 124 | LEU |
| 7 | AJ | 131 | LYS |
| 7 | AJ | 141 | VAL |
| 7 | AJ | 149 | ARG |
| 7 | AJ | 155 | ARG |
| 8 | AK | 3 | THR |
| 8 | AK | 19 | VAL |
| 8 | AK | 37 | ARG |
| 8 | AK | 54 | ASP |
| 8 | AK | 63 | LEU |
| 8 | AK | 68 | ARG |
| 8 | AK | 69 | ARG |
| 8 | AK | 75 | ARG |
| 8 | AK | 77 | GLU |
| 8 | AK | 80 | ILE |
| 8 | AK | 85 | ARG |
| 8 | AK | 87 | SER |
| 8 | AK | 95 | VAL |
| 8 | AK | 98 | LYS |
| 8 | AK | 105 | ARG |
| 8 | AK | 107 | LEU |
| 8 | AK | 112 | LEU |
| 8 | AK | 115 | SER |
| 8 | AK | 123 | GLU |
| 9 | AL | 2 | GLU |
| 9 | AL | 7 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AL | 9 | ARG |
| 9 | AL | 10 | ARG |
| 9 | AL | 16 | ARG |
| 9 | AL | 23 | ASN |
| 9 | AL | 25 | LYS |
| 9 | AL | 26 | VAL |
| 9 | AL | 35 | GLU |
| 9 | AL | 38 | GLN |
| 9 | AL | 42 | ARG |
| 9 | AL | 47 | LEU |
| 9 | AL | 64 | THR |
| 9 | AL | 65 | VAL |
| 9 | AL | 70 | LYS |
| 9 | AL | 75 | ASP |
| 9 | AL | 79 | LEU |
| 9 | AL | 85 | LEU |
| 9 | AL | 89 | ASN |
| 9 | AL | 93 | ARG |
| 9 | AL | 95 | LYS |
| 9 | AL | 99 | LEU |
| 9 | AL | 102 | LEU |
| 9 | AL | 111 | ARG |
| 9 | AL | 112 | LYS |
| 9 | AL | 114 | TYR |
| 9 | AL | 121 | ARG |
| 9 | AL | 124 | GLN |
| 10 | AM | 22 | LYS |
| 10 | AM | 24 | VAL |
| 10 | AM | 25 | GLU |
| 10 | AM | 33 | GLN |
| 10 | AM | 34 | VAL |
| 10 | AM | 35 | SER |
| 10 | AM | 42 | THR |
| 10 | AM | 44 | VAL |
| 10 | AM | 46 | ARG |
| 10 | AM | 48 | THR |
| 10 | AM | 49 | VAL |
| 10 | AM | 55 | LYS |
| 10 | AM | 62 | HIS |
| 10 | AM | 70 | ARG |
| 10 | AM | 74 | ILE |
| 10 | AM | 78 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | AM | 80 | LYS |
| 10 | AM | 85 | LEU |
| 10 | AM | 86 | MET |
| 10 | AM | 92 | THR |
| 10 | AM | 96 | ILE |
| 10 | AM | 100 | THR |
| 10 | AM | 101 | VAL |
| 11 | AN | 28 | THR |
| 11 | AN | 29 | ILE |
| 11 | AN | 30 | VAL |
| 11 | AN | 40 | ILE |
| 11 | AN | 41 | THR |
| 11 | AN | 48 | ILE |
| 11 | AN | 54 | ARG |
| 11 | AN | 63 | LEU |
| 11 | AN | 81 | ASP |
| 11 | AN | 84 | VAL |
| 11 | AN | 91 | ARG |
| 11 | AN | 104 | GLN |
| 11 | AN | 109 | VAL |
| 11 | AN | 114 | VAL |
| 11 | AN | 116 | HIS |
| 11 | AN | 124 | LYS |
| 12 | AO | 7 | ILE |
| 12 | AO | 20 | LYS |
| 12 | AO | 21 | LYS |
| 12 | AO | 59 | ARG |
| 12 | AO | 60 | LEU |
| 12 | AO | 78 | GLN |
| 12 | AO | 81 | SER |
| 12 | AO | 83 | VAL |
| 12 | AO | 85 | ILE |
| 12 | AO | 89 | ARG |
| 12 | AO | 91 | LYS |
| 12 | AO | 102 | ARG |
| 12 | AO | 114 | LYS |
| 12 | AO | 118 | SER |
| 12 | AO | 124 | LYS |
| 12 | AO | 127 | GLU |
| 13 | AP | 11 | ARG |
| 13 | AP | 13 | LYS |
| 13 | AP | 17 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | AP | 20 | THR |
| 13 | AP | 22 | ILE |
| 13 | AP | 34 | LEU |
| 13 | AP | 39 | ILE |
| 13 | AP | 45 | VAL |
| 13 | AP | 47 | ASP |
| 13 | AP | 54 | VAL |
| 13 | AP | 56 | LEU |
| 13 | AP | 64 | TRP |
| 13 | AP | 67 | GLU |
| 13 | AP | 69 | GLU |
| 13 | AP | 70 | LEU |
| 13 | AP | 78 | ILE |
| 13 | AP | 88 | ARG |
| 13 | AP | 101 | GLN |
| 13 | AP | 102 | ARG |
| 13 | AP | 105 | THR |
| 13 | AP | 108 | ARG |
| 13 | AP | 114 | ARG |
| 13 | AP | 116 | THR |
| 14 | AQ | 3 | ARG |
| 14 | AQ | 7 | ILE |
| 14 | AQ | 9 | LYS |
| 14 | AQ | 13 | THR |
| 14 | AQ | 17 | LYS |
| 14 | AQ | 18 | VAL |
| 14 | AQ | 23 | ARG |
| 14 | AQ | 24 | CYS |
| 14 | AQ | 27 | CYS |
| 14 | AQ | 32 | SER |
| 14 | AQ | 35 | ARG |
| 14 | AQ | 41 | ARG |
| 14 | AQ | 43 | CYS |
| 14 | AQ | 44 | LEU |
| 14 | AQ | 46 | GLU |
| 14 | AQ | 57 | ARG |
| 15 | AR | 25 | THR |
| 15 | AR | 31 | LEU |
| 15 | AR | 38 | ARG |
| 15 | AR | 39 | LEU |
| 15 | AR | 41 | GLU |
| 15 | AR | 47 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AR | 62 | GLN |
| 15 | AR | 65 | ARG |
| 15 | AR | 66 | LEU |
| 15 | AR | 71 | GLN |
| 15 | AR | 88 | ARG |
| 16 | AS | 2 | VAL |
| 16 | AS | 11 | SER |
| 16 | AS | 16 | HIS |
| 16 | AS | 18 | ARG |
| 16 | AS | 19 | ILE |
| 16 | AS | 20 | VAL |
| 16 | AS | 21 | VAL |
| 16 | AS | 22 | THR |
| 16 | AS | 25 | ARG |
| 16 | AS | 28 | ARG |
| 16 | AS | 53 | VAL |
| 16 | AS | 55 | ARG |
| 16 | AS | 58 | TYR |
| 16 | AS | 67 | THR |
| 16 | AS | 69 | THR |
| 16 | AS | 71 | ARG |
| 16 | AS | 72 | ARG |
| 16 | AS | 75 | ARG |
| 16 | AS | 82 | GLN |
| 17 | AT | 9 | VAL |
| 17 | AT | 17 | LYS |
| 17 | AT | 35 | VAL |
| 17 | AT | 45 | HIS |
| 17 | AT | 52 | LYS |
| 17 | AT | 57 | VAL |
| 17 | AT | 60 | ILE |
| 17 | AT | 62 | SER |
| 17 | AT | 67 | LYS |
| 17 | AT | 68 | ARG |
| 17 | AT | 74 | LEU |
| 17 | AT | 84 | LEU |
| 17 | AT | 101 | ARG |
| 18 | AU | 18 | ARG |
| 18 | AU | 26 | LEU |
| 18 | AU | 31 | LEU |
| 18 | AU | 32 | ARG |
| 18 | AU | 35 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | AU | 36 | ASN |
| 18 | AU | 42 | ARG |
| 18 | AU | 46 | GLU |
| 18 | AU | 61 | LYS |
| 18 | AU | 65 | ILE |
| 18 | AU | 68 | LYS |
| 18 | AU | 76 | LEU |
| 18 | AU | 82 | THR |
| 19 | AV | 7 | LYS |
| 19 | AV | 10 | PHE |
| 19 | AV | 15 | LEU |
| 19 | AV | 22 | LEU |
| 19 | AV | 28 | LYS |
| 19 | AV | 29 | ARG |
| 19 | AV | 30 | LEU |
| 19 | AV | 31 | ILE |
| 19 | AV | 35 | SER |
| 19 | AV | 37 | ARG |
| 19 | AV | 40 | ILE |
| 19 | AV | 43 | GLU |
| 19 | AV | 48 | THR |
| 19 | AV | 60 | VAL |
| 19 | AV | 61 | TYR |
| 19 | AV | 65 | ASN |
| 19 | AV | 66 | MET |
| 19 | AV | 77 | THR |
| 19 | AV | 81 | ARG |
| 19 | AV | 83 | HIS |
| 20 | AW | 8 | ARG |
| 20 | AW | 9 | ASN |
| 20 | AW | 13 | LEU |
| 20 | AW | 14 | LYS |
| 20 | AW | 24 | LEU |
| 20 | AW | 26 | ASN |
| 20 | AW | 29 | LYS |
| 20 | AW | 34 | LYS |
| 20 | AW | 36 | LEU |
| 20 | AW | 41 | ILE |
| 20 | AW | 50 | GLU |
| 20 | AW | 72 | LEU |
| 20 | AW | 73 | HIS |
| 20 | AW | 75 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AW | 84 | LEU |
| 20 | AW | 93 | GLU |
| 21 | AX | 15 | ARG |
| 21 | AX | 25 | LYS |
| 21 | AX | 26 | LYS |
| 27 | BD | 3 | VAL |
| 27 | BD | 17 | THR |
| 27 | BD | 26 | LYS |
| 27 | BD | 32 | SER |
| 27 | BD | 43 | ARG |
| 27 | BD | 44 | ASN |
| 27 | BD | 60 | ARG |
| 27 | BD | 61 | LEU |
| 27 | BD | 64 | ILE |
| 27 | BD | 65 | ILE |
| 27 | BD | 89 | SER |
| 27 | BD | 91 | ARG |
| 27 | BD | 94 | LEU |
| 27 | BD | 95 | LEU |
| 27 | BD | 99 | ASP |
| 27 | BD | 103 | ARG |
| 27 | BD | 111 | LEU |
| 27 | BD | 112 | GLN |
| 27 | BD | 115 | GLN |
| 27 | BD | 116 | GLN |
| 27 | BD | 117 | VAL |
| 27 | BD | 126 | GLN |
| 27 | BD | 127 | VAL |
| 27 | BD | 136 | ILE |
| 27 | BD | 141 | VAL |
| 27 | BD | 142 | VAL |
| 27 | BD | 155 | LEU |
| 27 | BD | 164 | GLN |
| 27 | BD | 166 | GLN |
| 27 | BD | 171 | ASP |
| 27 | BD | 183 | ARG |
| 27 | BD | 192 | THR |
| 27 | BD | 193 | VAL |
| 27 | BD | 202 | LYS |
| 27 | BD | 217 | ARG |
| 27 | BD | 221 | VAL |
| 27 | BD | 229 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | BD | 242 | ARG |
| 27 | BD | 257 | LEU |
| 27 | BD | 259 | THR |
| 27 | BD | 267 | SER |
| 27 | BD | 271 | ILE |
| 28 | BE | 2 | LYS |
| 28 | BE | 13 | ARG |
| 28 | BE | 16 | ARG |
| 28 | BE | 19 | ARG |
| 28 | BE | 25 | VAL |
| 28 | BE | 26 | ILE |
| 28 | BE | 27 | LEU |
| 28 | BE | 33 | VAL |
| 28 | BE | 40 | GLU |
| 28 | BE | 41 | LYS |
| 28 | BE | 42 | ASP |
| 28 | BE | 45 | THR |
| 28 | BE | 47 | VAL |
| 28 | BE | 48 | GLN |
| 28 | BE | 49 | LEU |
| 28 | BE | 52 | LEU |
| 28 | BE | 54 | GLN |
| 28 | BE | 57 | LYS |
| 28 | BE | 60 | ASN |
| 28 | BE | 63 | LEU |
| 28 | BE | 66 | HIS |
| 28 | BE | 67 | PHE |
| 28 | BE | 76 | ARG |
| 28 | BE | 81 | ILE |
| 28 | BE | 82 | ARG |
| 28 | BE | 89 | ASP |
| 28 | BE | 93 | VAL |
| 28 | BE | 95 | ILE |
| 28 | BE | 97 | LYS |
| 28 | BE | 101 | ARG |
| 28 | BE | 107 | THR |
| 28 | BE | 113 | PHE |
| 28 | BE | 116 | VAL |
| 28 | BE | 118 | LYS |
| 28 | BE | 119 | ARG |
| 28 | BE | 144 | ARG |
| 28 | BE | 146 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BE | 154 | LYS |
| 28 | BE | 163 | GLU |
| 28 | BE | 167 | VAL |
| 28 | BE | 170 | LEU |
| 28 | BE | 171 | GLU |
| 28 | BE | 175 | VAL |
| 28 | BE | 179 | GLU |
| 28 | BE | 181 | LEU |
| 28 | BE | 182 | LEU |
| 28 | BE | 183 | LEU |
| 28 | BE | 185 | LYS |
| 28 | BE | 197 | ILE |
| 28 | BE | 202 | LYS |
| 28 | BE | 203 | LYS |
| 29 | BF | 7 | TYR |
| 29 | BF | 8 | GLN |
| 29 | BF | 9 | ILE |
| 29 | BF | 15 | SER |
| 29 | BF | 27 | GLU |
| 29 | BF | 32 | LEU |
| 29 | BF | 33 | LEU |
| 29 | BF | 38 | ARG |
| 29 | BF | 43 | LYS |
| 29 | BF | 45 | ARG |
| 29 | BF | 46 | ARG |
| 29 | BF | 57 | VAL |
| 29 | BF | 64 | ILE |
| 29 | BF | 67 | GLN |
| 29 | BF | 70 | THR |
| 29 | BF | 82 | ILE |
| 29 | BF | 88 | VAL |
| 29 | BF | 106 | ARG |
| 29 | BF | 108 | LYS |
| 29 | BF | 117 | ARG |
| 29 | BF | 120 | GLU |
| 29 | BF | 127 | GLU |
| 29 | BF | 132 | VAL |
| 29 | BF | 136 | THR |
| 29 | BF | 158 | THR |
| 29 | BF | 161 | GLU |
| 29 | BF | 165 | ARG |
| 29 | BF | 168 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | BF | 181 | LEU |
| 29 | BF | 197 | ASP |
| 29 | BF | 203 | GLN |
| 29 | BF | 206 | ILE |
| 30 | BG | 3 | LEU |
| 30 | BG | 4 | ASP |
| 30 | BG | 10 | LYS |
| 30 | BG | 13 | GLU |
| 30 | BG | 16 | ARG |
| 30 | BG | 20 | ILE |
| 30 | BG | 31 | VAL |
| 30 | BG | 43 | LEU |
| 30 | BG | 45 | GLU |
| 30 | BG | 51 | ARG |
| 30 | BG | 58 | GLN |
| 30 | BG | 60 | LEU |
| 30 | BG | 63 | ILE |
| 30 | BG | 64 | THR |
| 30 | BG | 67 | LYS |
| 30 | BG | 70 | VAL |
| 30 | BG | 71 | THR |
| 30 | BG | 72 | ARG |
| 30 | BG | 75 | LYS |
| 30 | BG | 77 | ILE |
| 30 | BG | 81 | LYS |
| 30 | BG | 82 | LEU |
| 30 | BG | 83 | ARG |
| 30 | BG | 84 | LYS |
| 30 | BG | 90 | LEU |
| 30 | BG | 94 | LEU |
| 30 | BG | 96 | ARG |
| 30 | BG | 101 | ILE |
| 30 | BG | 104 | GLU |
| 30 | BG | 115 | ARG |
| 30 | BG | 118 | ARG |
| 30 | BG | 121 | ASN |
| 30 | BG | 128 | ARG |
| 30 | BG | 130 | ASN |
| 30 | BG | 133 | LEU |
| 30 | BG | 159 | VAL |
| 30 | BG | 165 | THR |
| 30 | BG | 167 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BG | 174 | GLU |
| 30 | BG | 175 | LEU |
| 31 | BH | 4 | ILE |
| 31 | BH | 7 | LEU |
| 31 | BH | 9 | ILE |
| 31 | BH | 23 | ARG |
| 31 | BH | 24 | VAL |
| 31 | BH | 41 | MET |
| 31 | BH | 42 | ARG |
| 31 | BH | 44 | VAL |
| 31 | BH | 45 | VAL |
| 31 | BH | 56 | SER |
| 31 | BH | 59 | ARG |
| 31 | BH | 77 | LYS |
| 31 | BH | 79 | VAL |
| 31 | BH | 80 | SER |
| 31 | BH | 81 | GLU |
| 31 | BH | 83 | TYR |
| 31 | BH | 89 | ILE |
| 31 | BH | 97 | ARG |
| 31 | BH | 105 | LEU |
| 31 | BH | 107 | VAL |
| 31 | BH | 113 | VAL |
| 31 | BH | 116 | GLU |
| 31 | BH | 122 | THR |
| 31 | BH | 129 | THR |
| 31 | BH | 132 | ARG |
| 31 | BH | 134 | SER |
| 31 | BH | 138 | LYS |
| 31 | BH | 139 | GLN |
| 31 | BH | 143 | GLN |
| 31 | BH | 153 | LYS |
| 31 | BH | 158 | HIS |
| 31 | BH | 164 | TYR |
| 31 | BH | 167 | GLU |
| 31 | BH | 170 | ARG |
| 31 | BH | 171 | LEU |
| 32 | BK | 2 | LYS |
| 32 | BK | 12 | LEU |
| 32 | BK | 20 | ASP |
| 32 | BK | 25 | TYR |
| 32 | BK | 35 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BK | 38 | LEU |
| 32 | BK | 41 | GLU |
| 32 | BK | 54 | GLN |
| 32 | BK | 57 | ARG |
| 32 | BK | 58 | LEU |
| 32 | BK | 64 | GLU |
| 32 | BK | 67 | ARG |
| 32 | BK | 68 | LEU |
| 32 | BK | 70 | GLU |
| 32 | BK | 71 | ILE |
| 32 | BK | 77 | LEU |
| 32 | BK | 78 | THR |
| 32 | BK | 81 | VAL |
| 32 | BK | 82 | ARG |
| 32 | BK | 85 | GLU |
| 32 | BK | 87 | LYS |
| 32 | BK | 92 | VAL |
| 32 | BK | 93 | THR |
| 32 | BK | 95 | LYS |
| 32 | BK | 101 | LEU |
| 32 | BK | 102 | SER |
| 32 | BK | 103 | ARG |
| 32 | BK | 107 | VAL |
| 32 | BK | 108 | THR |
| 32 | BK | 135 | GLU |
| 32 | BK | 140 | LEU |
| 33 | BM | 7 | LYS |
| 33 | BM | 9 | VAL |
| 33 | BM | 10 | GLU |
| 33 | BM | 28 | THR |
| 33 | BM | 32 | THR |
| 33 | BM | 34 | LEU |
| 33 | BM | 42 | TRP |
| 33 | BM | 43 | THR |
| 33 | BM | 45 | ASN |
| 33 | BM | 46 | VAL |
| 33 | BM | 48 | MET |
| 33 | BM | 60 | ILE |
| 33 | BM | 61 | ARG |
| 33 | BM | 63 | THR |
| 33 | BM | 67 | LEU |
| 33 | BM | 70 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | BM | 87 | LEU |
| 33 | BM | 89 | LYS |
| 33 | BM | 96 | GLU |
| 33 | BM | 97 | ARG |
| 33 | BM | 99 | LEU |
| 33 | BM | 115 | ARG |
| 33 | BM | 120 | LEU |
| 33 | BM | 122 | VAL |
| 33 | BM | 127 | ASP |
| 33 | BM | 130 | HIS |
| 33 | BM | 131 | GLN |
| 33 | BM | 133 | GLN |
| 33 | BM | 134 | ARG |
| 33 | BM | 138 | LEU |
| 34 | BN | 1 | MET |
| 34 | BN | 8 | LEU |
| 34 | BN | 9 | GLU |
| 34 | BN | 20 | MET |
| 34 | BN | 22 | ILE |
| 34 | BN | 23 | ARG |
| 34 | BN | 24 | VAL |
| 34 | BN | 35 | VAL |
| 34 | BN | 38 | VAL |
| 34 | BN | 47 | ILE |
| 34 | BN | 52 | VAL |
| 34 | BN | 53 | LYS |
| 34 | BN | 66 | LYS |
| 34 | BN | 68 | GLU |
| 34 | BN | 82 | ASN |
| 34 | BN | 94 | ARG |
| 34 | BN | 98 | VAL |
| 35 | BO | 3 | LEU |
| 35 | BO | 14 | LYS |
| 35 | BO | 15 | ARG |
| 35 | BO | 16 | ARG |
| 35 | BO | 21 | ARG |
| 35 | BO | 29 | LYS |
| 35 | BO | 30 | THR |
| 35 | BO | 32 | THR |
| 35 | BO | 41 | ARG |
| 35 | BO | 45 | LEU |
| 35 | BO | 46 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | BO | 49 | ARG |
| 35 | BO | 50 | ARG |
| 35 | BO | 61 | ARG |
| 35 | BO | 62 | LEU |
| 35 | BO | 64 | LYS |
| 35 | BO | 65 | ARG |
| 35 | BO | 68 | GLN |
| 35 | BO | 70 | GLN |
| 35 | BO | 75 | ILE |
| 35 | BO | 79 | ARG |
| 35 | BO | 88 | LEU |
| 35 | BO | 90 | ARG |
| 35 | BO | 92 | GLU |
| 35 | BO | 96 | THR |
| 35 | BO | 99 | LEU |
| 35 | BO | 100 | LEU |
| 35 | BO | 105 | LEU |
| 35 | BO | 106 | LEU |
| 35 | BO | 112 | LEU |
| 35 | BO | 123 | LEU |
| 35 | BO | 125 | VAL |
| 35 | BO | 135 | LEU |
| 35 | BO | 138 | LEU |
| 35 | BO | 144 | GLU |
| 35 | BO | 146 | VAL |
| 35 | BO | 147 | LEU |
| 35 | BO | 148 | LEU |
| 36 | BP | 5 | ARG |
| 36 | BP | 7 | MET |
| 36 | BP | 10 | ARG |
| 36 | BP | 17 | LEU |
| 36 | BP | 25 | ASP |
| 36 | BP | 26 | TYR |
| 36 | BP | 35 | VAL |
| 36 | BP | 45 | GLN |
| 36 | BP | 46 | GLN |
| 36 | BP | 52 | VAL |
| 36 | BP | 58 | PHE |
| 36 | BP | 59 | ARG |
| 36 | BP | 60 | ARG |
| 36 | BP | 63 | LYS |
| 36 | BP | 79 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BP | 82 | ARG |
| 36 | BP | 83 | MET |
| 36 | BP | 87 | LYS |
| 36 | BP | 90 | VAL |
| 36 | BP | 91 | GLU |
| 36 | BP | 103 | MET |
| 36 | BP | 109 | VAL |
| 36 | BP | 110 | THR |
| 36 | BP | 112 | GLU |
| 36 | BP | 129 | THR |
| 36 | BP | 134 | ARG |
| 36 | BP | 139 | GLU |
| 37 | B0 | 4 | LEU |
| 37 | B0 | 16 | HIS |
| 37 | B0 | 18 | LEU |
| 37 | B0 | 28 | LEU |
| 37 | B0 | 29 | LEU |
| 37 | B0 | 34 | ILE |
| 37 | B0 | 36 | THR |
| 37 | B0 | 37 | THR |
| 37 | B0 | 44 | LEU |
| 37 | B0 | 48 | VAL |
| 37 | B0 | 54 | LEU |
| 37 | B0 | 59 | ASP |
| 37 | B0 | 60 | LEU |
| 37 | B0 | 74 | LYS |
| 37 | B0 | 75 | LEU |
| 37 | B0 | 79 | LEU |
| 37 | B0 | 83 | ILE |
| 37 | B0 | 88 | ARG |
| 37 | B0 | 91 | GLN |
| 37 | B0 | 104 | ARG |
| 37 | B0 | 105 | ARG |
| 37 | B0 | 107 | ASP |
| 37 | B0 | 113 | LEU |
| 38 | BQ | 5 | THR |
| 38 | BQ | 19 | LYS |
| 38 | BQ | 20 | ARG |
| 38 | BQ | 24 | LEU |
| 38 | BQ | 30 | ARG |
| 38 | BQ | 31 | SER |
| 38 | BQ | 35 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | BQ | 36 | TYR |
| 38 | BQ | 43 | GLU |
| 38 | BQ | 50 | SER |
| 38 | BQ | 53 | SER |
| 38 | BQ | 54 | LEU |
| 38 | BQ | 56 | LEU |
| 38 | BQ | 58 | LEU |
| 38 | BQ | 69 | VAL |
| 38 | BQ | 73 | LEU |
| 38 | BQ | 83 | LYS |
| 38 | BQ | 93 | LYS |
| 38 | BQ | 97 | ARG |
| 38 | BQ | 101 | LEU |
| 38 | BQ | 106 | ARG |
| 38 | BQ | 111 | GLU |
| 39 | BR | 6 | LEU |
| 39 | BR | 11 | GLU |
| 39 | BR | 15 | VAL |
| 39 | BR | 17 | THR |
| 39 | BR | 27 | THR |
| 39 | BR | 30 | VAL |
| 39 | BR | 35 | LYS |
| 39 | BR | 41 | ARG |
| 39 | BR | 42 | ILE |
| 39 | BR | 49 | VAL |
| 39 | BR | 50 | ILE |
| 39 | BR | 53 | ARG |
| 39 | BR | 58 | ASN |
| 39 | BR | 59 | THR |
| 39 | BR | 61 | PHE |
| 39 | BR | 64 | ARG |
| 39 | BR | 74 | ARG |
| 39 | BR | 85 | LYS |
| 39 | BR | 86 | ILE |
| 39 | BR | 87 | ASP |
| 39 | BR | 88 | ILE |
| 39 | BR | 99 | LEU |
| 39 | BR | 106 | SER |
| 39 | BR | 108 | ARG |
| 39 | BR | 110 | ILE |
| 39 | BR | 112 | ARG |
| 39 | BR | 118 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BR | 128 | GLU |
| 40 | B1 | 3 | ARG |
| 40 | B1 | 5 | LYS |
| 40 | B1 | 8 | VAL |
| 40 | B1 | 13 | LYS |
| 40 | B1 | 27 | LEU |
| 40 | B1 | 34 | LYS |
| 40 | B1 | 52 | ARG |
| 40 | B1 | 70 | ARG |
| 40 | B1 | 74 | LEU |
| 40 | B1 | 79 | PHE |
| 40 | B1 | 89 | GLU |
| 40 | B1 | 95 | LEU |
| 40 | B1 | 97 | ASP |
| 40 | B1 | 98 | LEU |
| 40 | B1 | 108 | GLU |
| 40 | B1 | 111 | GLU |
| 40 | B1 | 112 | ARG |
| 41 | B2 | 1 | MET |
| 41 | B2 | 5 | VAL |
| 41 | B2 | 6 | LYS |
| 41 | B2 | 15 | GLU |
| 41 | B2 | 18 | LEU |
| 41 | B2 | 21 | ARG |
| 41 | B2 | 28 | GLU |
| 41 | B2 | 33 | VAL |
| 41 | B2 | 35 | LEU |
| 41 | B2 | 39 | LEU |
| 41 | B2 | 40 | LEU |
| 41 | B2 | 45 | THR |
| 41 | B2 | 47 | VAL |
| 41 | B2 | 57 | VAL |
| 41 | B2 | 68 | LYS |
| 41 | B2 | 70 | ILE |
| 41 | B2 | 72 | VAL |
| 41 | B2 | 74 | LYS |
| 41 | B2 | 78 | LYS |
| 41 | B2 | 88 | ARG |
| 41 | B2 | 99 | ILE |
| 42 | BS | 11 | ARG |
| 42 | BS | 16 | LYS |
| 42 | BS | 17 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BS | 28 | SER |
| 42 | BS | 37 | ARG |
| 42 | BS | 45 | TYR |
| 42 | BS | 51 | LEU |
| 42 | BS | 57 | ASN |
| 42 | BS | 67 | ASP |
| 42 | BS | 70 | TYR |
| 42 | BS | 76 | VAL |
| 42 | BS | 78 | GLU |
| 42 | BS | 88 | ARG |
| 42 | BS | 90 | ARG |
| 42 | BS | 92 | ARG |
| 42 | BS | 96 | ILE |
| 42 | BS | 100 | THR |
| 42 | BS | 106 | ILE |
| 42 | BS | 107 | LEU |
| 42 | BS | 111 | HIS |
| 43 | BT | 12 | VAL |
| 43 | BT | 23 | GLU |
| 43 | BT | 27 | THR |
| 43 | BT | 44 | GLU |
| 43 | BT | 45 | THR |
| 43 | BT | 57 | LEU |
| 43 | BT | 64 | LYS |
| 43 | BT | 65 | ARG |
| 43 | BT | 70 | LEU |
| 43 | BT | 80 | ILE |
| 43 | BT | 83 | VAL |
| 43 | BT | 87 | GLN |
| 43 | BT | 88 | LYS |
| 44 | BU | 3 | VAL |
| 44 | BU | 6 | HIS |
| 44 | BU | 26 | LYS |
| 44 | BU | 33 | LYS |
| 44 | BU | 38 | ILE |
| 44 | BU | 40 | GLU |
| 44 | BU | 44 | ILE |
| 44 | BU | 52 | SER |
| 44 | BU | 57 | GLN |
| 44 | BU | 61 | ILE |
| 44 | BU | 64 | GLU |
| 44 | BU | 67 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | BU | 76 | CYS |
| 44 | BU | 79 | CYS |
| 44 | BU | 81 | LYS |
| 44 | BU | 84 | ARG |
| 44 | BU | 86 | ARG |
| 44 | BU | 87 | LYS |
| 44 | BU | 90 | LEU |
| 44 | BU | 97 | ARG |
| 45 | BV | 2 | GLU |
| 45 | BV | 5 | LEU |
| 45 | BV | 16 | SER |
| 45 | BV | 19 | ARG |
| 45 | BV | 33 | LEU |
| 45 | BV | 41 | LEU |
| 45 | BV | 53 | ILE |
| 45 | BV | 59 | LEU |
| 45 | BV | 61 | LEU |
| 45 | BV | 71 | VAL |
| 45 | BV | 73 | GLN |
| 45 | BV | 76 | LEU |
| 45 | BV | 77 | ASP |
| 45 | BV | 80 | ARG |
| 45 | BV | 82 | ARG |
| 45 | BV | 86 | VAL |
| 45 | BV | 91 | LEU |
| 45 | BV | 92 | SER |
| 45 | BV | 93 | ASP |
| 45 | BV | 96 | VAL |
| 45 | BV | 97 | GLU |
| 45 | BV | 104 | PHE |
| 45 | BV | 111 | VAL |
| 45 | BV | 112 | ARG |
| 45 | BV | 117 | LEU |
| 45 | BV | 119 | GLU |
| 45 | BV | 121 | HIS |
| 45 | BV | 122 | ARG |
| 45 | BV | 128 | VAL |
| 45 | BV | 132 | ASN |
| 45 | BV | 144 | LEU |
| 45 | BV | 146 | ILE |
| 45 | BV | 148 | ASP |
| 45 | BV | 162 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | BV | 163 | LEU |
| 45 | BV | 165 | VAL |
| 45 | BV | 169 | GLU |
| 45 | BV | 175 | VAL |
| 46 | B3 | 11 | ARG |
| 46 | B3 | 20 | ARG |
| 46 | B3 | 36 | ILE |
| 46 | B3 | 40 | GLN |
| 46 | B3 | 53 | MET |
| 46 | B3 | 55 | ARG |
| 46 | B3 | 60 | PHE |
| 47 | BZ | 19 | GLN |
| 47 | BZ | 21 | ARG |
| 47 | BZ | 26 | ARG |
| 47 | BZ | 35 | THR |
| 47 | BZ | 40 | ARG |
| 47 | BZ | 41 | ARG |
| 47 | BZ | 50 | ARG |
| 47 | BZ | 62 | VAL |
| 47 | BZ | 75 | GLU |
| 47 | BZ | 78 | LYS |
| 47 | BZ | 80 | LEU |
| 47 | BZ | 81 | LYS |
| 47 | BZ | 82 | LEU |
| 47 | BZ | 83 | GLU |
| 47 | BZ | 85 | LEU |
| 47 | BZ | 88 | LYS |
| 47 | BZ | 91 | LYS |
| 47 | BZ | 97 | LEU |
| 48 | BW | 5 | GLU |
| 48 | BW | 7 | ARG |
| 48 | BW | 9 | GLN |
| 48 | BW | 16 | LEU |
| 48 | BW | 17 | SER |
| 48 | BW | 19 | VAL |
| 48 | BW | 23 | LYS |
| 48 | BW | 24 | LEU |
| 48 | BW | 32 | LEU |
| 48 | BW | 34 | GLU |
| 48 | BW | 35 | LEU |
| 48 | BW | 44 | LEU |
| 48 | BW | 47 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | BW | 50 | ILE |
| 48 | BW | 53 | LEU |
| 48 | BW | 54 | LYS |
| 48 | BW | 55 | ARG |
| 48 | BW | 62 | THR |
| 48 | BW | 64 | LEU |
| 48 | BW | 65 | ASN |
| 49 | BX | 6 | VAL |
| 49 | BX | 7 | LYS |
| 49 | BX | 8 | LEU |
| 49 | BX | 31 | LEU |
| 49 | BX | 32 | GLN |
| 49 | BX | 33 | GLN |
| 49 | BX | 40 | THR |
| 49 | BX | 44 | ARG |
| 49 | BX | 53 | LEU |
| 49 | BX | 54 | VAL |
| 50 | B4 | 10 | VAL |
| 50 | B4 | 14 | ILE |
| 50 | B4 | 15 | ILE |
| 50 | B4 | 16 | CYS |
| 50 | B4 | 22 | ILE |
| 50 | B4 | 27 | THR |
| 50 | B4 | 33 | VAL |
| 50 | B4 | 38 | LYS |
| 50 | B4 | 43 | TYR |
| 50 | B4 | 47 | GLN |
| 50 | B4 | 49 | PHE |
| 50 | B4 | 53 | GLU |
| 50 | B4 | 57 | GLU |
| 50 | B4 | 59 | PHE |
| 50 | B4 | 61 | ARG |
| 50 | B4 | 62 | ARG |
| 50 | B4 | 65 | ASP |
| 50 | B4 | 66 | SER |
| 51 | B5 | 3 | LYS |
| 51 | B5 | 4 | HIS |
| 51 | B5 | 6 | VAL |
| 51 | B5 | 11 | THR |
| 51 | B5 | 16 | ARG |
| 51 | B5 | 29 | THR |
| 51 | B5 | 36 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | B5 | 37 | LYS |
| 51 | B5 | 40 | LYS |
| 51 | B5 | 44 | THR |
| 51 | B5 | 48 | GLU |
| 51 | B5 | 51 | TYR |
| 51 | B5 | 52 | TYR |
| 51 | B5 | 55 | ARG |
| 51 | B5 | 56 | LYS |
| 51 | B5 | 58 | LEU |
| 52 | B6 | 10 | LEU |
| 52 | B6 | 12 | GLU |
| 52 | B6 | 13 | CYS |
| 52 | B6 | 16 | CYS |
| 52 | B6 | 17 | LYS |
| 52 | B6 | 18 | ARG |
| 52 | B6 | 25 | LYS |
| 52 | B6 | 26 | ASN |
| 52 | B6 | 27 | LYS |
| 52 | B6 | 28 | ARG |
| 52 | B6 | 32 | ASN |
| 52 | B6 | 34 | LEU |
| 52 | B6 | 36 | LEU |
| 52 | B6 | 39 | TYR |
| 52 | B6 | 42 | TRP |
| 52 | B6 | 44 | ARG |
| 52 | B6 | 45 | LYS |
| 53 | B7 | 4 | THR |
| 53 | B7 | 8 | ASN |
| 53 | B7 | 14 | LYS |
| 53 | B7 | 23 | ARG |
| 53 | B7 | 24 | THR |
| 53 | B7 | 43 | THR |
| 53 | B7 | 46 | VAL |
| 53 | B7 | 48 | LYS |
| 54 | B8 | 29 | LYS |
| 54 | B8 | 30 | ARG |
| 54 | B8 | 34 | TRP |
| 54 | B8 | 36 | LYS |
| 54 | B8 | 40 | GLU |
| 54 | B8 | 41 | ILE |
| 54 | B8 | 44 | LYS |
| 54 | B8 | 47 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | B8 | 50 | LEU |
| 54 | B8 | 56 | GLU |
| 54 | B8 | 58 | ILE |
| 2 | CE | 5 | ILE |
| 2 | CE | 16 | HIS |
| 2 | CE | 17 | PHE |
| 2 | CE | 19 | HIS |
| 2 | CE | 23 | ARG |
| 2 | CE | 24 | TRP |
| 2 | CE | 32 | ILE |
| 2 | CE | 37 | ASN |
| 2 | CE | 44 | LEU |
| 2 | CE | 53 | ARG |
| 2 | CE | 55 | PHE |
| 2 | CE | 56 | ARG |
| 2 | CE | 67 | THR |
| 2 | CE | 73 | THR |
| 2 | CE | 78 | GLN |
| 2 | CE | 80 | ILE |
| 2 | CE | 84 | GLU |
| 2 | CE | 87 | ARG |
| 2 | CE | 92 | TYR |
| 2 | CE | 96 | ARG |
| 2 | CE | 105 | PHE |
| 2 | CE | 107 | THR |
| 2 | CE | 110 | GLN |
| 2 | CE | 111 | ARG |
| 2 | CE | 114 | ARG |
| 2 | CE | 130 | ARG |
| 2 | CE | 137 | ARG |
| 2 | CE | 139 | LYS |
| 2 | CE | 140 | HIS |
| 2 | CE | 141 | GLU |
| 2 | CE | 144 | ARG |
| 2 | CE | 145 | LEU |
| 2 | CE | 147 | LYS |
| 2 | CE | 164 | VAL |
| 2 | CE | 165 | VAL |
| 2 | CE | 178 | ARG |
| 2 | CE | 185 | ILE |
| 2 | CE | 187 | LEU |
| 2 | CE | 196 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CE | 201 | ILE |
| 2 | CE | 206 | ASP |
| 2 | CE | 215 | LEU |
| 2 | CE | 222 | ILE |
| 2 | CE | 226 | ARG |
| 2 | CE | 230 | VAL |
| 2 | CE | 238 | LEU |
| 3 | CF | 5 | ILE |
| 3 | CF | 6 | HIS |
| 3 | CF | 16 | ARG |
| 3 | CF | 18 | TRP |
| 3 | CF | 21 | ARG |
| 3 | CF | 26 | LYS |
| 3 | CF | 27 | LYS |
| 3 | CF | 28 | GLN |
| 3 | CF | 29 | TYR |
| 3 | CF | 34 | LEU |
| 3 | CF | 36 | ASP |
| 3 | CF | 37 | GLN |
| 3 | CF | 42 | LEU |
| 3 | CF | 43 | LEU |
| 3 | CF | 63 | ASN |
| 3 | CF | 69 | HIS |
| 3 | CF | 76 | VAL |
| 3 | CF | 79 | ARG |
| 3 | CF | 83 | ARG |
| 3 | CF | 84 | ILE |
| 3 | CF | 85 | ARG |
| 3 | CF | 98 | ASN |
| 3 | CF | 99 | VAL |
| 3 | CF | 101 | LEU |
| 3 | CF | 120 | VAL |
| 3 | CF | 128 | PHE |
| 3 | CF | 131 | ARG |
| 3 | CF | 140 | ARG |
| 3 | CF | 175 | LEU |
| 3 | CF | 178 | LEU |
| 3 | CF | 184 | TYR |
| 3 | CF | 190 | ARG |
| 3 | CF | 192 | THR |
| 3 | CF | 196 | LEU |
| 3 | CF | 206 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CF | 207 | VAL |
| 4 | CG | 8 | VAL |
| 4 | CG | 9 | CYS |
| 4 | CG | 10 | ARG |
| 4 | CG | 11 | LEU |
| 4 | CG | 12 | CYS |
| 4 | CG | 13 | ARG |
| 4 | CG | 17 | VAL |
| 4 | CG | 19 | LEU |
| 4 | CG | 21 | LEU |
| 4 | CG | 22 | LYS |
| 4 | CG | 25 | ARG |
| 4 | CG | 26 | CYS |
| 4 | CG | 30 | LYS |
| 4 | CG | 36 | ARG |
| 4 | CG | 50 | ARG |
| 4 | CG | 58 | LEU |
| 4 | CG | 59 | ARG |
| 4 | CG | 84 | LYS |
| 4 | CG | 85 | LYS |
| 4 | CG | 96 | LEU |
| 4 | CG | 98 | GLU |
| 4 | CG | 106 | TYR |
| 4 | CG | 107 | ARG |
| 4 | CG | 112 | VAL |
| 4 | CG | 118 | ARG |
| 4 | CG | 119 | GLN |
| 4 | CG | 122 | ARG |
| 4 | CG | 131 | ARG |
| 4 | CG | 132 | ARG |
| 4 | CG | 135 | LEU |
| 4 | CG | 139 | ARG |
| 4 | CG | 141 | ARG |
| 4 | CG | 150 | GLU |
| 4 | CG | 155 | LEU |
| 4 | CG | 170 | VAL |
| 4 | CG | 177 | ASP |
| 4 | CG | 187 | ARG |
| 4 | CG | 191 | ARG |
| 4 | CG | 194 | LEU |
| 4 | CG | 200 | GLU |
| 5 | CH | 5 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CH | 6 | PHE |
| 5 | CH | 9 | LYS |
| 5 | CH | 11 | ILE |
| 5 | CH | 12 | LEU |
| 5 | CH | 13 | ILE |
| 5 | CH | 18 | ARG |
| 5 | CH | 20 | GLN |
| 5 | CH | 31 | LEU |
| 5 | CH | 41 | VAL |
| 5 | CH | 43 | LEU |
| 5 | CH | 53 | LEU |
| 5 | CH | 73 | ASN |
| 5 | CH | 75 | THR |
| 5 | CH | 76 | ILE |
| 5 | CH | 78 | HIS |
| 5 | CH | 79 | GLU |
| 5 | CH | 87 | SER |
| 5 | CH | 91 | LEU |
| 5 | CH | 101 | ILE |
| 5 | CH | 107 | ARG |
| 5 | CH | 116 | THR |
| 5 | CH | 136 | MET |
| 5 | CH | 141 | GLN |
| 5 | CH | 147 | ASP |
| 5 | CH | 153 | LYS |
| 5 | CH | 155 | GLU |
| 6 | CI | 2 | ARG |
| 6 | CI | 14 | LEU |
| 6 | CI | 15 | ASP |
| 6 | CI | 21 | LEU |
| 6 | CI | 27 | GLN |
| 6 | CI | 28 | ARG |
| 6 | CI | 45 | LEU |
| 6 | CI | 54 | LYS |
| 6 | CI | 55 | ASP |
| 6 | CI | 57 | GLN |
| 6 | CI | 63 | TYR |
| 6 | CI | 65 | VAL |
| 6 | CI | 75 | LEU |
| 6 | CI | 81 | ILE |
| 6 | CI | 87 | ARG |
| 6 | CI | 93 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CJ | 4 | ARG |
| 7 | CJ | 5 | ARG |
| 7 | CJ | 8 | GLU |
| 7 | CJ | 9 | VAL |
| 7 | CJ | 11 | GLN |
| 7 | CJ | 12 | LEU |
| 7 | CJ | 13 | GLN |
| 7 | CJ | 16 | LEU |
| 7 | CJ | 22 | LEU |
| 7 | CJ | 24 | THR |
| 7 | CJ | 37 | ASN |
| 7 | CJ | 38 | LEU |
| 7 | CJ | 41 | ARG |
| 7 | CJ | 47 | CYS |
| 7 | CJ | 49 | ILE |
| 7 | CJ | 51 | GLN |
| 7 | CJ | 53 | LYS |
| 7 | CJ | 60 | LYS |
| 7 | CJ | 63 | LYS |
| 7 | CJ | 72 | ARG |
| 7 | CJ | 75 | VAL |
| 7 | CJ | 78 | ARG |
| 7 | CJ | 85 | TYR |
| 7 | CJ | 86 | GLN |
| 7 | CJ | 87 | VAL |
| 7 | CJ | 89 | MET |
| 7 | CJ | 94 | ARG |
| 7 | CJ | 104 | LEU |
| 7 | CJ | 113 | GLU |
| 7 | CJ | 114 | ARG |
| 7 | CJ | 118 | VAL |
| 7 | CJ | 137 | LYS |
| 7 | CJ | 140 | ASP |
| 7 | CJ | 146 | GLU |
| 7 | CJ | 149 | ARG |
| 7 | CJ | 151 | TYR |
| 7 | CJ | 155 | ARG |
| 8 | CK | 1 | MET |
| 8 | CK | 8 | ASP |
| 8 | CK | 23 | SER |
| 8 | CK | 24 | THR |
| 8 | CK | 25 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CK | 30 | ARG |
| 8 | CK | 41 | ARG |
| 8 | CK | 52 | ASP |
| 8 | CK | 63 | LEU |
| 8 | CK | 77 | GLU |
| 8 | CK | 79 | VAL |
| 8 | CK | 82 | HIS |
| 8 | CK | 85 | ARG |
| 8 | CK | 88 | LYS |
| 8 | CK | 91 | ARG |
| 8 | CK | 92 | ARG |
| 8 | CK | 102 | ARG |
| 8 | CK | 104 | ARG |
| 8 | CK | 109 | ILE |
| 8 | CK | 112 | LEU |
| 8 | CK | 115 | SER |
| 8 | CK | 116 | LYS |
| 8 | CK | 123 | GLU |
| 8 | CK | 125 | ARG |
| 8 | CK | 137 | VAL |
| 9 | CL | 7 | THR |
| 9 | CL | 14 | VAL |
| 9 | CL | 16 | ARG |
| 9 | CL | 20 | ARG |
| 9 | CL | 23 | ASN |
| 9 | CL | 29 | ASN |
| 9 | CL | 38 | GLN |
| 9 | CL | 40 | LEU |
| 9 | CL | 56 | LEU |
| 9 | CL | 58 | HIS |
| 9 | CL | 71 | SER |
| 9 | CL | 78 | LYS |
| 9 | CL | 79 | LEU |
| 9 | CL | 88 | TYR |
| 9 | CL | 89 | ASN |
| 9 | CL | 91 | ASP |
| 9 | CL | 95 | LYS |
| 9 | CL | 97 | LYS |
| 9 | CL | 102 | LEU |
| 9 | CL | 104 | ARG |
| 9 | CL | 108 | VAL |
| 9 | CL | 110 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | CL | 112 | LYS |
| 9 | CL | 114 | TYR |
| 9 | CL | 117 | HIS |
| 9 | CL | 118 | LYS |
| 9 | CL | 120 | ARG |
| 9 | CL | 121 | ARG |
| 9 | CL | 125 | TYR |
| 10 | CM | 4 | ILE |
| 10 | CM | 13 | HIS |
| 10 | CM | 16 | LEU |
| 10 | CM | 19 | SER |
| 10 | CM | 21 | GLN |
| 10 | CM | 22 | LYS |
| 10 | CM | 25 | GLU |
| 10 | CM | 30 | SER |
| 10 | CM | 38 | ILE |
| 10 | CM | 40 | LEU |
| 10 | CM | 47 | PHE |
| 10 | CM | 48 | THR |
| 10 | CM | 49 | VAL |
| 10 | CM | 51 | ARG |
| 10 | CM | 55 | LYS |
| 10 | CM | 57 | LYS |
| 10 | CM | 61 | GLU |
| 10 | CM | 62 | HIS |
| 10 | CM | 72 | VAL |
| 10 | CM | 79 | ARG |
| 10 | CM | 80 | LYS |
| 10 | CM | 84 | GLN |
| 10 | CM | 85 | LEU |
| 10 | CM | 87 | THR |
| 10 | CM | 90 | LEU |
| 10 | CM | 95 | GLU |
| 10 | CM | 96 | ILE |
| 10 | CM | 98 | ILE |
| 10 | CM | 99 | LYS |
| 11 | CN | 12 | ARG |
| 11 | CN | 14 | VAL |
| 11 | CN | 18 | ARG |
| 11 | CN | 29 | ILE |
| 11 | CN | 30 | VAL |
| 11 | CN | 48 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | CN | 53 | SER |
| 11 | CN | 54 | ARG |
| 11 | CN | 57 | THR |
| 11 | CN | 63 | LEU |
| 11 | CN | 81 | ASP |
| 11 | CN | 83 | ILE |
| 11 | CN | 84 | VAL |
| 11 | CN | 112 | THR |
| 11 | CN | 117 | ASN |
| 11 | CN | 119 | CYS |
| 11 | CN | 120 | ARG |
| 12 | CO | 20 | LYS |
| 12 | CO | 23 | LYS |
| 12 | CO | 24 | VAL |
| 12 | CO | 27 | LEU |
| 12 | CO | 28 | LYS |
| 12 | CO | 33 | ARG |
| 12 | CO | 36 | VAL |
| 12 | CO | 41 | ARG |
| 12 | CO | 42 | THR |
| 12 | CO | 46 | LYS |
| 12 | CO | 47 | LYS |
| 12 | CO | 55 | VAL |
| 12 | CO | 60 | LEU |
| 12 | CO | 65 | GLU |
| 12 | CO | 70 | ILE |
| 12 | CO | 83 | VAL |
| 12 | CO | 84 | LEU |
| 12 | CO | 85 | ILE |
| 12 | CO | 102 | ARG |
| 12 | CO | 104 | VAL |
| 12 | CO | 111 | LYS |
| 12 | CO | 117 | ARG |
| 12 | CO | 118 | SER |
| 12 | CO | 122 | THR |
| 13 | CP | 3 | ARG |
| 13 | CP | 4 | ILE |
| 13 | CP | 19 | LEU |
| 13 | CP | 32 | GLU |
| 13 | CP | 54 | VAL |
| 13 | CP | 55 | ARG |
| 13 | CP | 58 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | CP | 63 | THR |
| 13 | CP | 64 | TRP |
| 13 | CP | 66 | LEU |
| 13 | CP | 70 | LEU |
| 13 | CP | 77 | ASN |
| 13 | CP | 82 | MET |
| 13 | CP | 83 | ASP |
| 13 | CP | 101 | GLN |
| 13 | CP | 103 | THR |
| 13 | CP | 105 | THR |
| 13 | CP | 108 | ARG |
| 13 | CP | 110 | ARG |
| 14 | CQ | 6 | LEU |
| 14 | CQ | 15 | LYS |
| 14 | CQ | 16 | PHE |
| 14 | CQ | 18 | VAL |
| 14 | CQ | 22 | THR |
| 14 | CQ | 23 | ARG |
| 14 | CQ | 43 | CYS |
| 14 | CQ | 44 | LEU |
| 14 | CQ | 46 | GLU |
| 14 | CQ | 60 | SER |
| 15 | CR | 3 | ILE |
| 15 | CR | 4 | THR |
| 15 | CR | 17 | ARG |
| 15 | CR | 22 | THR |
| 15 | CR | 26 | GLU |
| 15 | CR | 31 | LEU |
| 15 | CR | 35 | ARG |
| 15 | CR | 38 | ARG |
| 15 | CR | 41 | GLU |
| 15 | CR | 58 | MET |
| 15 | CR | 82 | ILE |
| 15 | CR | 83 | GLU |
| 15 | CR | 88 | ARG |
| 16 | CS | 2 | VAL |
| 16 | CS | 5 | ARG |
| 16 | CS | 8 | ARG |
| 16 | CS | 21 | VAL |
| 16 | CS | 45 | THR |
| 16 | CS | 47 | ASP |
| 16 | CS | 53 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | CS | 67 | THR |
| 16 | CS | 74 | LEU |
| 16 | CS | 82 | GLN |
| 17 | CT | 9 | VAL |
| 17 | CT | 52 | LYS |
| 17 | CT | 68 | ARG |
| 17 | CT | 74 | LEU |
| 17 | CT | 79 | SER |
| 17 | CT | 84 | LEU |
| 18 | CU | 21 | LYS |
| 18 | CU | 22 | VAL |
| 18 | CU | 23 | LYS |
| 18 | CU | 28 | GLU |
| 18 | CU | 29 | PHE |
| 18 | CU | 32 | ARG |
| 18 | CU | 44 | LEU |
| 18 | CU | 45 | SER |
| 18 | CU | 47 | THR |
| 18 | CU | 53 | ARG |
| 18 | CU | 54 | ARG |
| 18 | CU | 58 | LEU |
| 18 | CU | 82 | THR |
| 18 | CU | 83 | GLU |
| 18 | CU | 86 | VAL |
| 19 | CV | 14 | HIS |
| 19 | CV | 15 | LEU |
| 19 | CV | 22 | LEU |
| 19 | CV | 23 | ASN |
| 19 | CV | 25 | LYS |
| 19 | CV | 28 | LYS |
| 19 | CV | 33 | THR |
| 19 | CV | 36 | ARG |
| 19 | CV | 41 | VAL |
| 19 | CV | 60 | VAL |
| 19 | CV | 66 | MET |
| 19 | CV | 78 | ARG |
| 19 | CV | 79 | THR |
| 19 | CV | 83 | HIS |
| 20 | CW | 9 | ASN |
| 20 | CW | 10 | LEU |
| 20 | CW | 11 | SER |
| 20 | CW | 14 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CW | 24 | LEU |
| 20 | CW | 26 | ASN |
| 20 | CW | 27 | LYS |
| 20 | CW | 36 | LEU |
| 20 | CW | 39 | LYS |
| 20 | CW | 41 | ILE |
| 20 | CW | 50 | GLU |
| 20 | CW | 56 | MET |
| 20 | CW | 58 | LYS |
| 20 | CW | 68 | LYS |
| 20 | CW | 72 | LEU |
| 20 | CW | 73 | HIS |
| 20 | CW | 75 | ASN |
| 20 | CW | 81 | LYS |
| 20 | CW | 83 | ARG |
| 20 | CW | 84 | LEU |
| 20 | CW | 90 | GLN |
| 27 | DD | 3 | VAL |
| 27 | DD | 5 | LYS |
| 27 | DD | 20 | ASP |
| 27 | DD | 25 | THR |
| 27 | DD | 26 | LYS |
| 27 | DD | 27 | THR |
| 27 | DD | 28 | GLU |
| 27 | DD | 30 | GLU |
| 27 | DD | 31 | LYS |
| 27 | DD | 32 | SER |
| 27 | DD | 40 | THR |
| 27 | DD | 44 | ASN |
| 27 | DD | 46 | GLN |
| 27 | DD | 49 | ILE |
| 27 | DD | 61 | LEU |
| 27 | DD | 64 | ILE |
| 27 | DD | 65 | ILE |
| 27 | DD | 68 | LYS |
| 27 | DD | 69 | ARG |
| 27 | DD | 72 | LYS |
| 27 | DD | 88 | ARG |
| 27 | DD | 89 | SER |
| 27 | DD | 91 | ARG |
| 27 | DD | 94 | LEU |
| 27 | DD | 98 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | DD | 99 | ASP |
| 27 | DD | 103 | ARG |
| 27 | DD | 105 | ILE |
| 27 | DD | 106 | ILE |
| 27 | DD | 112 | GLN |
| 27 | DD | 116 | GLN |
| 27 | DD | 117 | VAL |
| 27 | DD | 140 | THR |
| 27 | DD | 141 | VAL |
| 27 | DD | 147 | LEU |
| 27 | DD | 157 | ARG |
| 27 | DD | 166 | GLN |
| 27 | DD | 176 | ARG |
| 27 | DD | 192 | THR |
| 27 | DD | 193 | VAL |
| 27 | DD | 198 | ASN |
| 27 | DD | 200 | ASP |
| 27 | DD | 202 | LYS |
| 27 | DD | 211 | ARG |
| 27 | DD | 217 | ARG |
| 27 | DD | 218 | ARG |
| 27 | DD | 244 | ARG |
| 27 | DD | 255 | LYS |
| 27 | DD | 257 | LEU |
| 27 | DD | 260 | ARG |
| 27 | DD | 266 | SER |
| 27 | DD | 271 | ILE |
| 28 | DE | 23 | VAL |
| 28 | DE | 26 | ILE |
| 28 | DE | 33 | VAL |
| 28 | DE | 35 | GLN |
| 28 | DE | 36 | ARG |
| 28 | DE | 37 | ARG |
| 28 | DE | 44 | TYR |
| 28 | DE | 49 | LEU |
| 28 | DE | 54 | GLN |
| 28 | DE | 58 | ARG |
| 28 | DE | 60 | ASN |
| 28 | DE | 61 | ARG |
| 28 | DE | 63 | LEU |
| 28 | DE | 67 | PHE |
| 28 | DE | 69 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | DE | 76 | ARG |
| 28 | DE | 77 | ILE |
| 28 | DE | 78 | LEU |
| 28 | DE | 79 | ARG |
| 28 | DE | 81 | ILE |
| 28 | DE | 82 | ARG |
| 28 | DE | 87 | GLU |
| 28 | DE | 91 | VAL |
| 28 | DE | 93 | VAL |
| 28 | DE | 95 | ILE |
| 28 | DE | 111 | ARG |
| 28 | DE | 116 | VAL |
| 28 | DE | 119 | ARG |
| 28 | DE | 128 | SER |
| 28 | DE | 135 | HIS |
| 28 | DE | 141 | ILE |
| 28 | DE | 144 | ARG |
| 28 | DE | 146 | THR |
| 28 | DE | 154 | LYS |
| 28 | DE | 175 | VAL |
| 28 | DE | 178 | GLU |
| 28 | DE | 179 | GLU |
| 28 | DE | 181 | LEU |
| 28 | DE | 182 | LEU |
| 28 | DE | 188 | VAL |
| 28 | DE | 197 | ILE |
| 28 | DE | 200 | GLU |
| 28 | DE | 201 | THR |
| 28 | DE | 203 | LYS |
| 29 | DF | 2 | LYS |
| 29 | DF | 7 | TYR |
| 29 | DF | 8 | GLN |
| 29 | DF | 11 | VAL |
| 29 | DF | 15 | SER |
| 29 | DF | 17 | ARG |
| 29 | DF | 19 | GLU |
| 29 | DF | 20 | LEU |
| 29 | DF | 24 | LEU |
| 29 | DF | 28 | ILE |
| 29 | DF | 33 | LEU |
| 29 | DF | 38 | ARG |
| 29 | DF | 45 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | DF | 48 | THR |
| 29 | DF | 53 | THR |
| 29 | DF | 62 | ARG |
| 29 | DF | 63 | LYS |
| 29 | DF | 67 | GLN |
| 29 | DF | 70 | THR |
| 29 | DF | 74 | ARG |
| 29 | DF | 83 | PHE |
| 29 | DF | 84 | VAL |
| 29 | DF | 88 | VAL |
| 29 | DF | 93 | LYS |
| 29 | DF | 100 | THR |
| 29 | DF | 104 | LYS |
| 29 | DF | 107 | LYS |
| 29 | DF | 116 | ASP |
| 29 | DF | 117 | ARG |
| 29 | DF | 123 | LEU |
| 29 | DF | 125 | LEU |
| 29 | DF | 140 | LEU |
| 29 | DF | 149 | ASP |
| 29 | DF | 153 | SER |
| 29 | DF | 158 | THR |
| 29 | DF | 165 | ARG |
| 29 | DF | 181 | LEU |
| 29 | DF | 183 | VAL |
| 29 | DF | 194 | MET |
| 29 | DF | 199 | TRP |
| 29 | DF | 201 | VAL |
| 29 | DF | 203 | GLN |
| 29 | DF | 205 | ARG |
| 30 | DG | 4 | ASP |
| 30 | DG | 13 | GLU |
| 30 | DG | 16 | ARG |
| 30 | DG | 22 | ARG |
| 30 | DG | 26 | GLN |
| 30 | DG | 27 | ASN |
| 30 | DG | 28 | VAL |
| 30 | DG | 31 | VAL |
| 30 | DG | 33 | ARG |
| 30 | DG | 34 | LEU |
| 30 | DG | 35 | GLU |
| 30 | DG | 40 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DG | 45 | GLU |
| 30 | DG | 47 | LYS |
| 30 | DG | 49 | ASP |
| 30 | DG | 52 | ILE |
| 30 | DG | 63 | ILE |
| 30 | DG | 67 | LYS |
| 30 | DG | 71 | THR |
| 30 | DG | 75 | LYS |
| 30 | DG | 76 | SER |
| 30 | DG | 81 | LYS |
| 30 | DG | 82 | LEU |
| 30 | DG | 83 | ARG |
| 30 | DG | 86 | MET |
| 30 | DG | 88 | ILE |
| 30 | DG | 90 | LEU |
| 30 | DG | 94 | LEU |
| 30 | DG | 96 | ARG |
| 30 | DG | 97 | ASP |
| 30 | DG | 108 | ASN |
| 30 | DG | 115 | ARG |
| 30 | DG | 117 | PHE |
| 30 | DG | 118 | ARG |
| 30 | DG | 128 | ARG |
| 30 | DG | 130 | ASN |
| 30 | DG | 137 | GLU |
| 30 | DG | 146 | TYR |
| 30 | DG | 148 | MET |
| 30 | DG | 162 | THR |
| 30 | DG | 165 | THR |
| 30 | DG | 173 | LEU |
| 31 | DH | 4 | ILE |
| 31 | DH | 7 | LEU |
| 31 | DH | 24 | VAL |
| 31 | DH | 30 | LYS |
| 31 | DH | 34 | GLU |
| 31 | DH | 37 | VAL |
| 31 | DH | 41 | MET |
| 31 | DH | 42 | ARG |
| 31 | DH | 43 | VAL |
| 31 | DH | 44 | VAL |
| 31 | DH | 50 | VAL |
| 31 | DH | 59 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | DH | 63 | SER |
| 31 | DH | 64 | LEU |
| 31 | DH | 72 | ILE |
| 31 | DH | 83 | TYR |
| 31 | DH | 86 | GLU |
| 31 | DH | 87 | LEU |
| 31 | DH | 89 | ILE |
| 31 | DH | 101 | ARG |
| 31 | DH | 103 | LEU |
| 31 | DH | 105 | LEU |
| 31 | DH | 106 | THR |
| 31 | DH | 125 | VAL |
| 31 | DH | 132 | ARG |
| 31 | DH | 136 | ILE |
| 31 | DH | 139 | GLN |
| 31 | DH | 143 | GLN |
| 31 | DH | 152 | ARG |
| 31 | DH | 153 | LYS |
| 31 | DH | 155 | SER |
| 31 | DH | 171 | LEU |
| 32 | DK | 7 | GLU |
| 32 | DK | 9 | LEU |
| 32 | DK | 11 | ASN |
| 32 | DK | 14 | ASP |
| 32 | DK | 37 | VAL |
| 32 | DK | 41 | GLU |
| 32 | DK | 44 | LEU |
| 32 | DK | 51 | ILE |
| 32 | DK | 52 | ARG |
| 32 | DK | 54 | GLN |
| 32 | DK | 56 | LYS |
| 32 | DK | 62 | LYS |
| 32 | DK | 74 | ASN |
| 32 | DK | 75 | LEU |
| 32 | DK | 76 | THR |
| 32 | DK | 77 | LEU |
| 32 | DK | 78 | THR |
| 32 | DK | 81 | VAL |
| 32 | DK | 82 | ARG |
| 32 | DK | 87 | LYS |
| 32 | DK | 88 | ILE |
| 32 | DK | 101 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DK | 102 | SER |
| 32 | DK | 104 | GLN |
| 32 | DK | 107 | VAL |
| 32 | DK | 109 | ILE |
| 32 | DK | 110 | ASP |
| 32 | DK | 113 | ARG |
| 32 | DK | 114 | LEU |
| 32 | DK | 117 | GLU |
| 32 | DK | 122 | GLU |
| 32 | DK | 123 | LEU |
| 32 | DK | 125 | GLU |
| 32 | DK | 128 | LEU |
| 32 | DK | 130 | TYR |
| 32 | DK | 133 | HIS |
| 32 | DK | 142 | VAL |
| 32 | DK | 144 | VAL |
| 33 | DM | 7 | LYS |
| 33 | DM | 28 | THR |
| 33 | DM | 32 | THR |
| 33 | DM | 33 | LEU |
| 33 | DM | 34 | LEU |
| 33 | DM | 35 | ARG |
| 33 | DM | 38 | HIS |
| 33 | DM | 43 | THR |
| 33 | DM | 45 | ASN |
| 33 | DM | 48 | MET |
| 33 | DM | 63 | THR |
| 33 | DM | 67 | LEU |
| 33 | DM | 69 | GLN |
| 33 | DM | 83 | LYS |
| 33 | DM | 87 | LEU |
| 33 | DM | 93 | THR |
| 33 | DM | 94 | HIS |
| 33 | DM | 97 | ARG |
| 33 | DM | 99 | LEU |
| 33 | DM | 127 | ASP |
| 33 | DM | 137 | LYS |
| 34 | DN | 3 | GLN |
| 34 | DN | 5 | GLN |
| 34 | DN | 8 | LEU |
| 34 | DN | 9 | GLU |
| 34 | DN | 14 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DN | 20 | MET |
| 34 | DN | 22 | ILE |
| 34 | DN | 24 | VAL |
| 34 | DN | 28 | SER |
| 34 | DN | 35 | VAL |
| 34 | DN | 38 | VAL |
| 34 | DN | 42 | SER |
| 34 | DN | 49 | ARG |
| 34 | DN | 87 | ILE |
| 34 | DN | 91 | LEU |
| 34 | DN | 94 | ARG |
| 34 | DN | 97 | ARG |
| 34 | DN | 98 | VAL |
| 34 | DN | 104 | ARG |
| 34 | DN | 108 | GLU |
| 34 | DN | 114 | ILE |
| 34 | DN | 117 | LEU |
| 35 | DO | 6 | LEU |
| 35 | DO | 7 | ARG |
| 35 | DO | 14 | LYS |
| 35 | DO | 15 | ARG |
| 35 | DO | 16 | ARG |
| 35 | DO | 21 | ARG |
| 35 | DO | 29 | LYS |
| 35 | DO | 30 | THR |
| 35 | DO | 36 | LYS |
| 35 | DO | 41 | ARG |
| 35 | DO | 45 | LEU |
| 35 | DO | 46 | LYS |
| 35 | DO | 49 | ARG |
| 35 | DO | 50 | ARG |
| 35 | DO | 61 | ARG |
| 35 | DO | 62 | LEU |
| 35 | DO | 64 | LYS |
| 35 | DO | 65 | ARG |
| 35 | DO | 68 | GLN |
| 35 | DO | 70 | GLN |
| 35 | DO | 75 | ILE |
| 35 | DO | 81 | GLN |
| 35 | DO | 85 | LEU |
| 35 | DO | 87 | ASP |
| 35 | DO | 95 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DO | 96 | THR |
| 35 | DO | 98 | GLU |
| 35 | DO | 100 | LEU |
| 35 | DO | 102 | ARG |
| 35 | DO | 105 | LEU |
| 35 | DO | 107 | LYS |
| 35 | DO | 110 | TYR |
| 35 | DO | 111 | ARG |
| 35 | DO | 112 | LEU |
| 35 | DO | 114 | ILE |
| 35 | DO | 117 | GLU |
| 35 | DO | 121 | LYS |
| 35 | DO | 124 | LYS |
| 35 | DO | 125 | VAL |
| 35 | DO | 135 | LEU |
| 35 | DO | 138 | LEU |
| 35 | DO | 144 | GLU |
| 35 | DO | 147 | LEU |
| 35 | DO | 148 | LEU |
| 36 | DP | 3 | MET |
| 36 | DP | 5 | ARG |
| 36 | DP | 21 | THR |
| 36 | DP | 25 | ASP |
| 36 | DP | 26 | TYR |
| 36 | DP | 35 | VAL |
| 36 | DP | 45 | GLN |
| 36 | DP | 59 | ARG |
| 36 | DP | 63 | LYS |
| 36 | DP | 65 | PHE |
| 36 | DP | 75 | THR |
| 36 | DP | 79 | LEU |
| 36 | DP | 80 | GLU |
| 36 | DP | 82 | ARG |
| 36 | DP | 83 | MET |
| 36 | DP | 87 | LYS |
| 36 | DP | 90 | VAL |
| 36 | DP | 103 | MET |
| 36 | DP | 109 | VAL |
| 36 | DP | 110 | THR |
| 36 | DP | 112 | GLU |
| 36 | DP | 113 | GLN |
| 36 | DP | 120 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | DP | 127 | ILE |
| 36 | DP | 133 | ARG |
| 36 | DP | 141 | GLN |
| 37 | D0 | 6 | SER |
| 37 | D0 | 16 | HIS |
| 37 | D0 | 18 | LEU |
| 37 | D0 | 26 | LYS |
| 37 | D0 | 28 | LEU |
| 37 | D0 | 29 | LEU |
| 37 | D0 | 33 | ARG |
| 37 | D0 | 35 | THR |
| 37 | D0 | 44 | LEU |
| 37 | D0 | 48 | VAL |
| 37 | D0 | 63 | ARG |
| 37 | D0 | 65 | LEU |
| 37 | D0 | 68 | ARG |
| 37 | D0 | 76 | VAL |
| 37 | D0 | 81 | ASP |
| 37 | D0 | 91 | GLN |
| 37 | D0 | 105 | ARG |
| 37 | D0 | 107 | ASP |
| 37 | D0 | 117 | VAL |
| 37 | D0 | 118 | GLU |
| 38 | DQ | 3 | ARG |
| 38 | DQ | 8 | GLU |
| 38 | DQ | 12 | PHE |
| 38 | DQ | 14 | VAL |
| 38 | DQ | 15 | ARG |
| 38 | DQ | 17 | ARG |
| 38 | DQ | 20 | ARG |
| 38 | DQ | 21 | THR |
| 38 | DQ | 24 | LEU |
| 38 | DQ | 30 | ARG |
| 38 | DQ | 35 | ILE |
| 38 | DQ | 36 | TYR |
| 38 | DQ | 39 | ILE |
| 38 | DQ | 40 | ILE |
| 38 | DQ | 41 | ASP |
| 38 | DQ | 42 | ASP |
| 38 | DQ | 50 | SER |
| 38 | DQ | 52 | SER |
| 38 | DQ | 53 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | DQ | 58 | LEU |
| 38 | DQ | 61 | ASN |
| 38 | DQ | 63 | THR |
| 38 | DQ | 65 | VAL |
| 38 | DQ | 71 | ARG |
| 38 | DQ | 73 | LEU |
| 38 | DQ | 78 | LEU |
| 38 | DQ | 83 | LYS |
| 38 | DQ | 84 | GLN |
| 38 | DQ | 87 | PHE |
| 38 | DQ | 89 | ARG |
| 38 | DQ | 101 | LEU |
| 38 | DQ | 103 | GLU |
| 38 | DQ | 106 | ARG |
| 38 | DQ | 110 | LEU |
| 39 | DR | 7 | ILE |
| 39 | DR | 8 | LYS |
| 39 | DR | 9 | LEU |
| 39 | DR | 11 | GLU |
| 39 | DR | 12 | SER |
| 39 | DR | 13 | ARG |
| 39 | DR | 23 | ARG |
| 39 | DR | 27 | THR |
| 39 | DR | 29 | ARG |
| 39 | DR | 30 | VAL |
| 39 | DR | 31 | SER |
| 39 | DR | 33 | LYS |
| 39 | DR | 42 | ILE |
| 39 | DR | 52 | ILE |
| 39 | DR | 53 | ARG |
| 39 | DR | 54 | ARG |
| 39 | DR | 66 | VAL |
| 39 | DR | 74 | ARG |
| 39 | DR | 86 | ILE |
| 39 | DR | 87 | ASP |
| 39 | DR | 88 | ILE |
| 39 | DR | 89 | VAL |
| 39 | DR | 90 | GLN |
| 39 | DR | 91 | ARG |
| 39 | DR | 93 | ARG |
| 39 | DR | 96 | ARG |
| 39 | DR | 98 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | DR | 105 | LEU |
| 39 | DR | 107 | ASP |
| 39 | DR | 112 | ARG |
| 39 | DR | 117 | ASP |
| 39 | DR | 121 | ILE |
| 39 | DR | 132 | LYS |
| 39 | DR | 134 | GLU |
| 39 | DR | 136 | GLN |
| 39 | DR | 137 | LYS |
| 40 | D1 | 20 | LEU |
| 40 | D1 | 31 | SER |
| 40 | D1 | 55 | ARG |
| 40 | D1 | 70 | ARG |
| 40 | D1 | 71 | GLN |
| 40 | D1 | 74 | LEU |
| 40 | D1 | 83 | LEU |
| 40 | D1 | 88 | ILE |
| 40 | D1 | 92 | ARG |
| 40 | D1 | 95 | LEU |
| 40 | D1 | 97 | ASP |
| 40 | D1 | 105 | VAL |
| 40 | D1 | 112 | ARG |
| 41 | D2 | 1 | MET |
| 41 | D2 | 7 | THR |
| 41 | D2 | 10 | LYS |
| 41 | D2 | 12 | TYR |
| 41 | D2 | 18 | LEU |
| 41 | D2 | 19 | LYS |
| 41 | D2 | 21 | ARG |
| 41 | D2 | 22 | VAL |
| 41 | D2 | 26 | ASP |
| 41 | D2 | 32 | THR |
| 41 | D2 | 34 | GLU |
| 41 | D2 | 35 | LEU |
| 41 | D2 | 38 | LEU |
| 41 | D2 | 40 | LEU |
| 41 | D2 | 47 | VAL |
| 41 | D2 | 57 | VAL |
| 41 | D2 | 61 | VAL |
| 41 | D2 | 62 | LEU |
| 41 | D2 | 66 | ARG |
| 41 | D2 | 69 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | D2 | 71 | LEU |
| 41 | D2 | 72 | VAL |
| 41 | D2 | 74 | LYS |
| 41 | D2 | 79 | VAL |
| 41 | D2 | 80 | GLN |
| 41 | D2 | 81 | TYR |
| 41 | D2 | 82 | ARG |
| 41 | D2 | 83 | ARG |
| 41 | D2 | 84 | LYS |
| 41 | D2 | 89 | GLN |
| 41 | D2 | 91 | TYR |
| 41 | D2 | 95 | LEU |
| 42 | DS | 2 | GLU |
| 42 | DS | 11 | ARG |
| 42 | DS | 13 | SER |
| 42 | DS | 15 | ARG |
| 42 | DS | 17 | VAL |
| 42 | DS | 19 | LEU |
| 42 | DS | 20 | VAL |
| 42 | DS | 29 | LEU |
| 42 | DS | 37 | ARG |
| 42 | DS | 39 | THR |
| 42 | DS | 40 | ASN |
| 42 | DS | 50 | VAL |
| 42 | DS | 51 | LEU |
| 42 | DS | 52 | GLU |
| 42 | DS | 61 | ASN |
| 42 | DS | 65 | LEU |
| 42 | DS | 67 | ASP |
| 42 | DS | 70 | TYR |
| 42 | DS | 76 | VAL |
| 42 | DS | 83 | LYS |
| 42 | DS | 88 | ARG |
| 42 | DS | 95 | ILE |
| 42 | DS | 98 | LYS |
| 42 | DS | 100 | THR |
| 42 | DS | 106 | ILE |
| 42 | DS | 107 | LEU |
| 42 | DS | 111 | HIS |
| 43 | DT | 15 | GLU |
| 43 | DT | 30 | VAL |
| 43 | DT | 36 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | DT | 48 | LYS |
| 43 | DT | 49 | VAL |
| 43 | DT | 52 | VAL |
| 43 | DT | 54 | VAL |
| 43 | DT | 55 | ASN |
| 43 | DT | 56 | THR |
| 43 | DT | 57 | LEU |
| 43 | DT | 60 | ARG |
| 43 | DT | 62 | LYS |
| 43 | DT | 63 | LYS |
| 43 | DT | 69 | TYR |
| 43 | DT | 76 | ARG |
| 43 | DT | 80 | ILE |
| 43 | DT | 82 | GLN |
| 44 | DU | 3 | VAL |
| 44 | DU | 4 | LYS |
| 44 | DU | 5 | MET |
| 44 | DU | 6 | HIS |
| 44 | DU | 13 | VAL |
| 44 | DU | 14 | LEU |
| 44 | DU | 20 | TYR |
| 44 | DU | 23 | ARG |
| 44 | DU | 26 | LYS |
| 44 | DU | 28 | LYS |
| 44 | DU | 31 | LEU |
| 44 | DU | 40 | GLU |
| 44 | DU | 43 | ASN |
| 44 | DU | 44 | ILE |
| 44 | DU | 50 | ARG |
| 44 | DU | 51 | VAL |
| 44 | DU | 57 | GLN |
| 44 | DU | 60 | PHE |
| 44 | DU | 62 | GLU |
| 44 | DU | 63 | LYS |
| 44 | DU | 71 | LYS |
| 44 | DU | 75 | ILE |
| 44 | DU | 76 | CYS |
| 44 | DU | 79 | CYS |
| 44 | DU | 81 | LYS |
| 44 | DU | 86 | ARG |
| 44 | DU | 89 | PHE |
| 44 | DU | 90 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | DU | 91 | GLU |
| 44 | DU | 95 | LYS |
| 44 | DU | 96 | ILE |
| 44 | DU | 97 | ARG |
| 44 | DU | 99 | CYS |
| 44 | DU | 102 | CYS |
| 45 | DV | 2 | GLU |
| 45 | DV | 14 | LYS |
| 45 | DV | 16 | SER |
| 45 | DV | 19 | ARG |
| 45 | DV | 23 | LYS |
| 45 | DV | 24 | LEU |
| 45 | DV | 27 | VAL |
| 45 | DV | 30 | ASN |
| 45 | DV | 32 | HIS |
| 45 | DV | 35 | ARG |
| 45 | DV | 37 | VAL |
| 45 | DV | 50 | GLN |
| 45 | DV | 52 | SER |
| 45 | DV | 60 | GLU |
| 45 | DV | 73 | GLN |
| 45 | DV | 74 | VAL |
| 45 | DV | 76 | LEU |
| 45 | DV | 79 | ARG |
| 45 | DV | 81 | ARG |
| 45 | DV | 87 | ASP |
| 45 | DV | 97 | GLU |
| 45 | DV | 103 | ARG |
| 45 | DV | 112 | ARG |
| 45 | DV | 117 | LEU |
| 45 | DV | 118 | GLN |
| 45 | DV | 119 | GLU |
| 45 | DV | 121 | HIS |
| 45 | DV | 148 | ASP |
| 45 | DV | 150 | LEU |
| 45 | DV | 163 | LEU |
| 45 | DV | 165 | VAL |
| 45 | DV | 166 | SER |
| 45 | DV | 170 | THR |
| 45 | DV | 179 | ASP |
| 46 | D3 | 9 | SER |
| 46 | D3 | 10 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | D3 | 12 | ASN |
| 46 | D3 | 16 | SER |
| 46 | D3 | 23 | VAL |
| 46 | D3 | 25 | ARG |
| 46 | D3 | 36 | ILE |
| 46 | D3 | 40 | GLN |
| 46 | D3 | 43 | THR |
| 46 | D3 | 44 | ARG |
| 46 | D3 | 50 | ASN |
| 46 | D3 | 55 | ARG |
| 46 | D3 | 68 | GLU |
| 46 | D3 | 70 | GLN |
| 46 | D3 | 74 | ARG |
| 47 | DZ | 3 | LYS |
| 47 | DZ | 25 | LYS |
| 47 | DZ | 38 | SER |
| 47 | DZ | 41 | ARG |
| 47 | DZ | 42 | GLN |
| 47 | DZ | 56 | GLN |
| 47 | DZ | 62 | VAL |
| 47 | DZ | 74 | VAL |
| 47 | DZ | 76 | ARG |
| 47 | DZ | 78 | LYS |
| 47 | DZ | 81 | LYS |
| 47 | DZ | 82 | LEU |
| 47 | DZ | 83 | GLU |
| 47 | DZ | 85 | LEU |
| 47 | DZ | 90 | ILE |
| 47 | DZ | 91 | LYS |
| 47 | DZ | 92 | LYS |
| 47 | DZ | 98 | LEU |
| 48 | DW | 5 | GLU |
| 48 | DW | 8 | LYS |
| 48 | DW | 10 | LEU |
| 48 | DW | 15 | LYS |
| 48 | DW | 16 | LEU |
| 48 | DW | 22 | GLU |
| 48 | DW | 24 | LEU |
| 48 | DW | 30 | ARG |
| 48 | DW | 35 | LEU |
| 48 | DW | 41 | ILE |
| 48 | DW | 44 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | DW | 47 | ASN |
| 48 | DW | 53 | LEU |
| 48 | DW | 60 | LEU |
| 49 | DX | 8 | LEU |
| 49 | DX | 17 | LYS |
| 49 | DX | 18 | ASP |
| 49 | DX | 24 | LYS |
| 49 | DX | 29 | ARG |
| 49 | DX | 32 | GLN |
| 49 | DX | 35 | ARG |
| 49 | DX | 40 | THR |
| 49 | DX | 53 | LEU |
| 50 | D4 | 1 | MET |
| 50 | D4 | 3 | GLU |
| 50 | D4 | 6 | HIS |
| 50 | D4 | 13 | ARG |
| 50 | D4 | 16 | CYS |
| 50 | D4 | 18 | CYS |
| 50 | D4 | 20 | ASN |
| 50 | D4 | 22 | ILE |
| 50 | D4 | 24 | THR |
| 50 | D4 | 30 | GLU |
| 50 | D4 | 44 | THR |
| 50 | D4 | 46 | GLN |
| 50 | D4 | 48 | ARG |
| 50 | D4 | 49 | PHE |
| 50 | D4 | 52 | THR |
| 50 | D4 | 53 | GLU |
| 50 | D4 | 60 | GLN |
| 50 | D4 | 61 | ARG |
| 50 | D4 | 62 | ARG |
| 51 | D5 | 3 | LYS |
| 51 | D5 | 4 | HIS |
| 51 | D5 | 6 | VAL |
| 51 | D5 | 11 | THR |
| 51 | D5 | 16 | ARG |
| 51 | D5 | 23 | HIS |
| 51 | D5 | 25 | LEU |
| 51 | D5 | 26 | THR |
| 51 | D5 | 29 | THR |
| 51 | D5 | 33 | CYS |
| 51 | D5 | 35 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | D5 | 48 | GLU |
| 51 | D5 | 52 | TYR |
| 51 | D5 | 56 | LYS |
| 52 | D6 | 9 | LEU |
| 52 | D6 | 10 | LEU |
| 52 | D6 | 17 | LYS |
| 52 | D6 | 29 | ASN |
| 52 | D6 | 30 | THR |
| 52 | D6 | 32 | ASN |
| 52 | D6 | 36 | LEU |
| 52 | D6 | 37 | ARG |
| 52 | D6 | 44 | ARG |
| 52 | D6 | 45 | LYS |
| 52 | D6 | 46 | HIS |
| 52 | D6 | 49 | HIS |
| 52 | D6 | 53 | LYS |
| 53 | D7 | 1 | MET |
| 53 | D7 | 4 | THR |
| 53 | D7 | 8 | ASN |
| 53 | D7 | 9 | ARG |
| 53 | D7 | 11 | LYS |
| 53 | D7 | 24 | THR |
| 53 | D7 | 32 | LYS |
| 53 | D7 | 46 | VAL |
| 53 | D7 | 48 | LYS |
| 53 | D7 | 49 | ARG |
| 54 | D8 | 6 | THR |
| 54 | D8 | 21 | LYS |
| 54 | D8 | 33 | ASN |
| 54 | D8 | 40 | GLU |
| 54 | D8 | 41 | ILE |
| 54 | D8 | 50 | LEU |
| 54 | D8 | 52 | LYS |
| 54 | D8 | 54 | GLU |
| 54 | D8 | 58 | ILE |
| 54 | D8 | 61 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (255) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AE | 19 | HIS |
| 2 | AE | 204 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AE | 212 | GLN |
| 3 | AF | 104 | GLN |
| 3 | AF | 108 | ASN |
| 3 | AF | 136 | GLN |
| 3 | AF | 162 | GLN |
| 3 | AF | 170 | GLN |
| 3 | AF | 176 | HIS |
| 3 | AF | 181 | ASN |
| 4 | AG | 42 | GLN |
| 4 | AG | 45 | GLN |
| 4 | AG | 119 | GLN |
| 4 | AG | 123 | HIS |
| 4 | AG | 160 | GLN |
| 4 | AG | 201 | GLN |
| 5 | AH | 20 | GLN |
| 5 | AH | 78 | HIS |
| 6 | AI | 18 | GLN |
| 6 | AI | 27 | GLN |
| 6 | AI | 57 | GLN |
| 6 | AI | 64 | GLN |
| 6 | AI | 100 | ASN |
| 9 | AL | 124 | GLN |
| 10 | AM | 33 | GLN |
| 10 | AM | 56 | HIS |
| 10 | AM | 62 | HIS |
| 10 | AM | 84 | GLN |
| 11 | AN | 104 | GLN |
| 12 | AO | 9 | GLN |
| 12 | AO | 49 | ASN |
| 12 | AO | 75 | HIS |
| 13 | AP | 62 | ASN |
| 13 | AP | 92 | HIS |
| 13 | AP | 101 | GLN |
| 13 | AP | 106 | ASN |
| 14 | AQ | 49 | HIS |
| 15 | AR | 37 | ASN |
| 16 | AS | 82 | GLN |
| 17 | AT | 16 | GLN |
| 17 | AT | 94 | ASN |
| 18 | AU | 36 | ASN |
| 19 | AV | 23 | ASN |
| 19 | AV | 56 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AV | 57 | HIS |
| 19 | AV | 65 | ASN |
| 19 | AV | 83 | HIS |
| 20 | AW | 9 | ASN |
| 27 | BD | 58 | HIS |
| 27 | BD | 116 | GLN |
| 27 | BD | 166 | GLN |
| 27 | BD | 186 | HIS |
| 27 | BD | 198 | ASN |
| 27 | BD | 220 | HIS |
| 28 | BE | 35 | GLN |
| 28 | BE | 55 | ASN |
| 28 | BE | 143 | ASN |
| 28 | BE | 192 | ASN |
| 29 | BF | 67 | GLN |
| 29 | BF | 69 | HIS |
| 29 | BF | 169 | ASN |
| 29 | BF | 203 | GLN |
| 30 | BG | 26 | GLN |
| 30 | BG | 40 | ASN |
| 30 | BG | 66 | GLN |
| 30 | BG | 108 | ASN |
| 30 | BG | 121 | ASN |
| 31 | BH | 143 | GLN |
| 31 | BH | 147 | ASN |
| 32 | BK | 139 | GLN |
| 33 | BM | 38 | HIS |
| 33 | BM | 128 | HIS |
| 33 | BM | 131 | GLN |
| 33 | BM | 133 | GLN |
| 34 | BN | 82 | ASN |
| 35 | BO | 9 | ASN |
| 35 | BO | 27 | HIS |
| 35 | BO | 84 | ASN |
| 35 | BO | 128 | HIS |
| 36 | BP | 12 | GLN |
| 36 | BP | 89 | ASN |
| 37 | B0 | 3 | HIS |
| 37 | B0 | 16 | HIS |
| 37 | B0 | 23 | ASN |
| 37 | B0 | 71 | GLN |
| 39 | BR | 43 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BR | 79 | HIS |
| 39 | BR | 84 | GLN |
| 40 | B1 | 44 | ASN |
| 40 | B1 | 49 | HIS |
| 40 | B1 | 94 | ASN |
| 41 | B2 | 11 | GLN |
| 41 | B2 | 89 | GLN |
| 42 | BS | 34 | ASN |
| 42 | BS | 40 | ASN |
| 42 | BS | 57 | ASN |
| 42 | BS | 62 | HIS |
| 42 | BS | 102 | HIS |
| 42 | BS | 111 | HIS |
| 43 | BT | 31 | HIS |
| 43 | BT | 55 | ASN |
| 43 | BT | 82 | GLN |
| 43 | BT | 87 | GLN |
| 44 | BU | 6 | HIS |
| 45 | BV | 75 | ASN |
| 45 | BV | 132 | ASN |
| 45 | BV | 151 | HIS |
| 46 | B3 | 17 | GLN |
| 46 | B3 | 35 | ASN |
| 46 | B3 | 40 | GLN |
| 47 | BZ | 56 | GLN |
| 47 | BZ | 66 | HIS |
| 48 | BW | 9 | GLN |
| 48 | BW | 43 | GLN |
| 48 | BW | 56 | GLN |
| 48 | BW | 65 | ASN |
| 49 | BX | 19 | GLN |
| 49 | BX | 32 | GLN |
| 49 | BX | 46 | ASN |
| 49 | BX | 52 | HIS |
| 50 | B4 | 47 | GLN |
| 51 | B5 | 4 | HIS |
| 51 | B5 | 23 | HIS |
| 51 | B5 | 43 | HIS |
| 52 | B6 | 49 | HIS |
| 53 | B7 | 8 | ASN |
| 53 | B7 | 36 | GLN |
| 54 | B8 | 35 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CE | 16 | HIS |
| 2 | CE | 78 | GLN |
| 2 | CE | 135 | GLN |
| 3 | CF | 3 | ASN |
| 3 | CF | 69 | HIS |
| 3 | CF | 98 | ASN |
| 3 | CF | 123 | GLN |
| 4 | CG | 43 | HIS |
| 4 | CG | 62 | GLN |
| 4 | CG | 77 | ASN |
| 4 | CG | 160 | GLN |
| 4 | CG | 201 | GLN |
| 5 | CH | 20 | GLN |
| 5 | CH | 141 | GLN |
| 6 | CI | 32 | ASN |
| 6 | CI | 57 | GLN |
| 6 | CI | 100 | ASN |
| 7 | CJ | 37 | ASN |
| 7 | CJ | 84 | ASN |
| 7 | CJ | 86 | GLN |
| 8 | CK | 82 | HIS |
| 9 | CL | 3 | GLN |
| 9 | CL | 89 | ASN |
| 9 | CL | 124 | GLN |
| 10 | CM | 13 | HIS |
| 10 | CM | 56 | HIS |
| 11 | CN | 38 | ASN |
| 11 | CN | 104 | GLN |
| 11 | CN | 117 | ASN |
| 12 | CO | 8 | ASN |
| 12 | CO | 49 | ASN |
| 12 | CO | 75 | HIS |
| 12 | CO | 80 | HIS |
| 14 | CQ | 49 | HIS |
| 15 | CR | 37 | ASN |
| 15 | CR | 46 | HIS |
| 16 | CS | 82 | GLN |
| 17 | CT | 26 | GLN |
| 19 | CV | 14 | HIS |
| 19 | CV | 56 | GLN |
| 19 | CV | 57 | HIS |
| 19 | CV | 65 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CW | 16 | HIS |
| 20 | CW | 26 | ASN |
| 27 | DD | 44 | ASN |
| 27 | DD | 58 | HIS |
| 27 | DD | 96 | HIS |
| 27 | DD | 143 | HIS |
| 27 | DD | 166 | GLN |
| 27 | DD | 186 | HIS |
| 27 | DD | 198 | ASN |
| 28 | DE | 48 | GLN |
| 28 | DE | 60 | ASN |
| 28 | DE | 66 | HIS |
| 28 | DE | 192 | ASN |
| 29 | DF | 169 | ASN |
| 30 | DG | 27 | ASN |
| 30 | DG | 40 | ASN |
| 30 | DG | 41 | GLN |
| 31 | DH | 74 | ASN |
| 31 | DH | 147 | ASN |
| 32 | DK | 11 | ASN |
| 32 | DK | 54 | GLN |
| 32 | DK | 104 | GLN |
| 32 | DK | 105 | HIS |
| 33 | DM | 45 | ASN |
| 33 | DM | 130 | HIS |
| 33 | DM | 133 | GLN |
| 34 | DN | 5 | GLN |
| 34 | DN | 82 | ASN |
| 35 | DO | 128 | HIS |
| 36 | DP | 123 | HIS |
| 37 | D0 | 11 | ASN |
| 37 | D0 | 13 | HIS |
| 37 | D0 | 16 | HIS |
| 37 | D0 | 23 | ASN |
| 37 | D0 | 24 | GLN |
| 37 | D0 | 53 | HIS |
| 38 | DQ | 95 | HIS |
| 39 | DR | 58 | ASN |
| 39 | DR | 79 | HIS |
| 39 | DR | 90 | GLN |
| 39 | DR | 136 | GLN |
| 40 | D1 | 49 | HIS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | D1 | 71 | GLN |
| 40 | D1 | 75 | ASN |
| 40 | D1 | 81 | HIS |
| 41 | D2 | 11 | GLN |
| 41 | D2 | 64 | HIS |
| 41 | D2 | 87 | HIS |
| 41 | D2 | 89 | GLN |
| 42 | DS | 57 | ASN |
| 42 | DS | 60 | ASN |
| 42 | DS | 61 | ASN |
| 42 | DS | 62 | HIS |
| 42 | DS | 102 | HIS |
| 43 | DT | 31 | HIS |
| 43 | DT | 41 | ASN |
| 43 | DT | 55 | ASN |
| 43 | DT | 82 | GLN |
| 43 | DT | 87 | GLN |
| 44 | DU | 43 | ASN |
| 45 | DV | 34 | ASN |
| 45 | DV | 50 | GLN |
| 45 | DV | 65 | GLN |
| 45 | DV | 75 | ASN |
| 45 | DV | 132 | ASN |
| 46 | D3 | 12 | ASN |
| 46 | D3 | 29 | GLN |
| 46 | D3 | 50 | ASN |
| 46 | D3 | 70 | GLN |
| 47 | DZ | 56 | GLN |
| 47 | DZ | 66 | HIS |
| 48 | DW | 9 | GLN |
| 48 | DW | 65 | ASN |
| 49 | DX | 19 | GLN |
| 49 | DX | 33 | GLN |
| 49 | DX | 46 | ASN |
| 49 | DX | 52 | HIS |
| 50 | D4 | 40 | HIS |
| 50 | D4 | 47 | GLN |
| 50 | D4 | 60 | GLN |
| 51 | D5 | 23 | HIS |
| 51 | D5 | 43 | HIS |
| 52 | D6 | 29 | ASN |
| 53 | D7 | 8 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | D7 | 36 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1505/1506 (99%) | 375 (24%) | 32 (2%) |
| 1 | CA | 1505/1506 (99%) | 409 (27%) | 41 (2%) |
| 22 | AB | 86/87 (98%) | 40 (46%) | 5 (5%) |
| 22 | CB | 86/87 (98%) | 46 (53%) | 2 (2%) |
| 23 | AC | 77/77 (100%) | 23 (29%) | 6 (7%) |
| 23 | AD | 76/77 (98%) | 28 (36%) | 1 (1%) |
| 23 | CC | 77/77 (100%) | 21 (27%) | 5 (6%) |
| 23 | CD | 76/77 (98%) | 26 (34%) | 1 (1%) |
| 24 | A1 | 9/10 (90%) | 3 (33%) | 1 (11%) |
| 24 | C1 | 9/10 (90%) | 3 (33%) | 0 |
| 25 | BA | 2911/2912 (99%) | 713 (24%) | 57 (1%) |
| 25 | DA | 2905/2912 (99%) | 763 (26%) | 57 (1%) |
| 26 | BB | 121/122 (99%) | 30 (24%) | 0 |
| 26 | DB | 121/122 (99%) | 39 (32%) | 0 |
| All | All | 9564/9582 (99%) | 2519 (26%) | 208 (2%) |

All (2519) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 6 | G |
| 1 | AA | 7 | G |
| 1 | AA | 8 | A |
| 1 | AA | 32 | A |
| 1 | AA | 33 | A |
| 1 | AA | 39 | G |
| 1 | AA | 48 | C |
| 1 | AA | 49 | U |
| 1 | AA | 50 | A |
| 1 | AA | 51 | A |
| 1 | AA | 54 | C |
| 1 | AA | 56 | U |
| 1 | AA | 61 | G |
| 1 | AA | 65 | U |
| 1 | AA | 66 | G |
| 1 | AA | 76 | G |
| 1 | AA | 78 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 80 | G |
| 1 | AA | 81 | G |
| 1 | AA | 84 | U |
| 1 | AA | 85 | U |
| 1 | AA | 86 | U |
| 1 | AA | 87 | A |
| 1 | AA | 88 | C |
| 1 | AA | 89 | U |
| 1 | AA | 90 | C |
| 1 | AA | 91 | C |
| 1 | AA | 92 | G |
| 1 | AA | 95 | G |
| 1 | AA | 99 | C |
| 1 | AA | 101 | A |
| 1 | AA | 116 | A |
| 1 | AA | 119 | A |
| 1 | AA | 120 | A |
| 1 | AA | 121 | C |
| 1 | AA | 123 | C |
| 1 | AA | 131 | C |
| 1 | AA | 143 | A |
| 1 | AA | 144 | G |
| 1 | AA | 154 | C |
| 1 | AA | 157 | G |
| 1 | AA | 158 | G |
| 1 | AA | 161 | A |
| 1 | AA | 163 | C |
| 1 | AA | 164 | U |
| 1 | AA | 168 | G |
| 1 | AA | 171 | A |
| 1 | AA | 173 | U |
| 1 | AA | 174 | C |
| 1 | AA | 188 | U |
| 1 | AA | 189 | U |
| 1 | AA | 190 | G |
| 1 | AA | 195 | A |
| 1 | AA | 197 | A |
| 1 | AA | 199 | G |
| 1 | AA | 201 | C |
| 1 | AA | 208 | U |
| 1 | AA | 209 | U |
| 1 | AA | 210 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 216 | G |
| 1 | AA | 226 | G |
| 1 | AA | 243 | A |
| 1 | AA | 245 | C |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 262 | A |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 268 | C |
| 1 | AA | 270 | A |
| 1 | AA | 281 | G |
| 1 | AA | 289 | G |
| 1 | AA | 313 | A |
| 1 | AA | 321 | A |
| 1 | AA | 328 | C |
| 1 | AA | 330 | C |
| 1 | AA | 332 | G |
| 1 | AA | 341 | C |
| 1 | AA | 342 | C |
| 1 | AA | 343 | U |
| 1 | AA | 344 | A |
| 1 | AA | 345 | C |
| 1 | AA | 346 | G |
| 1 | AA | 352 | C |
| 1 | AA | 353 | A |
| 1 | AA | 354 | G |
| 1 | AA | 365 | U |
| 1 | AA | 367 | U |
| 1 | AA | 372 | C |
| 1 | AA | 384 | G |
| 1 | AA | 390 | C |
| 1 | AA | 397 | A |
| 1 | AA | 398 | C |
| 1 | AA | 406 | G |
| 1 | AA | 411 | A |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 414 | A |
| 1 | AA | 415 | A |
| 1 | AA | 419 | C |
| 1 | AA | 422 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 424 | G |
| 1 | AA | 429 | U |
| 1 | AA | 430 | A |
| 1 | AA | 439 | A |
| 1 | AA | 452 | A |
| 1 | AA | 466 | C |
| 1 | AA | 467 | G |
| 1 | AA | 485 | G |
| 1 | AA | 487 | A |
| 1 | AA | 496 | A |
| 1 | AA | 497 | U |
| 1 | AA | 505 | G |
| 1 | AA | 509 | A |
| 1 | AA | 510 | A |
| 1 | AA | 511 | C |
| 1 | AA | 518 | C |
| 1 | AA | 521 | G |
| 1 | AA | 524 | G |
| 1 | AA | 527 | G |
| 1 | AA | 530 | G |
| 1 | AA | 531 | U |
| 1 | AA | 533 | A |
| 1 | AA | 534 | U |
| 1 | AA | 536 | C |
| 1 | AA | 545 | C |
| 1 | AA | 547 | A |
| 1 | AA | 559 | A |
| 1 | AA | 561 | U |
| 1 | AA | 562 | C |
| 1 | AA | 563 | A |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 576 | G |
| 1 | AA | 577 | G |
| 1 | AA | 579 | G |
| 1 | AA | 596 | C |
| 1 | AA | 606 | G |
| 1 | AA | 607 | A |
| 1 | AA | 608 | A |
| 1 | AA | 609 | A |
| 1 | AA | 616 | G |
| 1 | AA | 617 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 619 | U |
| 1 | AA | 622 | A |
| 1 | AA | 623 | C |
| 1 | AA | 630 | G |
| 1 | AA | 631 | G |
| 1 | AA | 632 | A |
| 1 | AA | 633 | G |
| 1 | AA | 639 | G |
| 1 | AA | 646 | U |
| 1 | AA | 651 | C |
| 1 | AA | 653 | A |
| 1 | AA | 665 | A |
| 1 | AA | 666 | G |
| 1 | AA | 687 | A |
| 1 | AA | 688 | G |
| 1 | AA | 701 | C |
| 1 | AA | 704 | A |
| 1 | AA | 723 | U |
| 1 | AA | 724 | G |
| 1 | AA | 731 | G |
| 1 | AA | 747 | C |
| 1 | AA | 748 | C |
| 1 | AA | 749 | C |
| 1 | AA | 751 | U |
| 1 | AA | 755 | G |
| 1 | AA | 766 | A |
| 1 | AA | 767 | A |
| 1 | AA | 773 | G |
| 1 | AA | 774 | G |
| 1 | AA | 777 | A |
| 1 | AA | 787 | A |
| 1 | AA | 792 | A |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 802 | A |
| 1 | AA | 805 | C |
| 1 | AA | 813 | U |
| 1 | AA | 815 | A |
| 1 | AA | 817 | C |
| 1 | AA | 820 | U |
| 1 | AA | 821 | G |
| 1 | AA | 827 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 828 | A |
| 1 | AA | 841 | U |
| 1 | AA | 842 | C |
| 1 | AA | 843 | U |
| 1 | AA | 848 | C |
| 1 | AA | 857 | C |
| 1 | AA | 859 | A |
| 1 | AA | 864 | A |
| 1 | AA | 871 | U |
| 1 | AA | 872 | A |
| 1 | AA | 884 | U |
| 1 | AA | 887 | G |
| 1 | AA | 902 | G |
| 1 | AA | 914 | A |
| 1 | AA | 926 | G |
| 1 | AA | 927 | G |
| 1 | AA | 934 | C |
| 1 | AA | 935 | A |
| 1 | AA | 936 | C |
| 1 | AA | 939 | G |
| 1 | AA | 940 | C |
| 1 | AA | 941 | G |
| 1 | AA | 960 | U |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 972 | C |
| 1 | AA | 974 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 978 | A |
| 1 | AA | 983 | A |
| 1 | AA | 991 | U |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 995 | C |
| 1 | AA | 1002 | G |
| 1 | AA | 1003 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1006 | C |
| 1 | AA | 1009 | G |
| 1 | AA | 1017 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1020 | U |
| 1 | AA | 1021 | G |
| 1 | AA | 1024 | G |
| 1 | AA | 1025 | U |
| 1 | AA | 1026 | G |
| 1 | AA | 1027 | C |
| 1 | AA | 1028 | C |
| 1 | AA | 1029 | G |
| 1 | AA | 1032(A) | G |
| 1 | AA | 1036 | G |
| 1 | AA | 1037 | C |
| 1 | AA | 1038 | C |
| 1 | AA | 1039 | C |
| 1 | AA | 1040 | U |
| 1 | AA | 1042 | G |
| 1 | AA | 1054 | C |
| 1 | AA | 1055 | A |
| 1 | AA | 1065 | U |
| 1 | AA | 1066 | C |
| 1 | AA | 1078 | U |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1101 | A |
| 1 | AA | 1103 | C |
| 1 | AA | 1113 | C |
| 1 | AA | 1123 | A |
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1126 | U |
| 1 | AA | 1127 | G |
| 1 | AA | 1129 | C |
| 1 | AA | 1131 | G |
| 1 | AA | 1132 | C |
| 1 | AA | 1133 | G |
| 1 | AA | 1136 | U |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1140 | C |
| 1 | AA | 1145 | C |
| 1 | AA | 1146 | A |
| 1 | AA | 1151 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1152 | A |
| 1 | AA | 1157 | A |
| 1 | AA | 1158 | C |
| 1 | AA | 1159 | U |
| 1 | AA | 1160 | G |
| 1 | AA | 1165 | C |
| 1 | AA | 1170 | A |
| 1 | AA | 1172 | C |
| 1 | AA | 1177 | G |
| 1 | AA | 1178 | G |
| 1 | AA | 1179 | A |
| 1 | AA | 1181 | G |
| 1 | AA | 1182 | G |
| 1 | AA | 1183 | A |
| 1 | AA | 1186 | G |
| 1 | AA | 1187 | G |
| 1 | AA | 1188 | A |
| 1 | AA | 1193 | G |
| 1 | AA | 1194 | U |
| 1 | AA | 1195 | C |
| 1 | AA | 1196 | U |
| 1 | AA | 1197 | G |
| 1 | AA | 1201 | A |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1224 | G |
| 1 | AA | 1225 | A |
| 1 | AA | 1227 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1241 | G |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | U |
| 1 | AA | 1258 | G |
| 1 | AA | 1270 | C |
| 1 | AA | 1272 | G |
| 1 | AA | 1273 | G |
| 1 | AA | 1275 | A |
| 1 | AA | 1278 | U |
| 1 | AA | 1279 | A |
| 1 | AA | 1280 | A |
| 1 | AA | 1281 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1282 | C |
| 1 | AA | 1286 | A |
| 1 | AA | 1287 | A |
| 1 | AA | 1288 | A |
| 1 | AA | 1290 | G |
| 1 | AA | 1291 | G |
| 1 | AA | 1300 | G |
| 1 | AA | 1301 | U |
| 1 | AA | 1302 | U |
| 1 | AA | 1303 | C |
| 1 | AA | 1305 | G |
| 1 | AA | 1313 | U |
| 1 | AA | 1317 | C |
| 1 | AA | 1319 | A |
| 1 | AA | 1322 | C |
| 1 | AA | 1323 | G |
| 1 | AA | 1331 | G |
| 1 | AA | 1334 | G |
| 1 | AA | 1336 | C |
| 1 | AA | 1337 | G |
| 1 | AA | 1346 | A |
| 1 | AA | 1347 | G |
| 1 | AA | 1350 | A |
| 1 | AA | 1353 | G |
| 1 | AA | 1356 | G |
| 1 | AA | 1361 | G |
| 1 | AA | 1363 | A |
| 1 | AA | 1365 | G |
| 1 | AA | 1370 | G |
| 1 | AA | 1373 | G |
| 1 | AA | 1377 | A |
| 1 | AA | 1378 | C |
| 1 | AA | 1381 | U |
| 1 | AA | 1388 | C |
| 1 | AA | 1397 | C |
| 1 | AA | 1398 | A |
| 1 | AA | 1401 | G |
| 1 | AA | 1406 | U |
| 1 | AA | 1416 | G |
| 1 | AA | 1419 | G |
| 1 | AA | 1442 | G |
| 1 | AA | 1443 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1446 | A |
| 1 | AA | 1447 | G |
| 1 | AA | 1449 | C |
| 1 | AA | 1450 | U |
| 1 | AA | 1452 | C |
| 1 | AA | 1453 | G |
| 1 | AA | 1454 | G |
| 1 | AA | 1487 | G |
| 1 | AA | 1492 | A |
| 1 | AA | 1493 | A |
| 1 | AA | 1497 | G |
| 1 | AA | 1499 | A |
| 1 | AA | 1502 | A |
| 1 | AA | 1503 | A |
| 1 | AA | 1504 | G |
| 1 | AA | 1505 | G |
| 1 | AA | 1506 | U |
| 1 | AA | 1507 | A |
| 1 | AA | 1517 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 1 | AA | 1531 | A |
| 22 | AB | 2 | C |
| 22 | AB | 7 | G |
| 22 | AB | 8 | U |
| 22 | AB | 9 | G |
| 22 | AB | 13 | G |
| 22 | AB | 14 | A |
| 22 | AB | 16 | U |
| 22 | AB | 17 | U |
| 22 | AB | 18 | G |
| 22 | AB | 19 | G |
| 22 | AB | 20 | U |
| 22 | AB | 21 | A |
| 22 | AB | 22 | G |
| 22 | AB | 23 | A |
| 22 | AB | 24 | C |
| 22 | AB | 26 | C |
| 22 | AB | 27 | G |
| 22 | AB | 34 | U |
| 22 | AB | 37 | G |
| 22 | AB | 39 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | AB | 41 | G |
| 22 | AB | 42 | U |
| 22 | AB | 43 | A |
| 22 | AB | 48 | C |
| 22 | AB | 49 | C |
| 22 | AB | 50 | A |
| 22 | AB | 51 | A |
| 22 | AB | 52 | U |
| 22 | AB | 55 | G |
| 22 | AB | 56 | G |
| 22 | AB | 58 | U |
| 22 | AB | 59 | U |
| 22 | AB | 60 | A |
| 22 | AB | 61 | C |
| 22 | AB | 71 | U |
| 22 | AB | 74 | C |
| 22 | AB | 76 | U |
| 22 | AB | 77 | C |
| 22 | AB | 85 | C |
| 22 | AB | 87 | A |
| 23 | AC | 2 | G |
| 23 | AC | 6 | G |
| 23 | AC | 9 | G |
| 23 | AC | 13 | C |
| 23 | AC | 14 | A |
| 23 | AC | 16 | C |
| 23 | AC | 18 | C |
| 23 | AC | 19 | G |
| 23 | AC | 20 | G |
| 23 | AC | 21 | U |
| 23 | AC | 22 | A |
| 23 | AC | 32 | G |
| 23 | AC | 38 | A |
| 23 | AC | 44 | A |
| 23 | AC | 45 | A |
| 23 | AC | 48 | U |
| 23 | AC | 49 | C |
| 23 | AC | 50 | G |
| 23 | AC | 52 | C |
| 23 | AC | 54 | G |
| 23 | AC | 60 | A |
| 23 | AC | 76 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | AC | 77 | A |
| 23 | AD | 6 | G |
| 23 | AD | 8 | U |
| 23 | AD | 9 | G |
| 23 | AD | 10 | G |
| 23 | AD | 13 | C |
| 23 | AD | 14 | A |
| 23 | AD | 15 | G |
| 23 | AD | 17 | C |
| 23 | AD | 19 | G |
| 23 | AD | 20 | G |
| 23 | AD | 21 | U |
| 23 | AD | 22 | A |
| 23 | AD | 23 | G |
| 23 | AD | 24 | C |
| 23 | AD | 40 | C |
| 23 | AD | 45 | A |
| 23 | AD | 46 | G |
| 23 | AD | 48 | U |
| 23 | AD | 49 | C |
| 23 | AD | 54 | G |
| 23 | AD | 58 | A |
| 23 | AD | 60 | A |
| 23 | AD | 61 | U |
| 23 | AD | 62 | C |
| 23 | AD | 68 | C |
| 23 | AD | 70 | C |
| 23 | AD | 74 | A |
| 23 | AD | 77 | A |
| 24 | A1 | 14 | U |
| 24 | A1 | 15 | U |
| 24 | A1 | 19 | U |
| 25 | BA | 2 | G |
| 25 | BA | 5 | A |
| 25 | BA | 12 | U |
| 25 | BA | 13 | A |
| 25 | BA | 15 | G |
| 25 | BA | 26 | G |
| 25 | BA | 33 | U |
| 25 | BA | 34 | C |
| 25 | BA | 35 | G |
| 25 | BA | 46 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BA | 51 | G |
| 25 | BA | 63 | U |
| 25 | BA | 71 | A |
| 25 | BA | 74 | A |
| 25 | BA | 75 | G |
| 25 | BA | 85 | G |
| 25 | BA | 95 | G |
| 25 | BA | 99 | U |
| 25 | BA | 101 | G |
| 25 | BA | 110 | G |
| 25 | BA | 118 | A |
| 25 | BA | 119 | A |
| 25 | BA | 120 | U |
| 25 | BA | 123 | G |
| 25 | BA | 125 | G |
| 25 | BA | 135 | G |
| 25 | BA | 138 | G |
| 25 | BA | 155 | C |
| 25 | BA | 162 | U |
| 25 | BA | 164 | U |
| 25 | BA | 165 | U |
| 25 | BA | 181 | A |
| 25 | BA | 188 | G |
| 25 | BA | 196 | A |
| 25 | BA | 197 | A |
| 25 | BA | 199 | A |
| 25 | BA | 214 | G |
| 25 | BA | 215 | G |
| 25 | BA | 216 | A |
| 25 | BA | 221 | A |
| 25 | BA | 222 | A |
| 25 | BA | 223 | A |
| 25 | BA | 227 | A |
| 25 | BA | 228 | A |
| 25 | BA | 229 | A |
| 25 | BA | 230 | U |
| 25 | BA | 232 | G |
| 25 | BA | 233 | A |
| 25 | BA | 248 | G |
| 25 | BA | 249 | C |
| 25 | BA | 250 | G |
| 25 | BA | 252 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | BA | 261 | G |
| 25 | BA | 264 | C |
| 25 | BA | 269 | U |
| 25 | BA | 270(I) | G |
| 25 | BA | 270(K) | C |
| 25 | BA | 270(L) | U |
| 25 | BA | 270(M) | U |
| 25 | BA | 270(N) | G |
| 25 | BA | 270(P) | C |
| 25 | BA | 271(C) | U |
| 25 | BA | 271 | G |
| 25 | BA | 274 | G |
| 25 | BA | 275 | G |
| 25 | BA | 278 | A |
| 25 | BA | 279 | C |
| 25 | BA | 299 | A |
| 25 | BA | 311 | A |
| 25 | BA | 315 | G |
| 25 | BA | 323 | G |
| 25 | BA | 324 | A |
| 25 | BA | 329 | G |
| 25 | BA | 330 | A |
| 25 | BA | 334 | C |
| 25 | BA | 335 | C |
| 25 | BA | 339 | U |
| 25 | BA | 352 | G |
| 25 | BA | 357 | A |
| 25 | BA | 360 | G |
| 25 | BA | 363 | G |
| 25 | BA | 363(E) | U |
| 25 | BA | 364 | C |
| 25 | BA | 372 | G |
| 25 | BA | 385 | C |
| 25 | BA | 386 | G |
| 25 | BA | 405 | U |
| 25 | BA | 411 | G |
| 25 | BA | 412 | A |
| 25 | BA | 418 | G |
| 25 | BA | 426 | C |
| 25 | BA | 428 | A |
| 25 | BA | 440 | G |
| 25 | BA | 444 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BA | 448 | U |
| 25 | BA | 454 | A |
| 25 | BA | 455 | C |
| 25 | BA | 457 | A |
| 25 | BA | 470 | A |
| 25 | BA | 471 | A |
| 25 | BA | 479 | A |
| 25 | BA | 481 | G |
| 25 | BA | 482 | A |
| 25 | BA | 491 | G |
| 25 | BA | 505 | A |
| 25 | BA | 509 | C |
| 25 | BA | 528 | A |
| 25 | BA | 529 | A |
| 25 | BA | 530 | G |
| 25 | BA | 531 | C |
| 25 | BA | 532 | A |
| 25 | BA | 533 | G |
| 25 | BA | 537 | C |
| 25 | BA | 539 | G |
| 25 | BA | 540 | G |
| 25 | BA | 546 | C |
| 25 | BA | 549 | G |
| 25 | BA | 556 | G |
| 25 | BA | 563 | G |
| 25 | BA | 564 | C |
| 25 | BA | 573 | G |
| 25 | BA | 575 | A |
| 25 | BA | 586 | A |
| 25 | BA | 588 | U |
| 25 | BA | 593 | G |
| 25 | BA | 603 | A |
| 25 | BA | 607 | U |
| 25 | BA | 613 | U |
| 25 | BA | 614 | U |
| 25 | BA | 617 | G |
| 25 | BA | 622 | G |
| 25 | BA | 627 | A |
| 25 | BA | 637 | A |
| 25 | BA | 640 | C |
| 25 | BA | 644 | A |
| 25 | BA | 645 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | BA | 646 | A |
| 25 | BA | 647 | G |
| 25 | BA | 649 | G |
| 25 | BA | 652 | C |
| 25 | BA | 653 | A |
| 25 | BA | 654(A) | A |
| 25 | BA | 654(C) | G |
| 25 | BA | 654(G) | C |
| 25 | BA | 654(I) | C |
| 25 | BA | 654(K) | C |
| 25 | BA | 654(L) | G |
| 25 | BA | 654(M) | C |
| 25 | BA | 654(N) | G |
| 25 | BA | 654(P) | G |
| 25 | BA | 654(T) | A |
| 25 | BA | 656 | G |
| 25 | BA | 686 | G |
| 25 | BA | 717 | G |
| 25 | BA | 730 | C |
| 25 | BA | 739 | G |
| 25 | BA | 745 | G |
| 25 | BA | 746 | A |
| 25 | BA | 753 | C |
| 25 | BA | 757 | U |
| 25 | BA | 763 | G |
| 25 | BA | 764 | A |
| 25 | BA | 765 | G |
| 25 | BA | 775 | G |
| 25 | BA | 776 | G |
| 25 | BA | 782 | A |
| 25 | BA | 784 | A |
| 25 | BA | 785 | G |
| 25 | BA | 789 | A |
| 25 | BA | 790 | C |
| 25 | BA | 791 | C |
| 25 | BA | 792 | G |
| 25 | BA | 802 | A |
| 25 | BA | 805 | G |
| 25 | BA | 810 | U |
| 25 | BA | 812 | C |
| 25 | BA | 819 | A |
| 25 | BA | 824 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BA | 827 | U |
| 25 | BA | 828 | U |
| 25 | BA | 836 | G |
| 25 | BA | 847 | U |
| 25 | BA | 857 | C |
| 25 | BA | 858 | U |
| 25 | BA | 859 | G |
| 25 | BA | 866 | A |
| 25 | BA | 878 | A |
| 25 | BA | 879 | G |
| 25 | BA | 880 | G |
| 25 | BA | 881 | G |
| 25 | BA | 882 | G |
| 25 | BA | 883 | G |
| 25 | BA | 884 | C |
| 25 | BA | 885 | C |
| 25 | BA | 886 | C |
| 25 | BA | 887 | A |
| 25 | BA | 888 | C |
| 25 | BA | 890 | A |
| 25 | BA | 893 | C |
| 25 | BA | 894 | C |
| 25 | BA | 895 | U |
| 25 | BA | 896 | A |
| 25 | BA | 897 | C |
| 25 | BA | 898 | C |
| 25 | BA | 899 | A |
| 25 | BA | 900 | A |
| 25 | BA | 901 | A |
| 25 | BA | 902 | C |
| 25 | BA | 906 | G |
| 25 | BA | 910 | A |
| 25 | BA | 917 | A |
| 25 | BA | 925 | C |
| 25 | BA | 926 | A |
| 25 | BA | 932 | G |
| 25 | BA | 938 | G |
| 25 | BA | 940 | G |
| 25 | BA | 941 | A |
| 25 | BA | 946 | G |
| 25 | BA | 961 | C |
| 25 | BA | 968 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 974 | G |
| 25 | BA | 974(A) | C |
| 25 | BA | 975 | G |
| 25 | BA | 983 | A |
| 25 | BA | 990 | A |
| 25 | BA | 995 | C |
| 25 | BA | 996 | A |
| 25 | BA | 999 | U |
| 25 | BA | 1003 | G |
| 25 | BA | 1005 | C |
| 25 | BA | 1010 | A |
| 25 | BA | 1011 | G |
| 25 | BA | 1012 | U |
| 25 | BA | 1013 | C |
| 25 | BA | 1015 | G |
| 25 | BA | 1020 | A |
| 25 | BA | 1022 | G |
| 25 | BA | 1023 | U |
| 25 | BA | 1025 | G |
| 25 | BA | 1026 | U |
| 25 | BA | 1027 | A |
| 25 | BA | 1033 | U |
| 25 | BA | 1037 | G |
| 25 | BA | 1044 | G |
| 25 | BA | 1045 | A |
| 25 | BA | 1046 | A |
| 25 | BA | 1047 | G |
| 25 | BA | 1050 | A |
| 25 | BA | 1054 | A |
| 25 | BA | 1055 | G |
| 25 | BA | 1056 | G |
| 25 | BA | 1057 | A |
| 25 | BA | 1060 | U |
| 25 | BA | 1061 | U |
| 25 | BA | 1062 | G |
| 25 | BA | 1066 | U |
| 25 | BA | 1067 | A |
| 25 | BA | 1068 | G |
| 25 | BA | 1070 | A |
| 25 | BA | 1071 | G |
| 25 | BA | 1073 | A |
| 25 | BA | 1075 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | BA | 1076 | C |
| 25 | BA | 1077 | A |
| 25 | BA | 1078 | U |
| 25 | BA | 1079 | C |
| 25 | BA | 1083 | U |
| 25 | BA | 1084 | A |
| 25 | BA | 1085 | A |
| 25 | BA | 1086 | A |
| 25 | BA | 1087 | G |
| 25 | BA | 1088 | A |
| 25 | BA | 1089 | G |
| 25 | BA | 1090 | U |
| 25 | BA | 1092 | C |
| 25 | BA | 1093 | G |
| 25 | BA | 1095 | A |
| 25 | BA | 1096 | A |
| 25 | BA | 1097 | U |
| 25 | BA | 1102 | C |
| 25 | BA | 1104 | C |
| 25 | BA | 1105 | U |
| 25 | BA | 1106 | G |
| 25 | BA | 1107 | G |
| 25 | BA | 1110 | G |
| 25 | BA | 1111 | A |
| 25 | BA | 1112 | G |
| 25 | BA | 1117 | G |
| 25 | BA | 1122 | G |
| 25 | BA | 1127 | A |
| 25 | BA | 1129 | A |
| 25 | BA | 1130 | U |
| 25 | BA | 1131 | G |
| 25 | BA | 1135 | C |
| 25 | BA | 1136 | G |
| 25 | BA | 1139 | G |
| 25 | BA | 1142 | U |
| 25 | BA | 1142(A) | A |
| 25 | BA | 1144 | G |
| 25 | BA | 1148 | A |
| 25 | BA | 1149 | G |
| 25 | BA | 1151 | G |
| 25 | BA | 1154 | G |
| 25 | BA | 1155 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 1170 | G |
| 25 | BA | 1171 | G |
| 25 | BA | 1176 | G |
| 25 | BA | 1178 | C |
| 25 | BA | 1179 | C |
| 25 | BA | 1180 | C |
| 25 | BA | 1195 | G |
| 25 | BA | 1204 | A |
| 25 | BA | 1205 | U |
| 25 | BA | 1210 | A |
| 25 | BA | 1211 | U |
| 25 | BA | 1218 | C |
| 25 | BA | 1220 | A |
| 25 | BA | 1230 | C |
| 25 | BA | 1241 | A |
| 25 | BA | 1242 | A |
| 25 | BA | 1244 | G |
| 25 | BA | 1253 | A |
| 25 | BA | 1256 | G |
| 25 | BA | 1265 | A |
| 25 | BA | 1269 | A |
| 25 | BA | 1271 | G |
| 25 | BA | 1272 | A |
| 25 | BA | 1273 | U |
| 25 | BA | 1287 | A |
| 25 | BA | 1298 | C |
| 25 | BA | 1300 | U |
| 25 | BA | 1301 | A |
| 25 | BA | 1303 | G |
| 25 | BA | 1312 | U |
| 25 | BA | 1313 | U |
| 25 | BA | 1314 | C |
| 25 | BA | 1328 | G |
| 25 | BA | 1329 | U |
| 25 | BA | 1338 | G |
| 25 | BA | 1341 | U |
| 25 | BA | 1345 | C |
| 25 | BA | 1349 | A |
| 25 | BA | 1352 | U |
| 25 | BA | 1358 | G |
| 25 | BA | 1359 | A |
| 25 | BA | 1360 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | BA | 1365 | A |
| 25 | BA | 1368 | G |
| 25 | BA | 1377 | G |
| 25 | BA | 1380 | G |
| 25 | BA | 1383 | C |
| 25 | BA | 1384 | A |
| 25 | BA | 1385 | G |
| 25 | BA | 1386 | C |
| 25 | BA | 1388 | G |
| 25 | BA | 1389 | G |
| 25 | BA | 1390 | U |
| 25 | BA | 1391 | U |
| 25 | BA | 1404 | C |
| 25 | BA | 1412 | A |
| 25 | BA | 1416 | G |
| 25 | BA | 1417 | C |
| 25 | BA | 1420 | U |
| 25 | BA | 1421 | G |
| 25 | BA | 1427 | A |
| 25 | BA | 1428 | C |
| 25 | BA | 1437 | C |
| 25 | BA | 1444(A) | A |
| 25 | BA | 1447 | G |
| 25 | BA | 1449 | A |
| 25 | BA | 1449(A) | G |
| 25 | BA | 1451 | C |
| 25 | BA | 1453 | A |
| 25 | BA | 1454 | U |
| 25 | BA | 1455 | G |
| 25 | BA | 1458 | C |
| 25 | BA | 1459 | G |
| 25 | BA | 1460 | A |
| 25 | BA | 1461 | G |
| 25 | BA | 1466 | G |
| 25 | BA | 1467 | C |
| 25 | BA | 1470 | G |
| 25 | BA | 1471 | A |
| 25 | BA | 1474 | C |
| 25 | BA | 1475 | G |
| 25 | BA | 1483 | G |
| 25 | BA | 1493 | C |
| 25 | BA | 1494 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 1495 | A |
| 25 | BA | 1497 | U |
| 25 | BA | 1504 | C |
| 25 | BA | 1506 | C |
| 25 | BA | 1507 | A |
| 25 | BA | 1508 | A |
| 25 | BA | 1509 | C |
| 25 | BA | 1510 | A |
| 25 | BA | 1511 | A |
| 25 | BA | 1514 | U |
| 25 | BA | 1520 | U |
| 25 | BA | 1522 | G |
| 25 | BA | 1526 | G |
| 25 | BA | 1533 | C |
| 25 | BA | 1534 | G |
| 25 | BA | 1535 | U |
| 25 | BA | 1536 | A |
| 25 | BA | 1537 | C |
| 25 | BA | 1538 | G |
| 25 | BA | 1540 | G |
| 25 | BA | 1543 | A |
| 25 | BA | 1545 | A |
| 25 | BA | 1548 | C |
| 25 | BA | 1554 | A |
| 25 | BA | 1558 | A |
| 25 | BA | 1559 | G |
| 25 | BA | 1560 | G |
| 25 | BA | 1566 | A |
| 25 | BA | 1569 | A |
| 25 | BA | 1578 | U |
| 25 | BA | 1579 | A |
| 25 | BA | 1585 | C |
| 25 | BA | 1586 | A |
| 25 | BA | 1597 | A |
| 25 | BA | 1608 | A |
| 25 | BA | 1609 | A |
| 25 | BA | 1610 | A |
| 25 | BA | 1617 | C |
| 25 | BA | 1618 | A |
| 25 | BA | 1639 | U |
| 25 | BA | 1640 | C |
| 25 | BA | 1641 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 1648 | C |
| 25 | BA | 1651 | G |
| 25 | BA | 1654 | A |
| 25 | BA | 1655 | A |
| 25 | BA | 1674 | G |
| 25 | BA | 1678 | G |
| 25 | BA | 1694 | C |
| 25 | BA | 1695 | G |
| 25 | BA | 1700 | A |
| 25 | BA | 1701 | A |
| 25 | BA | 1702 | G |
| 25 | BA | 1717 | G |
| 25 | BA | 1727 | U |
| 25 | BA | 1728 | G |
| 25 | BA | 1729 | A |
| 25 | BA | 1730 | U |
| 25 | BA | 1731 | G |
| 25 | BA | 1732 | A |
| 25 | BA | 1734 | C |
| 25 | BA | 1735 | C |
| 25 | BA | 1743 | G |
| 25 | BA | 1749 | A |
| 25 | BA | 1750 | G |
| 25 | BA | 1754 | C |
| 25 | BA | 1756 | G |
| 25 | BA | 1761 | C |
| 25 | BA | 1762 | A |
| 25 | BA | 1763 | G |
| 25 | BA | 1764 | G |
| 25 | BA | 1773 | A |
| 25 | BA | 1780 | A |
| 25 | BA | 1791 | A |
| 25 | BA | 1798 | U |
| 25 | BA | 1799 | G |
| 25 | BA | 1800 | C |
| 25 | BA | 1801 | G |
| 25 | BA | 1802 | A |
| 25 | BA | 1816 | G |
| 25 | BA | 1819 | A |
| 25 | BA | 1820 | U |
| 25 | BA | 1829 | A |
| 25 | BA | 1835 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 1839 | G |
| 25 | BA | 1847 | A |
| 25 | BA | 1858 | G |
| 25 | BA | 1861 | G |
| 25 | BA | 1869 | G |
| 25 | BA | 1870 | C |
| 25 | BA | 1878 | G |
| 25 | BA | 1882 | C |
| 25 | BA | 1885 | A |
| 25 | BA | 1886 | C |
| 25 | BA | 1887 | C |
| 25 | BA | 1889 | A |
| 25 | BA | 1900 | A |
| 25 | BA | 1906 | G |
| 25 | BA | 1914 | C |
| 25 | BA | 1916 | A |
| 25 | BA | 1926 | U |
| 25 | BA | 1929 | G |
| 25 | BA | 1930 | G |
| 25 | BA | 1931 | U |
| 25 | BA | 1936 | A |
| 25 | BA | 1937 | A |
| 25 | BA | 1938 | A |
| 25 | BA | 1955 | U |
| 25 | BA | 1956 | U |
| 25 | BA | 1963 | U |
| 25 | BA | 1967 | C |
| 25 | BA | 1969 | A |
| 25 | BA | 1970 | A |
| 25 | BA | 1971 | A |
| 25 | BA | 1972 | A |
| 25 | BA | 1982 | C |
| 25 | BA | 1984 | G |
| 25 | BA | 1993 | U |
| 25 | BA | 2020 | A |
| 25 | BA | 2023 | G |
| 25 | BA | 2031 | A |
| 25 | BA | 2032 | G |
| 25 | BA | 2033 | A |
| 25 | BA | 2043 | C |
| 25 | BA | 2051 | A |
| 25 | BA | 2055 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2056 | G |
| 25 | BA | 2060 | A |
| 25 | BA | 2061 | G |
| 25 | BA | 2062 | A |
| 25 | BA | 2069 | G |
| 25 | BA | 2096 | U |
| 25 | BA | 2099 | U |
| 25 | BA | 2100 | G |
| 25 | BA | 2111 | C |
| 25 | BA | 2112 | G |
| 25 | BA | 2113 | U |
| 25 | BA | 2114 | A |
| 25 | BA | 2115 | G |
| 25 | BA | 2116 | G |
| 25 | BA | 2118 | U |
| 25 | BA | 2120 | G |
| 25 | BA | 2122 | U |
| 25 | BA | 2126 | A |
| 25 | BA | 2127 | G |
| 25 | BA | 2128 | C |
| 25 | BA | 2129 | C |
| 25 | BA | 2131 | G |
| 25 | BA | 2132 | U |
| 25 | BA | 2133 | G |
| 25 | BA | 2135 | A |
| 25 | BA | 2136 | C |
| 25 | BA | 2139 | C |
| 25 | BA | 2144 | U |
| 25 | BA | 2146 | C |
| 25 | BA | 2148 | G |
| 25 | BA | 2151 | G |
| 25 | BA | 2157 | G |
| 25 | BA | 2158 | A |
| 25 | BA | 2159 | G |
| 25 | BA | 2165 | G |
| 25 | BA | 2166 | G |
| 25 | BA | 2168 | G |
| 25 | BA | 2169 | A |
| 25 | BA | 2170 | A |
| 25 | BA | 2171 | A |
| 25 | BA | 2173 | A |
| 25 | BA | 2176 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2181 | G |
| 25 | BA | 2185 | C |
| 25 | BA | 2189 | U |
| 25 | BA | 2190 | G |
| 25 | BA | 2191 | G |
| 25 | BA | 2192 | G |
| 25 | BA | 2198 | A |
| 25 | BA | 2205 | C |
| 25 | BA | 2210 | G |
| 25 | BA | 2211 | G |
| 25 | BA | 2212 | A |
| 25 | BA | 2213 | U |
| 25 | BA | 2215 | G |
| 25 | BA | 2225 | A |
| 25 | BA | 2226 | C |
| 25 | BA | 2238 | G |
| 25 | BA | 2239 | G |
| 25 | BA | 2262 | U |
| 25 | BA | 2263 | C |
| 25 | BA | 2264 | C |
| 25 | BA | 2269 | A |
| 25 | BA | 2275 | C |
| 25 | BA | 2283 | C |
| 25 | BA | 2287 | A |
| 25 | BA | 2304 | G |
| 25 | BA | 2307 | G |
| 25 | BA | 2308 | G |
| 25 | BA | 2309 | A |
| 25 | BA | 2310 | A |
| 25 | BA | 2311 | A |
| 25 | BA | 2319 | G |
| 25 | BA | 2320 | A |
| 25 | BA | 2321 | G |
| 25 | BA | 2325 | G |
| 25 | BA | 2327 | A |
| 25 | BA | 2334 | G |
| 25 | BA | 2336 | A |
| 25 | BA | 2342 | C |
| 25 | BA | 2343 | C |
| 25 | BA | 2346 | A |
| 25 | BA | 2347 | C |
| 25 | BA | 2350 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2352 | A |
| 25 | BA | 2360 | A |
| 25 | BA | 2377 | A |
| 25 | BA | 2379 | G |
| 25 | BA | 2383 | G |
| 25 | BA | 2385 | C |
| 25 | BA | 2394 | C |
| 25 | BA | 2402 | C |
| 25 | BA | 2403 | C |
| 25 | BA | 2406 | U |
| 25 | BA | 2408 | U |
| 25 | BA | 2410 | G |
| 25 | BA | 2423 | U |
| 25 | BA | 2425 | A |
| 25 | BA | 2428 | G |
| 25 | BA | 2429 | G |
| 25 | BA | 2430 | A |
| 25 | BA | 2434 | A |
| 25 | BA | 2435 | A |
| 25 | BA | 2439 | A |
| 25 | BA | 2440 | C |
| 25 | BA | 2441 | C |
| 25 | BA | 2448 | A |
| 25 | BA | 2468 | G |
| 25 | BA | 2474 | C |
| 25 | BA | 2476 | A |
| 25 | BA | 2478 | A |
| 25 | BA | 2487 | G |
| 25 | BA | 2498 | C |
| 25 | BA | 2502 | G |
| 25 | BA | 2504 | U |
| 25 | BA | 2505 | G |
| 25 | BA | 2506 | U |
| 25 | BA | 2518 | A |
| 25 | BA | 2525 | G |
| 25 | BA | 2529 | G |
| 25 | BA | 2554 | U |
| 25 | BA | 2566 | A |
| 25 | BA | 2567 | G |
| 25 | BA | 2573 | C |
| 25 | BA | 2582 | G |
| 25 | BA | 2584 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | BA | 2599 | G |
| 25 | BA | 2601 | C |
| 25 | BA | 2602 | A |
| 25 | BA | 2609 | U |
| 25 | BA | 2610 | C |
| 25 | BA | 2611 | U |
| 25 | BA | 2612 | C |
| 25 | BA | 2613 | U |
| 25 | BA | 2614 | A |
| 25 | BA | 2615 | U |
| 25 | BA | 2629 | A |
| 25 | BA | 2630 | G |
| 25 | BA | 2636 | U |
| 25 | BA | 2641 | G |
| 25 | BA | 2654 | A |
| 25 | BA | 2665 | A |
| 25 | BA | 2666 | C |
| 25 | BA | 2673 | G |
| 25 | BA | 2682 | U |
| 25 | BA | 2683 | C |
| 25 | BA | 2689 | U |
| 25 | BA | 2690 | C |
| 25 | BA | 2691 | C |
| 25 | BA | 2701 | C |
| 25 | BA | 2702 | U |
| 25 | BA | 2703 | C |
| 25 | BA | 2707 | G |
| 25 | BA | 2712 | U |
| 25 | BA | 2712(A) | A |
| 25 | BA | 2713 | A |
| 25 | BA | 2714 | G |
| 25 | BA | 2726 | U |
| 25 | BA | 2733 | A |
| 25 | BA | 2734 | A |
| 25 | BA | 2744 | G |
| 25 | BA | 2752 | C |
| 25 | BA | 2755 | C |
| 25 | BA | 2757 | A |
| 25 | BA | 2758 | A |
| 25 | BA | 2764 | A |
| 25 | BA | 2765 | A |
| 25 | BA | 2766 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2778 | A |
| 25 | BA | 2779 | U |
| 25 | BA | 2789 | C |
| 25 | BA | 2790 | A |
| 25 | BA | 2791 | C |
| 25 | BA | 2794 | C |
| 25 | BA | 2795 | G |
| 25 | BA | 2797 | U |
| 25 | BA | 2798 | C |
| 25 | BA | 2799 | A |
| 25 | BA | 2803 | C |
| 25 | BA | 2805 | G |
| 25 | BA | 2807 | G |
| 25 | BA | 2808 | U |
| 25 | BA | 2818 | G |
| 25 | BA | 2820 | A |
| 25 | BA | 2821 | A |
| 25 | BA | 2823 | A |
| 25 | BA | 2830 | G |
| 25 | BA | 2833 | G |
| 25 | BA | 2834 | G |
| 25 | BA | 2849 | U |
| 25 | BA | 2850 | A |
| 25 | BA | 2851 | A |
| 25 | BA | 2864 | G |
| 25 | BA | 2872 | G |
| 25 | BA | 2891 | G |
| 25 | BA | 2892 | A |
| 25 | BA | 2894 | G |
| 25 | BA | 2899 | G |
| 25 | BA | 2901 | C |
| 26 | BB | 1 | U |
| 26 | BB | 4 | C |
| 26 | BB | 7 | G |
| 26 | BB | 12 | C |
| 26 | BB | 13 | A |
| 26 | BB | 15 | A |
| 26 | BB | 21 | G |
| 26 | BB | 31 | C |
| 26 | BB | 32 | C |
| 26 | BB | 35 | U |
| 26 | BB | 38 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BB | 41 | U |
| 26 | BB | 42 | C |
| 26 | BB | 44 | G |
| 26 | BB | 45 | A |
| 26 | BB | 50 | G |
| 26 | BB | 52 | A |
| 26 | BB | 53 | A |
| 26 | BB | 56 | G |
| 26 | BB | 65 | C |
| 26 | BB | 72 | G |
| 26 | BB | 73 | A |
| 26 | BB | 74 | U |
| 26 | BB | 81 | G |
| 26 | BB | 82 | G |
| 26 | BB | 89 | G |
| 26 | BB | 95 | U |
| 26 | BB | 96 | G |
| 26 | BB | 105 | G |
| 26 | BB | 109 | G |
| 1 | CA | 7 | G |
| 1 | CA | 9 | G |
| 1 | CA | 22 | G |
| 1 | CA | 26 | A |
| 1 | CA | 31 | G |
| 1 | CA | 32 | A |
| 1 | CA | 39 | G |
| 1 | CA | 47 | C |
| 1 | CA | 48 | C |
| 1 | CA | 51 | A |
| 1 | CA | 54 | C |
| 1 | CA | 64 | G |
| 1 | CA | 65 | U |
| 1 | CA | 66 | G |
| 1 | CA | 73 | G |
| 1 | CA | 78 | G |
| 1 | CA | 79 | G |
| 1 | CA | 81 | G |
| 1 | CA | 84 | U |
| 1 | CA | 85 | U |
| 1 | CA | 86 | U |
| 1 | CA | 87 | A |
| 1 | CA | 90 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 91 | C |
| 1 | CA | 92 | G |
| 1 | CA | 95 | G |
| 1 | CA | 101 | A |
| 1 | CA | 116 | A |
| 1 | CA | 121 | C |
| 1 | CA | 131 | C |
| 1 | CA | 144 | G |
| 1 | CA | 161 | A |
| 1 | CA | 163 | C |
| 1 | CA | 169 | C |
| 1 | CA | 174 | C |
| 1 | CA | 182 | U |
| 1 | CA | 186 | C |
| 1 | CA | 187 | C |
| 1 | CA | 188 | U |
| 1 | CA | 189 | U |
| 1 | CA | 190 | G |
| 1 | CA | 191(A) | G |
| 1 | CA | 191(B) | G |
| 1 | CA | 191(D) | U |
| 1 | CA | 195 | A |
| 1 | CA | 197 | A |
| 1 | CA | 198 | G |
| 1 | CA | 208 | U |
| 1 | CA | 209 | U |
| 1 | CA | 210 | U |
| 1 | CA | 216 | G |
| 1 | CA | 226 | G |
| 1 | CA | 231 | G |
| 1 | CA | 240 | C |
| 1 | CA | 241 | C |
| 1 | CA | 243 | A |
| 1 | CA | 244 | U |
| 1 | CA | 245 | C |
| 1 | CA | 247 | G |
| 1 | CA | 250 | A |
| 1 | CA | 251 | G |
| 1 | CA | 253 | U |
| 1 | CA | 266 | G |
| 1 | CA | 267 | C |
| 1 | CA | 269 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 271 | C |
| 1 | CA | 274 | A |
| 1 | CA | 279 | A |
| 1 | CA | 280 | C |
| 1 | CA | 281 | G |
| 1 | CA | 289 | G |
| 1 | CA | 298 | A |
| 1 | CA | 321 | A |
| 1 | CA | 328 | C |
| 1 | CA | 329 | A |
| 1 | CA | 332 | G |
| 1 | CA | 340 | U |
| 1 | CA | 345 | C |
| 1 | CA | 346 | G |
| 1 | CA | 347 | G |
| 1 | CA | 350 | G |
| 1 | CA | 351 | G |
| 1 | CA | 352 | C |
| 1 | CA | 353 | A |
| 1 | CA | 354 | G |
| 1 | CA | 356 | A |
| 1 | CA | 367 | U |
| 1 | CA | 372 | C |
| 1 | CA | 397 | A |
| 1 | CA | 398 | C |
| 1 | CA | 406 | G |
| 1 | CA | 411 | A |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 414 | A |
| 1 | CA | 421 | U |
| 1 | CA | 422 | C |
| 1 | CA | 423 | G |
| 1 | CA | 429 | U |
| 1 | CA | 435 | C |
| 1 | CA | 439 | A |
| 1 | CA | 445 | G |
| 1 | CA | 451 | A |
| 1 | CA | 452 | A |
| 1 | CA | 465 | A |
| 1 | CA | 466 | C |
| 1 | CA | 467 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 476 | G |
| 1 | CA | 478 | A |
| 1 | CA | 482 | A |
| 1 | CA | 484 | G |
| 1 | CA | 485 | G |
| 1 | CA | 486 | U |
| 1 | CA | 496 | A |
| 1 | CA | 497 | U |
| 1 | CA | 498 | A |
| 1 | CA | 500 | G |
| 1 | CA | 504 | C |
| 1 | CA | 505 | G |
| 1 | CA | 506 | G |
| 1 | CA | 509 | A |
| 1 | CA | 510 | A |
| 1 | CA | 511 | C |
| 1 | CA | 513 | C |
| 1 | CA | 517 | G |
| 1 | CA | 518 | C |
| 1 | CA | 519 | C |
| 1 | CA | 521 | G |
| 1 | CA | 527 | G |
| 1 | CA | 530 | G |
| 1 | CA | 531 | U |
| 1 | CA | 532 | A |
| 1 | CA | 533 | A |
| 1 | CA | 535 | A |
| 1 | CA | 536 | C |
| 1 | CA | 544 | G |
| 1 | CA | 547 | A |
| 1 | CA | 553 | A |
| 1 | CA | 559 | A |
| 1 | CA | 561 | U |
| 1 | CA | 562 | C |
| 1 | CA | 564 | C |
| 1 | CA | 572 | A |
| 1 | CA | 573 | A |
| 1 | CA | 576 | G |
| 1 | CA | 601 | C |
| 1 | CA | 618 | C |
| 1 | CA | 620 | C |
| 1 | CA | 621 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 629 | G |
| 1 | CA | 630 | G |
| 1 | CA | 631 | G |
| 1 | CA | 632 | A |
| 1 | CA | 633 | G |
| 1 | CA | 634 | C |
| 1 | CA | 641 | U |
| 1 | CA | 651 | C |
| 1 | CA | 653 | A |
| 1 | CA | 656 | C |
| 1 | CA | 661 | G |
| 1 | CA | 665 | A |
| 1 | CA | 685 | G |
| 1 | CA | 686 | U |
| 1 | CA | 687 | A |
| 1 | CA | 688 | G |
| 1 | CA | 702 | A |
| 1 | CA | 703 | G |
| 1 | CA | 704 | A |
| 1 | CA | 707 | C |
| 1 | CA | 720 | C |
| 1 | CA | 721 | G |
| 1 | CA | 724 | G |
| 1 | CA | 731 | G |
| 1 | CA | 749 | C |
| 1 | CA | 755 | G |
| 1 | CA | 773 | G |
| 1 | CA | 777 | A |
| 1 | CA | 778 | G |
| 1 | CA | 792 | A |
| 1 | CA | 793 | U |
| 1 | CA | 794 | A |
| 1 | CA | 799 | G |
| 1 | CA | 800 | G |
| 1 | CA | 801 | U |
| 1 | CA | 802 | A |
| 1 | CA | 813 | U |
| 1 | CA | 816 | A |
| 1 | CA | 817 | C |
| 1 | CA | 819 | A |
| 1 | CA | 820 | U |
| 1 | CA | 821 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 827 | U |
| 1 | CA | 828 | A |
| 1 | CA | 836 | G |
| 1 | CA | 841 | U |
| 1 | CA | 842 | C |
| 1 | CA | 843 | U |
| 1 | CA | 848 | C |
| 1 | CA | 859 | A |
| 1 | CA | 870 | U |
| 1 | CA | 871 | U |
| 1 | CA | 885 | G |
| 1 | CA | 887 | G |
| 1 | CA | 889 | A |
| 1 | CA | 913 | A |
| 1 | CA | 914 | A |
| 1 | CA | 915 | A |
| 1 | CA | 926 | G |
| 1 | CA | 927 | G |
| 1 | CA | 934 | C |
| 1 | CA | 935 | A |
| 1 | CA | 936 | C |
| 1 | CA | 956 | U |
| 1 | CA | 958 | A |
| 1 | CA | 960 | U |
| 1 | CA | 961 | U |
| 1 | CA | 966 | G |
| 1 | CA | 968 | A |
| 1 | CA | 969 | A |
| 1 | CA | 971 | G |
| 1 | CA | 972 | C |
| 1 | CA | 974 | A |
| 1 | CA | 975 | A |
| 1 | CA | 976 | G |
| 1 | CA | 977 | A |
| 1 | CA | 978 | A |
| 1 | CA | 980 | C |
| 1 | CA | 981 | U |
| 1 | CA | 982 | U |
| 1 | CA | 988 | G |
| 1 | CA | 989 | C |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 993 | G |
| 1 | CA | 994 | A |
| 1 | CA | 995 | C |
| 1 | CA | 1004 | A |
| 1 | CA | 1005 | A |
| 1 | CA | 1006 | C |
| 1 | CA | 1009 | G |
| 1 | CA | 1013 | G |
| 1 | CA | 1014 | A |
| 1 | CA | 1016 | A |
| 1 | CA | 1022 | G |
| 1 | CA | 1024 | G |
| 1 | CA | 1025 | U |
| 1 | CA | 1027 | C |
| 1 | CA | 1028 | C |
| 1 | CA | 1028(B) | C |
| 1 | CA | 1029 | G |
| 1 | CA | 1030 | C |
| 1 | CA | 1032(A) | G |
| 1 | CA | 1032(B) | G |
| 1 | CA | 1036 | G |
| 1 | CA | 1039 | C |
| 1 | CA | 1040 | U |
| 1 | CA | 1042 | G |
| 1 | CA | 1045 | C |
| 1 | CA | 1046 | A |
| 1 | CA | 1052 | U |
| 1 | CA | 1053 | G |
| 1 | CA | 1054 | C |
| 1 | CA | 1055 | A |
| 1 | CA | 1066 | C |
| 1 | CA | 1067 | A |
| 1 | CA | 1068 | G |
| 1 | CA | 1081 | G |
| 1 | CA | 1084 | G |
| 1 | CA | 1086 | U |
| 1 | CA | 1092 | A |
| 1 | CA | 1094 | G |
| 1 | CA | 1095 | U |
| 1 | CA | 1101 | A |
| 1 | CA | 1106 | G |
| 1 | CA | 1113 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1118 | C |
| 1 | CA | 1122 | U |
| 1 | CA | 1123 | A |
| 1 | CA | 1124 | G |
| 1 | CA | 1125 | U |
| 1 | CA | 1126 | U |
| 1 | CA | 1127 | G |
| 1 | CA | 1128 | C |
| 1 | CA | 1129 | C |
| 1 | CA | 1130 | A |
| 1 | CA | 1131 | G |
| 1 | CA | 1133 | G |
| 1 | CA | 1136 | U |
| 1 | CA | 1137 | C |
| 1 | CA | 1139 | G |
| 1 | CA | 1146 | A |
| 1 | CA | 1147 | C |
| 1 | CA | 1152 | A |
| 1 | CA | 1154 | G |
| 1 | CA | 1157 | A |
| 1 | CA | 1158 | C |
| 1 | CA | 1159 | U |
| 1 | CA | 1160 | G |
| 1 | CA | 1171 | G |
| 1 | CA | 1178 | G |
| 1 | CA | 1179 | A |
| 1 | CA | 1180 | A |
| 1 | CA | 1181 | G |
| 1 | CA | 1182 | G |
| 1 | CA | 1183 | A |
| 1 | CA | 1184 | G |
| 1 | CA | 1185 | G |
| 1 | CA | 1187 | G |
| 1 | CA | 1196 | U |
| 1 | CA | 1201 | A |
| 1 | CA | 1202 | G |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1220 | G |
| 1 | CA | 1223 | C |
| 1 | CA | 1225 | A |
| 1 | CA | 1226 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1227 | A |
| 1 | CA | 1228 | C |
| 1 | CA | 1232 | U |
| 1 | CA | 1235 | U |
| 1 | CA | 1238 | A |
| 1 | CA | 1240 | U |
| 1 | CA | 1241 | G |
| 1 | CA | 1252 | A |
| 1 | CA | 1256 | A |
| 1 | CA | 1257 | U |
| 1 | CA | 1258 | G |
| 1 | CA | 1260 | C |
| 1 | CA | 1262 | C |
| 1 | CA | 1269 | A |
| 1 | CA | 1270 | C |
| 1 | CA | 1275 | A |
| 1 | CA | 1278 | U |
| 1 | CA | 1280 | A |
| 1 | CA | 1286 | A |
| 1 | CA | 1287 | A |
| 1 | CA | 1288 | A |
| 1 | CA | 1290 | G |
| 1 | CA | 1291 | G |
| 1 | CA | 1297 | C |
| 1 | CA | 1298 | C |
| 1 | CA | 1299 | A |
| 1 | CA | 1300 | G |
| 1 | CA | 1301 | U |
| 1 | CA | 1303 | C |
| 1 | CA | 1305 | G |
| 1 | CA | 1317 | C |
| 1 | CA | 1319 | A |
| 1 | CA | 1320 | C |
| 1 | CA | 1322 | C |
| 1 | CA | 1323 | G |
| 1 | CA | 1326 | C |
| 1 | CA | 1331 | G |
| 1 | CA | 1338 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1347 | G |
| 1 | CA | 1349 | A |
| 1 | CA | 1350 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1352 | C |
| 1 | CA | 1353 | G |
| 1 | CA | 1362(A) | C |
| 1 | CA | 1364 | U |
| 1 | CA | 1368 | G |
| 1 | CA | 1370 | G |
| 1 | CA | 1379 | G |
| 1 | CA | 1382 | C |
| 1 | CA | 1391 | U |
| 1 | CA | 1392 | G |
| 1 | CA | 1397 | C |
| 1 | CA | 1398 | A |
| 1 | CA | 1400 | C |
| 1 | CA | 1401 | G |
| 1 | CA | 1402 | C |
| 1 | CA | 1403 | C |
| 1 | CA | 1404 | C |
| 1 | CA | 1406 | U |
| 1 | CA | 1416 | G |
| 1 | CA | 1417 | G |
| 1 | CA | 1419 | G |
| 1 | CA | 1439 | C |
| 1 | CA | 1442 | G |
| 1 | CA | 1443 | G |
| 1 | CA | 1446 | A |
| 1 | CA | 1447 | G |
| 1 | CA | 1450 | U |
| 1 | CA | 1451 | A |
| 1 | CA | 1453 | G |
| 1 | CA | 1454 | G |
| 1 | CA | 1478 | C |
| 1 | CA | 1479 | C |
| 1 | CA | 1487 | G |
| 1 | CA | 1492 | A |
| 1 | CA | 1494 | G |
| 1 | CA | 1497 | G |
| 1 | CA | 1499 | A |
| 1 | CA | 1502 | A |
| 1 | CA | 1503 | A |
| 1 | CA | 1504 | G |
| 1 | CA | 1505 | G |
| 1 | CA | 1506 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1507 | A |
| 1 | CA | 1517 | G |
| 1 | CA | 1519 | A |
| 1 | CA | 1520 | G |
| 1 | CA | 1528 | U |
| 1 | CA | 1529 | G |
| 1 | CA | 1530 | G |
| 1 | CA | 1531 | A |
| 22 | CB | 2 | C |
| 22 | CB | 6 | G |
| 22 | CB | 7 | G |
| 22 | CB | 8 | U |
| 22 | CB | 9 | G |
| 22 | CB | 10 | G |
| 22 | CB | 11 | U |
| 22 | CB | 14 | A |
| 22 | CB | 17 | U |
| 22 | CB | 18 | G |
| 22 | CB | 19 | G |
| 22 | CB | 20 | U |
| 22 | CB | 21 | A |
| 22 | CB | 22 | G |
| 22 | CB | 23 | A |
| 22 | CB | 24 | C |
| 22 | CB | 25 | A |
| 22 | CB | 26 | C |
| 22 | CB | 27 | G |
| 22 | CB | 34 | U |
| 22 | CB | 37 | G |
| 22 | CB | 39 | U |
| 22 | CB | 41 | G |
| 22 | CB | 42 | U |
| 22 | CB | 43 | A |
| 22 | CB | 45 | U |
| 22 | CB | 46 | G |
| 22 | CB | 47 | C |
| 22 | CB | 48 | C |
| 22 | CB | 49 | C |
| 22 | CB | 50 | A |
| 22 | CB | 51 | A |
| 22 | CB | 52 | U |
| 22 | CB | 55 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | CB | 56 | G |
| 22 | CB | 60 | A |
| 22 | CB | 66 | U |
| 22 | CB | 67 | C |
| 22 | CB | 70 | G |
| 22 | CB | 71 | U |
| 22 | CB | 72 | C |
| 22 | CB | 74 | C |
| 22 | CB | 83 | U |
| 22 | CB | 85 | C |
| 22 | CB | 86 | C |
| 22 | CB | 87 | A |
| 23 | CC | 2 | G |
| 23 | CC | 8 | U |
| 23 | CC | 9 | G |
| 23 | CC | 16 | C |
| 23 | CC | 17 | C |
| 23 | CC | 18 | C |
| 23 | CC | 19 | G |
| 23 | CC | 20 | G |
| 23 | CC | 21 | U |
| 23 | CC | 22 | A |
| 23 | CC | 23 | G |
| 23 | CC | 31 | G |
| 23 | CC | 43 | G |
| 23 | CC | 48 | U |
| 23 | CC | 49 | C |
| 23 | CC | 50 | G |
| 23 | CC | 53 | G |
| 23 | CC | 61 | U |
| 23 | CC | 68 | C |
| 23 | CC | 69 | C |
| 23 | CC | 77 | A |
| 23 | CD | 9 | G |
| 23 | CD | 14 | A |
| 23 | CD | 15 | G |
| 23 | CD | 16 | C |
| 23 | CD | 17 | C |
| 23 | CD | 19 | G |
| 23 | CD | 21 | U |
| 23 | CD | 23 | G |
| 23 | CD | 24 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | CD | 25 | U |
| 23 | CD | 28 | U |
| 23 | CD | 36 | A |
| 23 | CD | 39 | A |
| 23 | CD | 40 | C |
| 23 | CD | 46 | G |
| 23 | CD | 48 | U |
| 23 | CD | 49 | C |
| 23 | CD | 54 | G |
| 23 | CD | 57 | C |
| 23 | CD | 59 | A |
| 23 | CD | 60 | A |
| 23 | CD | 62 | C |
| 23 | CD | 68 | C |
| 23 | CD | 70 | C |
| 23 | CD | 74 | A |
| 23 | CD | 77 | A |
| 24 | C1 | 14 | U |
| 24 | C1 | 19 | U |
| 24 | C1 | 22 | U |
| 25 | DA | 5 | A |
| 25 | DA | 34 | C |
| 25 | DA | 36 | G |
| 25 | DA | 46 | C |
| 25 | DA | 49 | A |
| 25 | DA | 50 | U |
| 25 | DA | 55 | G |
| 25 | DA | 58 | G |
| 25 | DA | 60 | G |
| 25 | DA | 69 | C |
| 25 | DA | 71 | A |
| 25 | DA | 72 | U |
| 25 | DA | 74 | A |
| 25 | DA | 75 | G |
| 25 | DA | 90 | U |
| 25 | DA | 91 | A |
| 25 | DA | 94 | G |
| 25 | DA | 95 | G |
| 25 | DA | 101 | G |
| 25 | DA | 102 | G |
| 25 | DA | 118 | A |
| 25 | DA | 119 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | DA | 120 | U |
| 25 | DA | 125 | G |
| 25 | DA | 129 | C |
| 25 | DA | 138 | G |
| 25 | DA | 148 | C |
| 25 | DA | 153 | C |
| 25 | DA | 154 | G |
| 25 | DA | 155 | C |
| 25 | DA | 172 | C |
| 25 | DA | 173 | G |
| 25 | DA | 174 | C |
| 25 | DA | 175 | G |
| 25 | DA | 182 | A |
| 25 | DA | 196 | A |
| 25 | DA | 199 | A |
| 25 | DA | 205 | G |
| 25 | DA | 206 | U |
| 25 | DA | 214 | G |
| 25 | DA | 215 | G |
| 25 | DA | 216 | A |
| 25 | DA | 217 | G |
| 25 | DA | 221 | A |
| 25 | DA | 222 | A |
| 25 | DA | 225 | A |
| 25 | DA | 228 | A |
| 25 | DA | 229 | A |
| 25 | DA | 233 | A |
| 25 | DA | 239 | U |
| 25 | DA | 245 | G |
| 25 | DA | 248 | G |
| 25 | DA | 249 | C |
| 25 | DA | 250 | G |
| 25 | DA | 252 | G |
| 25 | DA | 270(K) | C |
| 25 | DA | 270(L) | U |
| 25 | DA | 270(M) | U |
| 25 | DA | 270(O) | U |
| 25 | DA | 270(Q) | C |
| 25 | DA | 271(C) | U |
| 25 | DA | 271 | G |
| 25 | DA | 273(C) | C |
| 25 | DA | 273(D) | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | DA | 274 | G |
| 25 | DA | 275 | G |
| 25 | DA | 276 | A |
| 25 | DA | 278 | A |
| 25 | DA | 279 | C |
| 25 | DA | 285 | C |
| 25 | DA | 287 | C |
| 25 | DA | 289 | A |
| 25 | DA | 298 | G |
| 25 | DA | 308 | G |
| 25 | DA | 311 | A |
| 25 | DA | 312 | G |
| 25 | DA | 317 | G |
| 25 | DA | 324 | A |
| 25 | DA | 329 | G |
| 25 | DA | 330 | A |
| 25 | DA | 331 | A |
| 25 | DA | 333 | G |
| 25 | DA | 334 | C |
| 25 | DA | 342 | G |
| 25 | DA | 352 | G |
| 25 | DA | 354 | G |
| 25 | DA | 356 | G |
| 25 | DA | 363 | G |
| 25 | DA | 363(B) | G |
| 25 | DA | 363(E) | U |
| 25 | DA | 363(F) | A |
| 25 | DA | 386 | G |
| 25 | DA | 394 | A |
| 25 | DA | 395 | U |
| 25 | DA | 396 | G |
| 25 | DA | 399 | G |
| 25 | DA | 405 | U |
| 25 | DA | 406 | G |
| 25 | DA | 411 | G |
| 25 | DA | 412 | A |
| 25 | DA | 414 | C |
| 25 | DA | 419 | C |
| 25 | DA | 428 | A |
| 25 | DA | 443 | A |
| 25 | DA | 444 | C |
| 25 | DA | 448 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | DA | 454 | A |
| 25 | DA | 455 | C |
| 25 | DA | 457 | A |
| 25 | DA | 459 | U |
| 25 | DA | 470 | A |
| 25 | DA | 481 | G |
| 25 | DA | 485 | C |
| 25 | DA | 501 | A |
| 25 | DA | 504 | U |
| 25 | DA | 505 | A |
| 25 | DA | 508 | G |
| 25 | DA | 509 | C |
| 25 | DA | 512 | G |
| 25 | DA | 529 | A |
| 25 | DA | 530 | G |
| 25 | DA | 531 | C |
| 25 | DA | 532 | A |
| 25 | DA | 533 | G |
| 25 | DA | 543 | C |
| 25 | DA | 547 | A |
| 25 | DA | 556 | G |
| 25 | DA | 557 | U |
| 25 | DA | 563 | G |
| 25 | DA | 567 | A |
| 25 | DA | 568 | U |
| 25 | DA | 573 | G |
| 25 | DA | 575 | A |
| 25 | DA | 584 | C |
| 25 | DA | 588 | U |
| 25 | DA | 593 | G |
| 25 | DA | 595 | C |
| 25 | DA | 603 | A |
| 25 | DA | 607 | U |
| 25 | DA | 609(A) | G |
| 25 | DA | 614 | U |
| 25 | DA | 617 | G |
| 25 | DA | 620 | G |
| 25 | DA | 621 | A |
| 25 | DA | 622 | G |
| 25 | DA | 627 | A |
| 25 | DA | 637 | A |
| 25 | DA | 644 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | DA | 645 | C |
| 25 | DA | 646 | A |
| 25 | DA | 647 | G |
| 25 | DA | 650 | C |
| 25 | DA | 651 | G |
| 25 | DA | 654 | A |
| 25 | DA | 654(A) | A |
| 25 | DA | 654(F) | C |
| 25 | DA | 654(G) | C |
| 25 | DA | 654(I) | C |
| 25 | DA | 654(J) | A |
| 25 | DA | 654(K) | C |
| 25 | DA | 654(L) | G |
| 25 | DA | 654(N) | G |
| 25 | DA | 654(Q) | C |
| 25 | DA | 654(R) | C |
| 25 | DA | 654(T) | A |
| 25 | DA | 669 | G |
| 25 | DA | 670 | A |
| 25 | DA | 673 | C |
| 25 | DA | 686 | G |
| 25 | DA | 706 | A |
| 25 | DA | 707 | G |
| 25 | DA | 708 | C |
| 25 | DA | 717 | G |
| 25 | DA | 719 | C |
| 25 | DA | 720 | C |
| 25 | DA | 722 | A |
| 25 | DA | 730 | C |
| 25 | DA | 745 | G |
| 25 | DA | 752 | A |
| 25 | DA | 753 | C |
| 25 | DA | 757 | U |
| 25 | DA | 762 | U |
| 25 | DA | 765 | G |
| 25 | DA | 768 | G |
| 25 | DA | 776 | G |
| 25 | DA | 778 | G |
| 25 | DA | 779 | U |
| 25 | DA | 782 | A |
| 25 | DA | 784 | A |
| 25 | DA | 785 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DA | 789 | A |
| 25 | DA | 792 | G |
| 25 | DA | 793 | A |
| 25 | DA | 805 | G |
| 25 | DA | 812 | C |
| 25 | DA | 814 | C |
| 25 | DA | 819 | A |
| 25 | DA | 827 | U |
| 25 | DA | 828 | U |
| 25 | DA | 832 | G |
| 25 | DA | 845 | G |
| 25 | DA | 848 | G |
| 25 | DA | 856 | C |
| 25 | DA | 857 | C |
| 25 | DA | 859 | G |
| 25 | DA | 869 | G |
| 25 | DA | 878 | A |
| 25 | DA | 879 | G |
| 25 | DA | 881 | G |
| 25 | DA | 882 | G |
| 25 | DA | 884 | C |
| 25 | DA | 886 | C |
| 25 | DA | 887 | A |
| 25 | DA | 888 | C |
| 25 | DA | 889 | C |
| 25 | DA | 890 | A |
| 25 | DA | 894 | C |
| 25 | DA | 896 | A |
| 25 | DA | 897 | C |
| 25 | DA | 899 | A |
| 25 | DA | 900 | A |
| 25 | DA | 901 | A |
| 25 | DA | 903 | C |
| 25 | DA | 905 | U |
| 25 | DA | 906 | G |
| 25 | DA | 907 | U |
| 25 | DA | 910 | A |
| 25 | DA | 914 | C |
| 25 | DA | 915 | C |
| 25 | DA | 917 | A |
| 25 | DA | 925 | C |
| 25 | DA | 932 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 933 | A |
| 25 | DA | 934 | G |
| 25 | DA | 938 | G |
| 25 | DA | 941 | A |
| 25 | DA | 944 | G |
| 25 | DA | 945 | A |
| 25 | DA | 946 | G |
| 25 | DA | 959 | A |
| 25 | DA | 960 | A |
| 25 | DA | 961 | C |
| 25 | DA | 974 | G |
| 25 | DA | 983 | A |
| 25 | DA | 989 | G |
| 25 | DA | 990 | A |
| 25 | DA | 991 | C |
| 25 | DA | 996 | A |
| 25 | DA | 997 | G |
| 25 | DA | 998 | C |
| 25 | DA | 1005 | C |
| 25 | DA | 1012 | U |
| 25 | DA | 1013 | C |
| 25 | DA | 1016 | G |
| 25 | DA | 1020 | A |
| 25 | DA | 1022 | G |
| 25 | DA | 1023 | U |
| 25 | DA | 1024 | G |
| 25 | DA | 1025 | G |
| 25 | DA | 1026 | U |
| 25 | DA | 1033 | U |
| 25 | DA | 1037 | G |
| 25 | DA | 1044 | G |
| 25 | DA | 1045 | A |
| 25 | DA | 1048 | A |
| 25 | DA | 1054 | A |
| 25 | DA | 1057 | A |
| 25 | DA | 1060 | U |
| 25 | DA | 1061 | U |
| 25 | DA | 1062 | G |
| 25 | DA | 1065 | U |
| 25 | DA | 1066 | U |
| 25 | DA | 1067 | A |
| 25 | DA | 1070 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | DA | 1071 | G |
| 25 | DA | 1072 | C |
| 25 | DA | 1073 | A |
| 25 | DA | 1074 | G |
| 25 | DA | 1076 | C |
| 25 | DA | 1085 | A |
| 25 | DA | 1086 | A |
| 25 | DA | 1087 | G |
| 25 | DA | 1088 | A |
| 25 | DA | 1090 | U |
| 25 | DA | 1093 | G |
| 25 | DA | 1095 | A |
| 25 | DA | 1096 | A |
| 25 | DA | 1098 | A |
| 25 | DA | 1099 | G |
| 25 | DA | 1100 | C |
| 25 | DA | 1105 | U |
| 25 | DA | 1108 | U |
| 25 | DA | 1111 | A |
| 25 | DA | 1112 | G |
| 25 | DA | 1115 | G |
| 25 | DA | 1122 | G |
| 25 | DA | 1127 | A |
| 25 | DA | 1128 | A |
| 25 | DA | 1129 | A |
| 25 | DA | 1130 | U |
| 25 | DA | 1135 | C |
| 25 | DA | 1136 | G |
| 25 | DA | 1137 | G |
| 25 | DA | 1139 | G |
| 25 | DA | 1141 | U |
| 25 | DA | 1142(A) | A |
| 25 | DA | 1143 | A |
| 25 | DA | 1154 | G |
| 25 | DA | 1155 | A |
| 25 | DA | 1160 | G |
| 25 | DA | 1170 | G |
| 25 | DA | 1171 | G |
| 25 | DA | 1173 | G |
| 25 | DA | 1174 | A |
| 25 | DA | 1175 | U |
| 25 | DA | 1176 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 1177 | A |
| 25 | DA | 1178 | C |
| 25 | DA | 1183 | G |
| 25 | DA | 1190 | G |
| 25 | DA | 1204 | A |
| 25 | DA | 1205 | U |
| 25 | DA | 1210 | A |
| 25 | DA | 1211 | U |
| 25 | DA | 1212 | G |
| 25 | DA | 1217 | C |
| 25 | DA | 1220 | A |
| 25 | DA | 1221 | C |
| 25 | DA | 1237 | A |
| 25 | DA | 1245 | G |
| 25 | DA | 1247 | A |
| 25 | DA | 1250 | G |
| 25 | DA | 1253 | A |
| 25 | DA | 1255 | U |
| 25 | DA | 1256 | G |
| 25 | DA | 1269 | A |
| 25 | DA | 1271 | G |
| 25 | DA | 1272 | A |
| 25 | DA | 1273 | U |
| 25 | DA | 1275 | A |
| 25 | DA | 1284 | A |
| 25 | DA | 1287 | A |
| 25 | DA | 1298 | C |
| 25 | DA | 1300 | U |
| 25 | DA | 1301 | A |
| 25 | DA | 1304 | C |
| 25 | DA | 1313 | U |
| 25 | DA | 1314 | C |
| 25 | DA | 1319 | G |
| 25 | DA | 1325 | G |
| 25 | DA | 1329 | U |
| 25 | DA | 1332 | G |
| 25 | DA | 1342 | A |
| 25 | DA | 1347 | G |
| 25 | DA | 1348 | G |
| 25 | DA | 1352 | U |
| 25 | DA | 1359 | A |
| 25 | DA | 1360 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | DA | 1365 | A |
| 25 | DA | 1368 | G |
| 25 | DA | 1379 | A |
| 25 | DA | 1384 | A |
| 25 | DA | 1385 | G |
| 25 | DA | 1386 | C |
| 25 | DA | 1389 | G |
| 25 | DA | 1390 | U |
| 25 | DA | 1391 | U |
| 25 | DA | 1395 | A |
| 25 | DA | 1397 | U |
| 25 | DA | 1405 | U |
| 25 | DA | 1406 | U |
| 25 | DA | 1407 | C |
| 25 | DA | 1416 | G |
| 25 | DA | 1417 | C |
| 25 | DA | 1419 | A |
| 25 | DA | 1420 | U |
| 25 | DA | 1421 | G |
| 25 | DA | 1427 | A |
| 25 | DA | 1428 | C |
| 25 | DA | 1437 | C |
| 25 | DA | 1443 | G |
| 25 | DA | 1444(A) | A |
| 25 | DA | 1445 | C |
| 25 | DA | 1449 | A |
| 25 | DA | 1449(A) | G |
| 25 | DA | 1451 | C |
| 25 | DA | 1460 | A |
| 25 | DA | 1461 | G |
| 25 | DA | 1467 | C |
| 25 | DA | 1471 | A |
| 25 | DA | 1472 | A |
| 25 | DA | 1475 | G |
| 25 | DA | 1482 | U |
| 25 | DA | 1483 | G |
| 25 | DA | 1486 | A |
| 25 | DA | 1488 | G |
| 25 | DA | 1490 | A |
| 25 | DA | 1493 | C |
| 25 | DA | 1506 | C |
| 25 | DA | 1507 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 1508 | A |
| 25 | DA | 1509 | C |
| 25 | DA | 1510 | A |
| 25 | DA | 1515 | C |
| 25 | DA | 1522 | G |
| 25 | DA | 1527 | G |
| 25 | DA | 1528 | A |
| 25 | DA | 1534 | G |
| 25 | DA | 1535 | U |
| 25 | DA | 1536 | A |
| 25 | DA | 1537 | C |
| 25 | DA | 1538 | G |
| 25 | DA | 1541 | U |
| 25 | DA | 1543 | A |
| 25 | DA | 1544 | C |
| 25 | DA | 1546 | C |
| 25 | DA | 1547 | C |
| 25 | DA | 1548 | C |
| 25 | DA | 1554 | A |
| 25 | DA | 1558 | A |
| 25 | DA | 1559 | G |
| 25 | DA | 1560 | G |
| 25 | DA | 1566 | A |
| 25 | DA | 1569 | A |
| 25 | DA | 1578 | U |
| 25 | DA | 1580 | A |
| 25 | DA | 1582 | C |
| 25 | DA | 1586 | A |
| 25 | DA | 1587 | A |
| 25 | DA | 1588 | C |
| 25 | DA | 1589 | C |
| 25 | DA | 1596 | A |
| 25 | DA | 1597 | A |
| 25 | DA | 1598 | C |
| 25 | DA | 1608 | A |
| 25 | DA | 1609 | A |
| 25 | DA | 1610 | A |
| 25 | DA | 1616 | A |
| 25 | DA | 1619 | G |
| 25 | DA | 1625 | C |
| 25 | DA | 1639 | U |
| 25 | DA | 1640 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 1648 | C |
| 25 | DA | 1654 | A |
| 25 | DA | 1655 | A |
| 25 | DA | 1660 | C |
| 25 | DA | 1661 | G |
| 25 | DA | 1674 | G |
| 25 | DA | 1675 | C |
| 25 | DA | 1678 | G |
| 25 | DA | 1688 | U |
| 25 | DA | 1696 | G |
| 25 | DA | 1700 | A |
| 25 | DA | 1701 | A |
| 25 | DA | 1718 | G |
| 25 | DA | 1725 | G |
| 25 | DA | 1726 | G |
| 25 | DA | 1728 | G |
| 25 | DA | 1729 | A |
| 25 | DA | 1741 | C |
| 25 | DA | 1743 | G |
| 25 | DA | 1756 | G |
| 25 | DA | 1758 | G |
| 25 | DA | 1762 | A |
| 25 | DA | 1763 | G |
| 25 | DA | 1764 | G |
| 25 | DA | 1773 | A |
| 25 | DA | 1780 | A |
| 25 | DA | 1782 | C |
| 25 | DA | 1791 | A |
| 25 | DA | 1800 | C |
| 25 | DA | 1801 | G |
| 25 | DA | 1802 | A |
| 25 | DA | 1812 | A |
| 25 | DA | 1816 | G |
| 25 | DA | 1819 | A |
| 25 | DA | 1820 | U |
| 25 | DA | 1827 | C |
| 25 | DA | 1828 | G |
| 25 | DA | 1829 | A |
| 25 | DA | 1835 | G |
| 25 | DA | 1839 | G |
| 25 | DA | 1847 | A |
| 25 | DA | 1857 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 1858 | G |
| 25 | DA | 1861 | G |
| 25 | DA | 1863 | G |
| 25 | DA | 1864 | U |
| 25 | DA | 1869 | G |
| 25 | DA | 1878 | G |
| 25 | DA | 1882 | C |
| 25 | DA | 1883 | G |
| 25 | DA | 1888 | G |
| 25 | DA | 1889 | A |
| 25 | DA | 1896 | G |
| 25 | DA | 1900 | A |
| 25 | DA | 1906 | G |
| 25 | DA | 1909 | C |
| 25 | DA | 1913 | A |
| 25 | DA | 1916 | A |
| 25 | DA | 1917 | U |
| 25 | DA | 1919 | A |
| 25 | DA | 1929 | G |
| 25 | DA | 1930 | G |
| 25 | DA | 1936 | A |
| 25 | DA | 1937 | A |
| 25 | DA | 1938 | A |
| 25 | DA | 1940 | U |
| 25 | DA | 1955 | U |
| 25 | DA | 1956 | U |
| 25 | DA | 1963 | U |
| 25 | DA | 1967 | C |
| 25 | DA | 1968 | G |
| 25 | DA | 1970 | A |
| 25 | DA | 1971 | A |
| 25 | DA | 1972 | A |
| 25 | DA | 1981 | A |
| 25 | DA | 1991 | U |
| 25 | DA | 1993 | U |
| 25 | DA | 1994 | C |
| 25 | DA | 2023 | G |
| 25 | DA | 2031 | A |
| 25 | DA | 2032 | G |
| 25 | DA | 2033 | A |
| 25 | DA | 2036 | C |
| 25 | DA | 2039 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 2043 | C |
| 25 | DA | 2049 | G |
| 25 | DA | 2055 | C |
| 25 | DA | 2056 | G |
| 25 | DA | 2059 | A |
| 25 | DA | 2060 | A |
| 25 | DA | 2061 | G |
| 25 | DA | 2062 | A |
| 25 | DA | 2063 | C |
| 25 | DA | 2066 | C |
| 25 | DA | 2067 | G |
| 25 | DA | 2069 | G |
| 25 | DA | 2071 | A |
| 25 | DA | 2082 | A |
| 25 | DA | 2097 | C |
| 25 | DA | 2099 | U |
| 25 | DA | 2100 | G |
| 25 | DA | 2105 | C |
| 25 | DA | 2107 | C |
| 25 | DA | 2108 | C |
| 25 | DA | 2111 | C |
| 25 | DA | 2112 | G |
| 25 | DA | 2113 | U |
| 25 | DA | 2114 | A |
| 25 | DA | 2115 | G |
| 25 | DA | 2116 | G |
| 25 | DA | 2118 | U |
| 25 | DA | 2119 | A |
| 25 | DA | 2120 | G |
| 25 | DA | 2123 | G |
| 25 | DA | 2126 | A |
| 25 | DA | 2127 | G |
| 25 | DA | 2128 | C |
| 25 | DA | 2129 | C |
| 25 | DA | 2130 | U |
| 25 | DA | 2131 | G |
| 25 | DA | 2132 | U |
| 25 | DA | 2133 | G |
| 25 | DA | 2135 | A |
| 25 | DA | 2136 | C |
| 25 | DA | 2137 | C |
| 25 | DA | 2139 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DA | 2141 | G |
| 25 | DA | 2145 | C |
| 25 | DA | 2146 | C |
| 25 | DA | 2147 | G |
| 25 | DA | 2148 | G |
| 25 | DA | 2152 | G |
| 25 | DA | 2158 | A |
| 25 | DA | 2164 | C |
| 25 | DA | 2166 | G |
| 25 | DA | 2168 | G |
| 25 | DA | 2169 | A |
| 25 | DA | 2170 | A |
| 25 | DA | 2171 | A |
| 25 | DA | 2172 | U |
| 25 | DA | 2173 | A |
| 25 | DA | 2174 | C |
| 25 | DA | 2175 | C |
| 25 | DA | 2182 | G |
| 25 | DA | 2189 | U |
| 25 | DA | 2190 | G |
| 25 | DA | 2192 | G |
| 25 | DA | 2193 | G |
| 25 | DA | 2198 | A |
| 25 | DA | 2210 | G |
| 25 | DA | 2211 | G |
| 25 | DA | 2212 | A |
| 25 | DA | 2213 | U |
| 25 | DA | 2215 | G |
| 25 | DA | 2225 | A |
| 25 | DA | 2226 | C |
| 25 | DA | 2238 | G |
| 25 | DA | 2239 | G |
| 25 | DA | 2240 | C |
| 25 | DA | 2245 | U |
| 25 | DA | 2246 | G |
| 25 | DA | 2262 | U |
| 25 | DA | 2267 | A |
| 25 | DA | 2272 | U |
| 25 | DA | 2273 | A |
| 25 | DA | 2275 | C |
| 25 | DA | 2276 | G |
| 25 | DA | 2279 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 2280 | G |
| 25 | DA | 2282 | G |
| 25 | DA | 2283 | C |
| 25 | DA | 2285 | C |
| 25 | DA | 2286 | A |
| 25 | DA | 2287 | A |
| 25 | DA | 2297 | C |
| 25 | DA | 2298 | A |
| 25 | DA | 2304 | G |
| 25 | DA | 2307 | G |
| 25 | DA | 2308 | G |
| 25 | DA | 2309 | A |
| 25 | DA | 2311 | A |
| 25 | DA | 2312 | U |
| 25 | DA | 2315 | G |
| 25 | DA | 2316 | C |
| 25 | DA | 2319 | G |
| 25 | DA | 2322 | A |
| 25 | DA | 2324 | C |
| 25 | DA | 2325 | G |
| 25 | DA | 2333 | A |
| 25 | DA | 2335 | A |
| 25 | DA | 2337 | G |
| 25 | DA | 2342 | C |
| 25 | DA | 2343 | C |
| 25 | DA | 2346 | A |
| 25 | DA | 2347 | C |
| 25 | DA | 2350 | C |
| 25 | DA | 2383 | G |
| 25 | DA | 2385 | C |
| 25 | DA | 2388 | A |
| 25 | DA | 2391 | G |
| 25 | DA | 2392 | A |
| 25 | DA | 2394 | C |
| 25 | DA | 2400 | G |
| 25 | DA | 2402 | C |
| 25 | DA | 2406 | U |
| 25 | DA | 2410 | G |
| 25 | DA | 2414 | G |
| 25 | DA | 2422 | A |
| 25 | DA | 2423 | U |
| 25 | DA | 2425 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 2429 | G |
| 25 | DA | 2430 | A |
| 25 | DA | 2431 | U |
| 25 | DA | 2434 | A |
| 25 | DA | 2435 | A |
| 25 | DA | 2439 | A |
| 25 | DA | 2440 | C |
| 25 | DA | 2441 | C |
| 25 | DA | 2445 | G |
| 25 | DA | 2447 | G |
| 25 | DA | 2448 | A |
| 25 | DA | 2466 | C |
| 25 | DA | 2469 | A |
| 25 | DA | 2470 | G |
| 25 | DA | 2471 | C |
| 25 | DA | 2472 | G |
| 25 | DA | 2476 | A |
| 25 | DA | 2484 | G |
| 25 | DA | 2487 | G |
| 25 | DA | 2502 | G |
| 25 | DA | 2504 | U |
| 25 | DA | 2505 | G |
| 25 | DA | 2506 | U |
| 25 | DA | 2507 | C |
| 25 | DA | 2518 | A |
| 25 | DA | 2523 | G |
| 25 | DA | 2525 | G |
| 25 | DA | 2529 | G |
| 25 | DA | 2532 | G |
| 25 | DA | 2543 | G |
| 25 | DA | 2553 | G |
| 25 | DA | 2554 | U |
| 25 | DA | 2566 | A |
| 25 | DA | 2567 | G |
| 25 | DA | 2569 | G |
| 25 | DA | 2571 | C |
| 25 | DA | 2572 | A |
| 25 | DA | 2573 | C |
| 25 | DA | 2584 | U |
| 25 | DA | 2585 | U |
| 25 | DA | 2601 | C |
| 25 | DA | 2602 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | DA | 2603 | G |
| 25 | DA | 2609 | U |
| 25 | DA | 2611 | U |
| 25 | DA | 2612 | C |
| 25 | DA | 2613 | U |
| 25 | DA | 2615 | U |
| 25 | DA | 2629 | A |
| 25 | DA | 2630 | G |
| 25 | DA | 2655 | G |
| 25 | DA | 2665 | A |
| 25 | DA | 2673 | G |
| 25 | DA | 2682 | U |
| 25 | DA | 2689 | U |
| 25 | DA | 2690 | C |
| 25 | DA | 2703 | C |
| 25 | DA | 2704 | C |
| 25 | DA | 2707 | G |
| 25 | DA | 2712(A) | A |
| 25 | DA | 2713 | A |
| 25 | DA | 2714 | G |
| 25 | DA | 2726 | U |
| 25 | DA | 2733 | A |
| 25 | DA | 2734 | A |
| 25 | DA | 2739 | U |
| 25 | DA | 2744 | G |
| 25 | DA | 2748 | A |
| 25 | DA | 2750 | A |
| 25 | DA | 2751 | G |
| 25 | DA | 2752 | C |
| 25 | DA | 2754 | U |
| 25 | DA | 2758 | A |
| 25 | DA | 2761 | G |
| 25 | DA | 2762 | G |
| 25 | DA | 2764 | A |
| 25 | DA | 2765 | A |
| 25 | DA | 2766 | G |
| 25 | DA | 2777 | G |
| 25 | DA | 2778 | A |
| 25 | DA | 2779 | U |
| 25 | DA | 2790 | A |
| 25 | DA | 2791 | C |
| 25 | DA | 2794 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 2797 | U |
| 25 | DA | 2798 | C |
| 25 | DA | 2799 | A |
| 25 | DA | 2803 | C |
| 25 | DA | 2807 | G |
| 25 | DA | 2808 | U |
| 25 | DA | 2811 | G |
| 25 | DA | 2818 | G |
| 25 | DA | 2820 | A |
| 25 | DA | 2821 | A |
| 25 | DA | 2833 | G |
| 25 | DA | 2834 | G |
| 25 | DA | 2835 | A |
| 25 | DA | 2839 | G |
| 25 | DA | 2845 | G |
| 25 | DA | 2847 | U |
| 25 | DA | 2848 | G |
| 25 | DA | 2849 | U |
| 25 | DA | 2860 | A |
| 25 | DA | 2872 | G |
| 25 | DA | 2873 | A |
| 25 | DA | 2880 | C |
| 25 | DA | 2892 | A |
| 25 | DA | 2893 | G |
| 25 | DA | 2894 | G |
| 25 | DA | 2896 | C |
| 25 | DA | 2897 | U |
| 26 | DB | 0 | A |
| 26 | DB | 3 | C |
| 26 | DB | 8 | U |
| 26 | DB | 9 | G |
| 26 | DB | 13 | A |
| 26 | DB | 15 | A |
| 26 | DB | 16 | G |
| 26 | DB | 24 | G |
| 26 | DB | 25 | A |
| 26 | DB | 26 | A |
| 26 | DB | 28 | C |
| 26 | DB | 29 | A |
| 26 | DB | 30 | C |
| 26 | DB | 31 | C |
| 26 | DB | 32 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 26 | DB | 40 | U |
| 26 | DB | 42 | C |
| 26 | DB | 44 | G |
| 26 | DB | 45 | A |
| 26 | DB | 46 | A |
| 26 | DB | 47 | C |
| 26 | DB | 65 | C |
| 26 | DB | 73 | A |
| 26 | DB | 74 | U |
| 26 | DB | 75 | G |
| 26 | DB | 81 | G |
| 26 | DB | 82 | G |
| 26 | DB | 88 | C |
| 26 | DB | 89 | G |
| 26 | DB | 89(A) | A |
| 26 | DB | 90 | C |
| 26 | DB | 100 | G |
| 26 | DB | 101 | A |
| 26 | DB | 105 | G |
| 26 | DB | 108 | C |
| 26 | DB | 109 | G |
| 26 | DB | 112 | G |
| 26 | DB | 115 | G |
| 26 | DB | 119 | A |

All (208) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 31 | G |
| 1 | AA | 49 | U |
| 1 | AA | 50 | A |
| 1 | AA | 115 | G |
| 1 | AA | 119 | A |
| 1 | AA | 244 | U |
| 1 | AA | 266 | G |
| 1 | AA | 412 | A |
| 1 | AA | 428 | G |
| 1 | AA | 429 | U |
| 1 | AA | 484 | G |
| 1 | AA | 509 | A |
| 1 | AA | 530 | G |
| 1 | AA | 560 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 687 | A |
| 1 | AA | 703 | G |
| 1 | AA | 748 | C |
| 1 | AA | 812 | C |
| 1 | AA | 820 | U |
| 1 | AA | 842 | C |
| 1 | AA | 871 | U |
| 1 | AA | 913 | A |
| 1 | AA | 975 | A |
| 1 | AA | 992 | U |
| 1 | AA | 1025 | U |
| 1 | AA | 1027 | C |
| 1 | AA | 1065 | U |
| 1 | AA | 1178 | G |
| 1 | AA | 1285 | A |
| 1 | AA | 1498 | U |
| 1 | AA | 1503 | A |
| 1 | AA | 1504 | G |
| 22 | AB | 18 | G |
| 22 | AB | 19 | G |
| 22 | AB | 20 | U |
| 22 | AB | 23 | A |
| 22 | AB | 71 | U |
| 23 | AC | 1 | C |
| 23 | AC | 19 | G |
| 23 | AC | 20 | G |
| 23 | AC | 21 | U |
| 23 | AC | 48 | U |
| 23 | AC | 61 | U |
| 23 | AD | 13 | C |
| 24 | A1 | 14 | U |
| 25 | BA | 74 | A |
| 25 | BA | 196 | A |
| 25 | BA | 222 | A |
| 25 | BA | 229 | A |
| 25 | BA | 270(L) | U |
| 25 | BA | 271(B) | G |
| 25 | BA | 271(C) | U |
| 25 | BA | 404 | C |
| 25 | BA | 587 | C |
| 25 | BA | 654(S) | G |
| 25 | BA | 685 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | BA | 752 | A |
| 25 | BA | 764 | A |
| 25 | BA | 856 | C |
| 25 | BA | 881 | G |
| 25 | BA | 974(A) | C |
| 25 | BA | 1022 | G |
| 25 | BA | 1026 | U |
| 25 | BA | 1060 | U |
| 25 | BA | 1069 | A |
| 25 | BA | 1085 | A |
| 25 | BA | 1130 | U |
| 25 | BA | 1175 | U |
| 25 | BA | 1178 | C |
| 25 | BA | 1210 | A |
| 25 | BA | 1312 | U |
| 25 | BA | 1379 | A |
| 25 | BA | 1427 | A |
| 25 | BA | 1510 | A |
| 25 | BA | 1536 | A |
| 25 | BA | 1558 | A |
| 25 | BA | 1608 | A |
| 25 | BA | 1609 | A |
| 25 | BA | 1617 | C |
| 25 | BA | 1653 | G |
| 25 | BA | 1694 | C |
| 25 | BA | 1762 | A |
| 25 | BA | 1799 | G |
| 25 | BA | 1819 | A |
| 25 | BA | 1899 | G |
| 25 | BA | 1937 | A |
| 25 | BA | 1955 | U |
| 25 | BA | 1992 | G |
| 25 | BA | 2157 | G |
| 25 | BA | 2211 | G |
| 25 | BA | 2346 | A |
| 25 | BA | 2402 | C |
| 25 | BA | 2422 | A |
| 25 | BA | 2428 | G |
| 25 | BA | 2439 | A |
| 25 | BA | 2566 | A |
| 25 | BA | 2610 | C |
| 25 | BA | 2613 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2681 | C |
| 25 | BA | 2689 | U |
| 25 | BA | 2751 | G |
| 25 | BA | 2756 | U |
| 1 | CA | 31 | G |
| 1 | CA | 64 | G |
| 1 | CA | 89 | U |
| 1 | CA | 115 | G |
| 1 | CA | 197 | A |
| 1 | CA | 201 | C |
| 1 | CA | 209 | U |
| 1 | CA | 243 | A |
| 1 | CA | 250 | A |
| 1 | CA | 266 | G |
| 1 | CA | 279 | A |
| 1 | CA | 328 | C |
| 1 | CA | 345 | C |
| 1 | CA | 353 | A |
| 1 | CA | 412 | A |
| 1 | CA | 485 | G |
| 1 | CA | 509 | A |
| 1 | CA | 560 | U |
| 1 | CA | 575 | G |
| 1 | CA | 631 | G |
| 1 | CA | 632 | A |
| 1 | CA | 687 | A |
| 1 | CA | 748 | C |
| 1 | CA | 793 | U |
| 1 | CA | 812 | C |
| 1 | CA | 913 | A |
| 1 | CA | 974 | A |
| 1 | CA | 992 | U |
| 1 | CA | 1067 | A |
| 1 | CA | 1126 | U |
| 1 | CA | 1128 | C |
| 1 | CA | 1183 | A |
| 1 | CA | 1285 | A |
| 1 | CA | 1297 | C |
| 1 | CA | 1300 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1442 | G |
| 1 | CA | 1449 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 1498 | U |
| 1 | CA | 1503 | A |
| 1 | CA | 1529 | G |
| 22 | CB | 21 | A |
| 22 | CB | 48 | C |
| 23 | CC | 1 | C |
| 23 | CC | 19 | G |
| 23 | CC | 20 | G |
| 23 | CC | 21 | U |
| 23 | CC | 48 | U |
| 23 | CD | 13 | C |
| 25 | DA | 49 | A |
| 25 | DA | 71 | A |
| 25 | DA | 74 | A |
| 25 | DA | 101 | G |
| 25 | DA | 128 | C |
| 25 | DA | 148 | C |
| 25 | DA | 196 | A |
| 25 | DA | 204 | A |
| 25 | DA | 205 | G |
| 25 | DA | 278 | A |
| 25 | DA | 654(S) | G |
| 25 | DA | 669 | G |
| 25 | DA | 685 | A |
| 25 | DA | 752 | A |
| 25 | DA | 856 | C |
| 25 | DA | 877 | U |
| 25 | DA | 886 | C |
| 25 | DA | 888 | C |
| 25 | DA | 893 | C |
| 25 | DA | 945 | A |
| 25 | DA | 990 | A |
| 25 | DA | 1022 | G |
| 25 | DA | 1085 | A |
| 25 | DA | 1171 | G |
| 25 | DA | 1210 | A |
| 25 | DA | 1300 | U |
| 25 | DA | 1420 | U |
| 25 | DA | 1427 | A |
| 25 | DA | 1460 | A |
| 25 | DA | 1558 | A |
| 25 | DA | 1608 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | DA | 1653 | G |
| 25 | DA | 1762 | A |
| 25 | DA | 1819 | A |
| 25 | DA | 1955 | U |
| 25 | DA | 1992 | G |
| 25 | DA | 2126 | A |
| 25 | DA | 2191 | G |
| 25 | DA | 2210 | G |
| 25 | DA | 2211 | G |
| 25 | DA | 2225 | A |
| 25 | DA | 2275 | C |
| 25 | DA | 2282 | G |
| 25 | DA | 2311 | A |
| 25 | DA | 2406 | U |
| 25 | DA | 2422 | A |
| 25 | DA | 2439 | A |
| 25 | DA | 2447 | G |
| 25 | DA | 2602 | A |
| 25 | DA | 2610 | C |
| 25 | DA | 2611 | U |
| 25 | DA | 2689 | U |
| 25 | DA | 2776 | A |
| 25 | DA | 2778 | A |
| 25 | DA | 2790 | A |
| 25 | DA | 2859 | G |
| 25 | DA | 2893 | G |

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1700 ligands modelled in this entry, 1700 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | 1506/1506 (100%) | -0.57 | 4 (0%) 91 48 | 50, 98, 179, 234 | 0 |
| 1 | CA | 1506/1506 (100%) | -0.58 | 2 (0%) 93 63 | 62, 109, 181, 235 | 0 |
| 2 | AE | 237/256 (92%) | 0.08 | 2 (0%) 83 26 | 103, 136, 174, 185 | 0 |
| 2 | CE | 237/256 (92%) | 0.24 | 3 (1%) 74 19 | 114, 151, 185, 201 | 0 |
| 3 | AF | 205/239 (85%) | 0.64 | 12 (5%) 22 5 | 84, 111, 144, 153 | 0 |
| 3 | CF | 206/239 (86%) | 1.16 | 38 (18%) 2 1 | 118, 138, 166, 174 | 0 |
| 4 | AG | 208/208 (100%) | 0.14 | 4 (1%) 64 13 | 80, 105, 129, 142 | 0 |
| 4 | CG | 208/208 (100%) | 0.17 | 2 (0%) 79 22 | 77, 102, 123, 136 | 0 |
| 5 | AH | 151/162 (93%) | 0.09 | 0 100 100 | 74, 97, 118, 152 | 0 |
| 5 | CH | 151/162 (93%) | 0.12 | 0 100 100 | 91, 112, 134, 153 | 0 |
| 6 | AI | 101/101 (100%) | 0.45 | 5 (4%) 28 6 | 76, 99, 115, 137 | 0 |
| 6 | CI | 101/101 (100%) | 0.36 | 0 100 100 | 74, 95, 116, 141 | 0 |
| 7 | AJ | 155/156 (99%) | 0.26 | 8 (5%) 26 6 | 99, 114, 145, 155 | 0 |
| 7 | CJ | 155/156 (99%) | 0.22 | 6 (3%) 37 7 | 102, 122, 149, 156 | 0 |
| 8 | AK | 138/138 (100%) | -0.12 | 0 100 100 | 84, 103, 117, 122 | 0 |
| 8 | CK | 138/138 (100%) | -0.24 | 0 100 100 | 94, 116, 128, 136 | 0 |
| 9 | AL | 127/128 (99%) | -0.33 | 0 100 100 | 85, 133, 153, 160 | 0 |
| 9 | CL | 127/128 (99%) | -0.06 | 2 (1%) 68 16 | 107, 145, 160, 164 | 0 |
| 10 | AM | 99/105 (94%) | 0.14 | 0 100 100 | 81, 132, 162, 165 | 0 |
| 10 | CM | 99/105 (94%) | 0.26 | 0 100 100 | 111, 149, 165, 170 | 0 |
| 11 | AN | 119/129 (92%) | 0.72 | 7 (5%) 22 5 | 64, 97, 128, 154 | 0 |
| 11 | CN | 119/129 (92%) | 0.71 | 6 (5%) 28 6 | 79, 101, 134, 158 | 0 |
| 12 | AO | 125/132 (94%) | 0.44 | 7 (5%) 24 5 | 63, 73, 105, 151 | 0 |
| 12 | CO | 125/132 (94%) | 0.82 | 15 (12%) 5 1 | 75, 98, 124, 160 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 13 | AP | 116/126 (92%) | 0.00 | 1 (0%) 81 24 | 86, 117, 136, 145 | 0 |
| 13 | CP | 117/126 (92%) | 0.20 | 6 (5%) 27 6 | 106, 146, 161, 164 | 0 |
| 14 | AQ | 60/61 (98%) | -0.04 | 0 100 100 | 86, 101, 115, 126 | 0 |
| 14 | CQ | 60/61 (98%) | 0.73 | 6 (10%) 8 2 | 118, 132, 146, 153 | 0 |
| 15 | AR | 88/89 (98%) | -0.02 | 1 (1%) 77 21 | 72, 93, 114, 117 | 0 |
| 15 | CR | 88/89 (98%) | 0.06 | 1 (1%) 77 21 | 73, 104, 127, 133 | 0 |
| 16 | AS | 84/88 (95%) | -0.16 | 0 100 100 | 90, 107, 133, 165 | 0 |
| 16 | CS | 84/88 (95%) | -0.23 | 0 100 100 | 81, 96, 120, 153 | 0 |
| 17 | AT | 100/105 (95%) | -0.04 | 1 (1%) 79 22 | 82, 100, 118, 130 | 0 |
| 17 | CT | 100/105 (95%) | 0.00 | 1 (1%) 79 22 | 82, 102, 125, 137 | 0 |
| 18 | AU | 72/88 (81%) | 0.37 | 1 (1%) 72 18 | 78, 99, 132, 159 | 0 |
| 18 | CU | 72/88 (81%) | 0.32 | 5 (6%) 17 4 | 85, 106, 144, 157 | 0 |
| 19 | AV | 78/93 (83%) | -0.11 | 0 100 100 | 100, 122, 137, 144 | 0 |
| 19 | CV | 78/93 (83%) | 0.01 | 0 100 100 | 136, 154, 174, 177 | 0 |
| 20 | AW | 99/106 (93%) | -0.11 | 0 100 100 | 93, 115, 144, 155 | 0 |
| 20 | CW | 99/106 (93%) | 0.01 | 0 100 100 | 83, 109, 143, 157 | 0 |
| 21 | AX | 25/27 (92%) | -0.38 | 0 100 100 | 88, 109, 125, 147 | 0 |
| 21 | CX | 25/27 (92%) | 0.11 | 0 100 100 | 112, 133, 148, 160 | 0 |
| 22 | AB | 87/87 (100%) | 1.20 | 22 (25%) 1 1 | 78, 145, 185, 196 | 0 |
| 22 | CB | 87/87 (100%) | 2.80 | 37 (42%) 1 0 | 92, 148, 188, 200 | 0 |
| 23 | AC | 77/77 (100%) | -0.24 | 0 100 100 | 63, 100, 132, 147 | 0 |
| 23 | AD | 77/77 (100%) | 0.21 | 5 (6%) 18 4 | 71, 218, 232, 234 | 0 |
| 23 | CC | 77/77 (100%) | -0.16 | 1 (1%) 74 19 | 73, 107, 141, 153 | 0 |
| 23 | CD | 77/77 (100%) | 0.36 | 9 (11%) 5 2 | 77, 219, 231, 234 | 0 |
| 24 | A1 | 10/10 (100%) | 0.89 | 2 (20%) 2 1 | 67, 81, 112, 112 | 0 |
| 24 | C1 | 10/10 (100%) | 0.78 | 2 (20%) 2 1 | 81, 98, 118, 124 | 0 |
| 25 | BA | 2912/2912 (100%) | -0.37 | 31 (1%) 77 21 | 36, 66, 200, 234 | 0 |
| 25 | DA | 2907/2912 (99%) | -0.32 | 34 (1%) 75 20 | 45, 80, 220, 235 | 0 |
| 26 | BB | 122/122 (100%) | -0.64 | 1 (0%) 83 26 | 66, 91, 110, 169 | 0 |
| 26 | DB | 122/122 (100%) | -0.53 | 2 (1%) 68 16 | 84, 120, 141, 189 | 0 |
| 27 | BD | 272/276 (98%) | 0.08 | 0 100 100 | 35, 57, 79, 96 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 27 | DD | 272/276 (98%) | 0.21 | 3 (1%) 77 21 | 42, 67, 88, 119 | 0 |
| 28 | BE | 205/206 (99%) | 0.20 | 3 (1%) 70 16 | 43, 77, 123, 132 | 0 |
| 28 | DE | 205/206 (99%) | 0.18 | 5 (2%) 56 11 | 52, 88, 137, 159 | 0 |
| 29 | BF | 202/210 (96%) | -0.08 | 0 100 100 | 38, 70, 108, 123 | 0 |
| 29 | DF | 208/210 (99%) | 0.39 | 9 (4%) 34 7 | 48, 94, 152, 175 | 0 |
| 30 | BG | 181/182 (99%) | 0.36 | 6 (3%) 44 8 | 81, 101, 130, 142 | 0 |
| 30 | DG | 181/182 (99%) | 0.71 | 14 (7%) 13 3 | 112, 135, 155, 162 | 0 |
| 31 | BH | 170/180 (94%) | 0.25 | 4 (2%) 56 11 | 74, 104, 121, 146 | 0 |
| 31 | DH | 170/180 (94%) | 0.76 | 15 (8%) 10 3 | 148, 188, 209, 218 | 0 |
| 32 | BK | 146/148 (98%) | 0.13 | 1 (0%) 84 28 | 69, 121, 137, 142 | 0 |
| 32 | DK | 146/148 (98%) | 0.32 | 1 (0%) 84 28 | 77, 120, 143, 150 | 0 |
| 33 | BM | 138/140 (98%) | 0.14 | 1 (0%) 84 28 | 57, 81, 116, 129 | 0 |
| 33 | DM | 138/140 (98%) | -0.07 | 0 100 100 | 71, 102, 133, 143 | 0 |
| 34 | BN | 122/122 (100%) | 0.21 | 0 100 100 | 48, 67, 83, 97 | 0 |
| 34 | DN | 122/122 (100%) | 0.33 | 0 100 100 | 62, 82, 102, 118 | 0 |
| 35 | BO | 150/150 (100%) | -0.00 | 2 (1%) 74 19 | 42, 77, 106, 153 | 0 |
| 35 | DO | 150/150 (100%) | 0.64 | 11 (7%) 15 3 | 44, 99, 135, 171 | 0 |
| 36 | BP | 141/141 (100%) | 0.35 | 5 (3%) 42 8 | 52, 78, 99, 125 | 0 |
| 36 | DP | 141/141 (100%) | 0.65 | 10 (7%) 16 4 | 58, 98, 129, 148 | 0 |
| 37 | B0 | 118/118 (100%) | 0.15 | 0 100 100 | 50, 76, 94, 110 | 0 |
| 37 | D0 | 117/118 (99%) | -0.04 | 0 100 100 | 50, 75, 97, 113 | 0 |
| 38 | BQ | 111/112 (99%) | 0.07 | 0 100 100 | 70, 88, 110, 127 | 0 |
| 38 | DQ | 111/112 (99%) | 0.17 | 2 (1%) 65 14 | 83, 117, 139, 159 | 0 |
| 39 | BR | 137/146 (93%) | 0.16 | 3 (2%) 59 12 | 60, 82, 134, 163 | 0 |
| 39 | DR | 137/146 (93%) | 0.18 | 0 100 100 | 69, 93, 154, 174 | 0 |
| 40 | B1 | 117/118 (99%) | -0.15 | 2 (1%) 67 15 | 44, 70, 101, 132 | 0 |
| 40 | D1 | 117/118 (99%) | -0.03 | 0 100 100 | 58, 89, 131, 152 | 0 |
| 41 | B2 | 101/101 (100%) | 0.01 | 1 (0%) 79 22 | 48, 92, 115, 132 | 0 |
| 41 | D2 | 101/101 (100%) | 0.29 | 1 (0%) 79 22 | 58, 115, 133, 142 | 0 |
| 42 | BS | 113/113 (100%) | 0.07 | 3 (2%) 52 10 | 41, 65, 97, 147 | 0 |
| 42 | DS | 113/113 (100%) | 0.33 | 2 (1%) 65 14 | 54, 69, 104, 148 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 43 | BT | 92/96 (95%) | 0.06 | 2 (2%) 59 12 | 49, 63, 87, 104 | 0 |
| 43 | DT | 92/96 (95%) | 0.27 | 4 (4%) 34 7 | 64, 80, 104, 121 | 0 |
| 44 | BU | 102/110 (92%) | 0.37 | 6 (5%) 22 5 | 67, 92, 142, 159 | 0 |
| 44 | DU | 102/110 (92%) | 0.79 | 16 (15%) 3 1 | 82, 109, 160, 176 | 0 |
| 45 | BV | 175/206 (84%) | 1.09 | 28 (16%) 3 1 | 80, 117, 179, 183 | 0 |
| 45 | DV | 179/206 (86%) | 1.52 | 50 (27%) 1 0 | 110, 151, 199, 206 | 0 |
| 46 | B3 | 76/85 (89%) | -0.14 | 1 (1%) 74 19 | 52, 68, 83, 117 | 0 |
| 46 | D3 | 77/85 (90%) | 0.23 | 1 (1%) 74 19 | 65, 86, 108, 141 | 0 |
| 47 | BZ | 97/98 (98%) | 0.27 | 6 (6%) 20 5 | 46, 64, 122, 151 | 0 |
| 47 | DZ | 97/98 (98%) | 0.41 | 3 (3%) 47 9 | 54, 77, 126, 148 | 0 |
| 48 | BW | 66/72 (91%) | 0.04 | 1 (1%) 70 16 | 55, 73, 90, 120 | 0 |
| 48 | DW | 69/72 (95%) | 0.05 | 2 (2%) 49 9 | 77, 100, 130, 167 | 0 |
| 49 | BX | 59/60 (98%) | 0.14 | 1 (1%) 67 15 | 60, 75, 105, 120 | 0 |
| 49 | DX | 59/60 (98%) | 0.10 | 1 (1%) 67 15 | 73, 98, 130, 153 | 0 |
| 50 | B4 | 66/71 (92%) | 0.88 | 6 (9%) 9 2 | 111, 146, 164, 173 | 0 |
| 50 | D4 | 63/71 (88%) | 1.46 | 18 (28%) 1 0 | 140, 176, 185, 191 | 0 |
| 51 | B5 | 59/60 (98%) | 0.66 | 9 (15%) 3 1 | 43, 80, 163, 168 | 0 |
| 51 | D5 | 58/60 (96%) | 0.46 | 6 (10%) 7 2 | 52, 78, 167, 178 | 0 |
| 52 | B6 | 45/54 (83%) | 1.19 | 7 (15%) 3 1 | 105, 134, 156, 160 | 0 |
| 52 | D6 | 45/54 (83%) | 1.94 | 21 (46%) 1 0 | 121, 156, 173, 176 | 0 |
| 53 | B7 | 49/49 (100%) | 0.02 | 2 (4%) 35 7 | 35, 45, 88, 118 | 0 |
| 53 | D7 | 49/49 (100%) | 0.25 | 2 (4%) 35 7 | 44, 54, 112, 131 | 0 |
| 54 | B8 | 61/65 (93%) | 0.06 | 0 100 100 | 51, 64, 81, 102 | 0 |
| 54 | D8 | 61/65 (93%) | 0.73 | 2 (3%) 44 8 | 65, 79, 94, 123 | 0 |
| All | All | 21104/21634 (97%) | -0.01 | 591 (2%) 50 10 | 35, 96, 177, 235 | 0 |

All (591) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 22 | CB | 54 | G | 13.6 |
| 22 | CB | 52 | U | 12.9 |
| 22 | CB | 53 | A | 12.8 |
| 22 | CB | 82 | G | 12.2 |
| 22 | CB | 51 | A | 11.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 29 | DF | 1 | MET | 10.8 |
| 25 | DA | 654(J) | A | 10.0 |
| 22 | CB | 55 | G | 9.8 |
| 35 | DO | 150 | ALA | 9.3 |
| 22 | CB | 17 | U | 9.3 |
| 25 | BA | 2798 | C | 9.2 |
| 45 | DV | 112 | ARG | 9.1 |
| 25 | BA | 2901 | C | 8.9 |
| 12 | AO | 129 | ALA | 8.8 |
| 22 | CB | 83 | U | 8.6 |
| 25 | DA | 2901 | C | 8.3 |
| 25 | DA | 654(K) | C | 8.3 |
| 22 | CB | 47 | C | 8.1 |
| 25 | DA | 654(I) | C | 7.8 |
| 22 | AB | 84 | A | 7.6 |
| 25 | BA | 1536 | A | 7.5 |
| 22 | CB | 16 | U | 7.4 |
| 11 | AN | 11 | LYS | 7.4 |
| 51 | D5 | 59 | GLU | 7.4 |
| 22 | AB | 83 | U | 7.2 |
| 45 | DV | 179 | ASP | 7.0 |
| 11 | AN | 12 | ARG | 6.9 |
| 35 | DO | 149 | GLU | 6.8 |
| 11 | CN | 13 | GLN | 6.8 |
| 22 | CB | 80 | C | 6.8 |
| 45 | DV | 147 | GLY | 6.8 |
| 22 | CB | 48 | C | 6.7 |
| 25 | BA | 654(K) | C | 6.7 |
| 51 | B5 | 54 | GLY | 6.6 |
| 22 | CB | 81 | G | 6.5 |
| 22 | CB | 50 | A | 6.5 |
| 22 | AB | 1 | G | 6.5 |
| 25 | DA | 2902 | C | 6.5 |
| 1 | AA | 86 | U | 6.4 |
| 52 | D6 | 13 | CYS | 6.3 |
| 22 | CB | 56 | G | 6.3 |
| 7 | AJ | 78 | ARG | 6.2 |
| 25 | BA | 1534 | G | 6.2 |
| 28 | DE | 69 | LYS | 6.1 |
| 25 | BA | 1 | G | 6.1 |
| 51 | B5 | 2 | ALA | 6.1 |
| 53 | B7 | 49 | ARG | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 25 | BA | 2 | G | 6.0 |
| 22 | CB | 49 | C | 5.9 |
| 22 | CB | 87 | A | 5.9 |
| 25 | BA | 2799 | A | 5.8 |
| 25 | DA | 1535 | U | 5.7 |
| 35 | DO | 110 | TYR | 5.7 |
| 12 | CO | 129 | ALA | 5.7 |
| 22 | CB | 1 | G | 5.7 |
| 25 | BA | 163 | U | 5.6 |
| 25 | BA | 2797 | U | 5.6 |
| 22 | CB | 57 | C | 5.6 |
| 17 | CT | 101 | ARG | 5.6 |
| 35 | BO | 149 | GLU | 5.5 |
| 25 | BA | 2902 | C | 5.5 |
| 51 | B5 | 59 | GLU | 5.5 |
| 25 | DA | 2798 | C | 5.4 |
| 22 | CB | 4 | G | 5.4 |
| 28 | BE | 205 | ALA | 5.4 |
| 28 | BE | 79 | ARG | 5.4 |
| 47 | BZ | 98 | LEU | 5.4 |
| 22 | AB | 51 | A | 5.3 |
| 42 | BS | 113 | LYS | 5.3 |
| 25 | DA | 654(L) | G | 5.3 |
| 29 | DF | 208 | GLY | 5.2 |
| 12 | CO | 64 | TYR | 5.2 |
| 25 | DA | 2 | G | 5.2 |
| 18 | CU | 88 | LYS | 5.1 |
| 22 | CB | 84 | A | 5.0 |
| 47 | DZ | 96 | LYS | 5.0 |
| 42 | DS | 113 | LYS | 4.9 |
| 23 | AD | 18 | C | 4.9 |
| 25 | BA | 4 | C | 4.8 |
| 52 | D6 | 50 | ARG | 4.8 |
| 24 | A1 | 14 | U | 4.8 |
| 24 | C1 | 14 | U | 4.8 |
| 51 | B5 | 55 | ARG | 4.8 |
| 45 | DV | 146 | ILE | 4.8 |
| 25 | DA | 1509 | C | 4.7 |
| 25 | BA | 2900 | A | 4.7 |
| 31 | DH | 32 | GLU | 4.7 |
| 36 | DP | 1 | MET | 4.7 |
| 45 | DV | 162 | GLU | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 18 | AU | 88 | LYS | 4.7 |
| 11 | CN | 12 | ARG | 4.7 |
| 25 | BA | 654(J) | A | 4.7 |
| 50 | D4 | 40 | HIS | 4.6 |
| 11 | CN | 129 | SER | 4.6 |
| 45 | DV | 121 | HIS | 4.6 |
| 51 | D5 | 60 | VAL | 4.6 |
| 22 | AB | 79 | U | 4.6 |
| 22 | CB | 46 | G | 4.5 |
| 49 | BX | 60 | GLU | 4.5 |
| 22 | AB | 52 | U | 4.5 |
| 25 | DA | 1177 | A | 4.4 |
| 25 | DA | 887 | A | 4.4 |
| 25 | DA | 2799 | A | 4.3 |
| 22 | AB | 17 | U | 4.3 |
| 25 | DA | 2797 | U | 4.3 |
| 53 | D7 | 49 | ARG | 4.3 |
| 25 | DA | 888 | C | 4.3 |
| 22 | AB | 53 | A | 4.2 |
| 51 | B5 | 53 | ALA | 4.2 |
| 52 | B6 | 19 | ARG | 4.2 |
| 25 | DA | 1176 | G | 4.2 |
| 30 | DG | 139 | LEU | 4.1 |
| 23 | CD | 37 | U | 4.1 |
| 23 | CD | 35 | C | 4.1 |
| 52 | D6 | 14 | THR | 4.1 |
| 41 | D2 | 45 | THR | 4.1 |
| 31 | DH | 99 | VAL | 4.0 |
| 50 | D4 | 12 | ALA | 4.0 |
| 45 | DV | 119 | GLU | 4.0 |
| 25 | DA | 654(M) | C | 4.0 |
| 47 | BZ | 96 | LYS | 4.0 |
| 44 | DU | 49 | VAL | 4.0 |
| 44 | DU | 48 | ALA | 4.0 |
| 29 | DF | 2 | LYS | 4.0 |
| 27 | DD | 26 | LYS | 4.0 |
| 52 | B6 | 50 | ARG | 4.0 |
| 45 | DV | 145 | GLU | 4.0 |
| 3 | CF | 79 | ARG | 3.9 |
| 12 | AO | 128 | ALA | 3.9 |
| 30 | BG | 182 | LYS | 3.9 |
| 45 | BV | 106 | GLY | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 45 | DV | 168 | GLU | 3.9 |
| 22 | AB | 16 | U | 3.9 |
| 25 | BA | 654(L) | G | 3.9 |
| 7 | AJ | 154 | TYR | 3.9 |
| 31 | DH | 48 | GLY | 3.8 |
| 3 | CF | 45 | LYS | 3.8 |
| 25 | BA | 3 | U | 3.8 |
| 45 | DV | 107 | THR | 3.8 |
| 47 | DZ | 98 | LEU | 3.8 |
| 3 | CF | 146 | ALA | 3.8 |
| 25 | DA | 654(F) | C | 3.8 |
| 25 | DA | 2900 | A | 3.8 |
| 28 | DE | 70 | ALA | 3.8 |
| 17 | AT | 101 | ARG | 3.8 |
| 46 | D3 | 85 | ALA | 3.7 |
| 7 | AJ | 85 | TYR | 3.7 |
| 45 | DV | 155 | LEU | 3.7 |
| 22 | CB | 77 | C | 3.7 |
| 7 | AJ | 153 | HIS | 3.7 |
| 25 | BA | 2795 | G | 3.7 |
| 25 | BA | 2899 | G | 3.7 |
| 38 | DQ | 60 | GLY | 3.7 |
| 11 | AN | 129 | SER | 3.7 |
| 44 | DU | 46 | LYS | 3.7 |
| 3 | CF | 60 | ALA | 3.7 |
| 13 | CP | 4 | ILE | 3.7 |
| 45 | DV | 172 | ALA | 3.7 |
| 30 | DG | 34 | LEU | 3.7 |
| 45 | DV | 138 | GLU | 3.6 |
| 45 | DV | 178 | GLU | 3.6 |
| 44 | DU | 50 | ARG | 3.6 |
| 31 | DH | 25 | LYS | 3.6 |
| 45 | BV | 99 | TYR | 3.6 |
| 45 | DV | 113 | ALA | 3.6 |
| 45 | BV | 107 | THR | 3.6 |
| 25 | BA | 654(F) | C | 3.6 |
| 54 | D8 | 35 | GLN | 3.6 |
| 45 | DV | 144 | LEU | 3.6 |
| 25 | DA | 1536 | A | 3.6 |
| 29 | DF | 12 | LEU | 3.6 |
| 53 | B7 | 48 | LYS | 3.5 |
| 25 | DA | 654(O) | G | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 22 | CB | 2 | C | 3.5 |
| 45 | DV | 152 | ALA | 3.5 |
| 3 | CF | 53 | ALA | 3.5 |
| 28 | BE | 204 | ALA | 3.5 |
| 3 | CF | 131 | ARG | 3.5 |
| 7 | AJ | 84 | ASN | 3.5 |
| 22 | AB | 18 | G | 3.5 |
| 22 | CB | 85 | C | 3.5 |
| 3 | AF | 131 | ARG | 3.5 |
| 45 | DV | 148 | ASP | 3.5 |
| 22 | AB | 81 | G | 3.5 |
| 50 | D4 | 28 | LYS | 3.5 |
| 45 | DV | 141 | VAL | 3.5 |
| 25 | DA | 3 | U | 3.5 |
| 42 | BS | 111 | HIS | 3.5 |
| 45 | DV | 150 | LEU | 3.5 |
| 52 | D6 | 21 | TYR | 3.5 |
| 51 | D5 | 53 | ALA | 3.4 |
| 1 | AA | 85 | U | 3.4 |
| 50 | D4 | 10 | VAL | 3.4 |
| 50 | D4 | 13 | ARG | 3.4 |
| 47 | DZ | 97 | LEU | 3.4 |
| 3 | CF | 135 | LYS | 3.4 |
| 12 | CO | 128 | ALA | 3.4 |
| 45 | BV | 172 | ALA | 3.4 |
| 13 | CP | 6 | GLY | 3.4 |
| 23 | CC | 1 | C | 3.4 |
| 44 | DU | 47 | LYS | 3.4 |
| 52 | D6 | 27 | LYS | 3.4 |
| 25 | BA | 654(P) | G | 3.4 |
| 31 | BH | 18 | GLU | 3.3 |
| 11 | CN | 128 | ALA | 3.3 |
| 18 | CU | 46 | GLU | 3.3 |
| 35 | DO | 148 | LEU | 3.3 |
| 22 | AB | 48 | C | 3.3 |
| 30 | DG | 182 | LYS | 3.3 |
| 50 | D4 | 42 | PHE | 3.3 |
| 3 | CF | 199 | LYS | 3.3 |
| 40 | B1 | 118 | GLY | 3.3 |
| 23 | CD | 18 | C | 3.3 |
| 36 | DP | 105 | GLU | 3.3 |
| 51 | B5 | 58 | LEU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 45 | BV | 145 | GLU | 3.3 |
| 22 | AB | 82 | G | 3.2 |
| 35 | DO | 64 | LYS | 3.2 |
| 44 | DU | 52 | SER | 3.2 |
| 45 | BV | 171 | ILE | 3.2 |
| 31 | DH | 18 | GLU | 3.2 |
| 50 | D4 | 63 | TYR | 3.2 |
| 45 | DV | 9 | TYR | 3.2 |
| 12 | CO | 21 | LYS | 3.2 |
| 12 | CO | 19 | ARG | 3.2 |
| 13 | CP | 7 | VAL | 3.2 |
| 22 | CB | 86 | C | 3.2 |
| 47 | BZ | 92 | LYS | 3.2 |
| 45 | DV | 142 | SER | 3.2 |
| 3 | CF | 206 | GLU | 3.2 |
| 35 | DO | 106 | LEU | 3.2 |
| 45 | DV | 173 | ALA | 3.2 |
| 44 | DU | 53 | PRO | 3.1 |
| 22 | AB | 54 | G | 3.1 |
| 48 | BW | 43 | GLN | 3.1 |
| 22 | CB | 24 | C | 3.1 |
| 44 | BU | 52 | SER | 3.1 |
| 11 | CN | 11 | LYS | 3.1 |
| 51 | B5 | 60 | VAL | 3.1 |
| 24 | A1 | 13 | U | 3.1 |
| 39 | BR | 1 | MET | 3.1 |
| 52 | D6 | 49 | HIS | 3.1 |
| 44 | BU | 50 | ARG | 3.1 |
| 23 | CD | 38 | A | 3.1 |
| 25 | DA | 2899 | G | 3.1 |
| 45 | DV | 143 | GLY | 3.1 |
| 52 | D6 | 45 | LYS | 3.1 |
| 30 | BG | 80 | PHE | 3.1 |
| 52 | D6 | 52 | VAL | 3.1 |
| 48 | DW | 43 | GLN | 3.1 |
| 44 | DU | 29 | GLU | 3.0 |
| 45 | DV | 169 | GLU | 3.0 |
| 52 | D6 | 51 | GLU | 3.0 |
| 45 | DV | 111 | VAL | 3.0 |
| 25 | DA | 654(H) | G | 3.0 |
| 28 | DE | 59 | VAL | 3.0 |
| 11 | AN | 128 | ALA | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 12 | CO | 127 | GLU | 3.0 |
| 41 | B2 | 36 | PRO | 3.0 |
| 3 | AF | 94 | LEU | 3.0 |
| 7 | AJ | 79 | ARG | 3.0 |
| 50 | B4 | 28 | LYS | 3.0 |
| 45 | DV | 122 | ARG | 3.0 |
| 25 | DA | 1067 | A | 3.0 |
| 45 | BV | 108 | PRO | 3.0 |
| 25 | BA | 5 | A | 3.0 |
| 44 | BU | 99 | CYS | 3.0 |
| 50 | B4 | 3 | GLU | 3.0 |
| 50 | D4 | 54 | GLY | 3.0 |
| 45 | BV | 146 | ILE | 3.0 |
| 3 | AF | 72 | LYS | 3.0 |
| 9 | CL | 115 | GLY | 3.0 |
| 44 | DU | 88 | LYS | 3.0 |
| 22 | CB | 18 | G | 3.0 |
| 40 | B1 | 117 | GLN | 3.0 |
| 7 | CJ | 78 | ARG | 3.0 |
| 12 | CO | 28 | LYS | 3.0 |
| 44 | DU | 63 | LYS | 3.0 |
| 52 | B6 | 34 | LEU | 2.9 |
| 28 | DE | 54 | GLN | 2.9 |
| 12 | AO | 64 | TYR | 2.9 |
| 36 | DP | 66 | ILE | 2.9 |
| 3 | CF | 46 | GLU | 2.9 |
| 45 | BV | 60 | GLU | 2.9 |
| 22 | AB | 80 | C | 2.9 |
| 45 | DV | 55 | HIS | 2.9 |
| 33 | BM | 134 | ARG | 2.9 |
| 50 | D4 | 55 | ARG | 2.9 |
| 22 | AB | 4 | G | 2.9 |
| 50 | D4 | 30 | GLU | 2.9 |
| 36 | BP | 136 | ALA | 2.9 |
| 3 | CF | 108 | ASN | 2.9 |
| 50 | D4 | 29 | PRO | 2.9 |
| 24 | C1 | 13 | U | 2.9 |
| 42 | DS | 112 | GLY | 2.9 |
| 27 | DD | 35 | LYS | 2.9 |
| 23 | CD | 40 | C | 2.9 |
| 25 | BA | 654(G) | C | 2.9 |
| 45 | DV | 106 | GLY | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | CF | 198 | VAL | 2.9 |
| 13 | CP | 8 | GLU | 2.9 |
| 45 | BV | 1 | MET | 2.8 |
| 3 | CF | 44 | GLU | 2.8 |
| 22 | CB | 19 | G | 2.8 |
| 25 | BA | 2898 | U | 2.8 |
| 7 | CJ | 82 | GLY | 2.8 |
| 13 | CP | 5 | ALA | 2.8 |
| 31 | DH | 29 | PRO | 2.8 |
| 12 | AO | 19 | ARG | 2.8 |
| 51 | D5 | 58 | LEU | 2.8 |
| 30 | BG | 137 | GLU | 2.8 |
| 50 | B4 | 31 | ILE | 2.8 |
| 52 | D6 | 18 | ARG | 2.8 |
| 26 | BB | 1(M) | A | 2.8 |
| 45 | DV | 176 | PRO | 2.8 |
| 12 | CO | 126 | LYS | 2.8 |
| 1 | AA | 84 | U | 2.8 |
| 45 | BV | 117 | LEU | 2.8 |
| 39 | BR | 21 | GLU | 2.8 |
| 46 | B3 | 85 | ALA | 2.7 |
| 7 | CJ | 79 | ARG | 2.7 |
| 22 | CB | 3 | C | 2.7 |
| 22 | CB | 78 | C | 2.7 |
| 52 | D6 | 30 | THR | 2.7 |
| 3 | AF | 193 | TYR | 2.7 |
| 52 | D6 | 42 | TRP | 2.7 |
| 30 | DG | 82 | LEU | 2.7 |
| 45 | BV | 155 | LEU | 2.7 |
| 52 | B6 | 53 | LYS | 2.7 |
| 52 | B6 | 29 | ASN | 2.7 |
| 9 | CL | 127 | LYS | 2.7 |
| 45 | DV | 177 | PRO | 2.7 |
| 1 | AA | 345 | C | 2.7 |
| 45 | DV | 109 | ALA | 2.7 |
| 52 | B6 | 18 | ARG | 2.7 |
| 12 | CO | 65 | GLU | 2.7 |
| 45 | BV | 2 | GLU | 2.7 |
| 45 | BV | 173 | ALA | 2.7 |
| 30 | DG | 39 | ILE | 2.7 |
| 1 | CA | 1029 | G | 2.7 |
| 52 | D6 | 24 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | DH | 95 | ARG | 2.7 |
| 43 | BT | 92 | LEU | 2.7 |
| 3 | CF | 52 | LEU | 2.7 |
| 25 | DA | 2139 | C | 2.6 |
| 2 | AE | 96 | ARG | 2.6 |
| 28 | DE | 205 | ALA | 2.6 |
| 2 | CE | 5 | ILE | 2.6 |
| 43 | DT | 68 | ARG | 2.6 |
| 31 | BH | 155 | SER | 2.6 |
| 29 | DF | 21 | ALA | 2.6 |
| 43 | DT | 92 | LEU | 2.6 |
| 53 | D7 | 47 | ARG | 2.6 |
| 30 | DG | 108 | ASN | 2.6 |
| 3 | AF | 201 | TYR | 2.6 |
| 35 | BO | 150 | ALA | 2.6 |
| 23 | AD | 33 | C | 2.6 |
| 25 | BA | 546 | C | 2.6 |
| 4 | AG | 181 | MET | 2.6 |
| 7 | CJ | 86 | GLN | 2.6 |
| 18 | CU | 42 | ARG | 2.6 |
| 23 | CD | 36 | A | 2.6 |
| 44 | DU | 62 | GLU | 2.6 |
| 2 | AE | 77 | ALA | 2.6 |
| 3 | CF | 6 | HIS | 2.6 |
| 36 | BP | 91 | GLU | 2.6 |
| 3 | CF | 103 | VAL | 2.6 |
| 25 | DA | 4 | C | 2.6 |
| 3 | CF | 185 | GLY | 2.6 |
| 45 | BV | 160 | GLY | 2.6 |
| 25 | BA | 1535 | U | 2.6 |
| 3 | CF | 109 | PRO | 2.5 |
| 45 | BV | 168 | GLU | 2.5 |
| 45 | BV | 142 | SER | 2.5 |
| 45 | BV | 150 | LEU | 2.5 |
| 47 | BZ | 93 | GLU | 2.5 |
| 43 | DT | 89 | ILE | 2.5 |
| 43 | DT | 69 | TYR | 2.5 |
| 3 | CF | 147 | LYS | 2.5 |
| 14 | CQ | 50 | LYS | 2.5 |
| 45 | DV | 137 | ILE | 2.5 |
| 12 | AO | 28 | LYS | 2.5 |
| 12 | CO | 68 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 52 | D6 | 22 | ALA | 2.5 |
| 32 | DK | 125 | GLU | 2.5 |
| 45 | DV | 50 | GLN | 2.5 |
| 52 | D6 | 26 | ASN | 2.5 |
| 6 | AI | 48 | LEU | 2.5 |
| 3 | AF | 199 | LYS | 2.5 |
| 25 | BA | 654(E) | C | 2.5 |
| 22 | CB | 76 | U | 2.5 |
| 3 | CF | 155 | GLY | 2.5 |
| 36 | DP | 63 | LYS | 2.5 |
| 12 | CO | 60 | LEU | 2.5 |
| 3 | CF | 143 | GLU | 2.5 |
| 3 | CF | 56 | ASP | 2.5 |
| 14 | CQ | 39 | LEU | 2.5 |
| 22 | AB | 3 | C | 2.5 |
| 4 | AG | 163 | GLU | 2.5 |
| 36 | BP | 133 | ARG | 2.5 |
| 44 | DU | 58 | GLY | 2.5 |
| 45 | BV | 170 | THR | 2.5 |
| 3 | AF | 166 | GLU | 2.5 |
| 3 | CF | 204 | LEU | 2.5 |
| 22 | CB | 5 | A | 2.5 |
| 30 | BG | 2 | PRO | 2.5 |
| 22 | AB | 49 | C | 2.5 |
| 45 | DV | 68 | PRO | 2.4 |
| 45 | DV | 163 | LEU | 2.4 |
| 49 | DX | 60 | GLU | 2.4 |
| 25 | DA | 1095 | A | 2.4 |
| 3 | CF | 65 | ALA | 2.4 |
| 30 | DG | 146 | TYR | 2.4 |
| 36 | DP | 104 | PHE | 2.4 |
| 6 | AI | 47 | ARG | 2.4 |
| 23 | AD | 37 | U | 2.4 |
| 25 | BA | 164 | U | 2.4 |
| 31 | DH | 45 | VAL | 2.4 |
| 6 | AI | 46 | ARG | 2.4 |
| 35 | DO | 147 | LEU | 2.4 |
| 30 | DG | 177 | GLY | 2.4 |
| 45 | DV | 110 | GLY | 2.4 |
| 3 | AF | 200 | ALA | 2.4 |
| 12 | CO | 37 | CYS | 2.4 |
| 3 | CF | 77 | ILE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 45 | DV | 5 | LEU | 2.4 |
| 6 | AI | 57 | GLN | 2.4 |
| 23 | CD | 17 | C | 2.4 |
| 45 | BV | 4 | ARG | 2.4 |
| 51 | D5 | 55 | ARG | 2.4 |
| 52 | D6 | 9 | LEU | 2.4 |
| 22 | CB | 58 | U | 2.4 |
| 35 | DO | 111 | ARG | 2.4 |
| 38 | DQ | 108 | GLY | 2.4 |
| 7 | AJ | 156 | TRP | 2.4 |
| 30 | DG | 58 | GLN | 2.4 |
| 50 | D4 | 8 | LYS | 2.4 |
| 29 | DF | 11 | VAL | 2.4 |
| 45 | DV | 139 | VAL | 2.4 |
| 12 | CO | 69 | TYR | 2.3 |
| 22 | CB | 72 | C | 2.3 |
| 45 | DV | 108 | PRO | 2.3 |
| 50 | B4 | 55 | ARG | 2.3 |
| 3 | AF | 135 | LYS | 2.3 |
| 45 | DV | 156 | LYS | 2.3 |
| 29 | DF | 20 | LEU | 2.3 |
| 50 | D4 | 41 | PRO | 2.3 |
| 11 | AN | 127 | LYS | 2.3 |
| 44 | BU | 53 | PRO | 2.3 |
| 3 | CF | 105 | GLU | 2.3 |
| 44 | DU | 79 | CYS | 2.3 |
| 13 | CP | 3 | ARG | 2.3 |
| 22 | AB | 85 | C | 2.3 |
| 25 | DA | 1537 | C | 2.3 |
| 22 | CB | 79 | U | 2.3 |
| 30 | DG | 152 | LEU | 2.3 |
| 45 | BV | 70 | LEU | 2.3 |
| 25 | DA | 654(G) | C | 2.3 |
| 29 | DF | 27 | GLU | 2.3 |
| 36 | BP | 32 | TYR | 2.3 |
| 45 | BV | 98 | MET | 2.3 |
| 13 | AP | 8 | GLU | 2.3 |
| 52 | D6 | 25 | LYS | 2.3 |
| 7 | CJ | 81 | GLY | 2.3 |
| 14 | CQ | 25 | VAL | 2.3 |
| 22 | AB | 56 | G | 2.3 |
| 23 | AD | 48 | U | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 32 | BK | 113 | ARG | 2.3 |
| 35 | DO | 61 | ARG | 2.3 |
| 18 | CU | 23 | LYS | 2.3 |
| 52 | D6 | 53 | LYS | 2.3 |
| 52 | D6 | 23 | THR | 2.3 |
| 11 | AN | 81 | ASP | 2.3 |
| 47 | BZ | 97 | LEU | 2.3 |
| 15 | AR | 89 | GLY | 2.3 |
| 44 | DU | 86 | ARG | 2.3 |
| 12 | AO | 127 | GLU | 2.3 |
| 4 | CG | 35 | ARG | 2.3 |
| 25 | BA | 654(H) | G | 2.3 |
| 25 | DA | 1093 | G | 2.3 |
| 45 | DV | 171 | ILE | 2.3 |
| 22 | CB | 45 | U | 2.3 |
| 3 | CF | 64 | VAL | 2.2 |
| 3 | AF | 122 | GLU | 2.2 |
| 15 | CR | 2 | PRO | 2.2 |
| 45 | DV | 140 | ASP | 2.2 |
| 31 | DH | 24 | VAL | 2.2 |
| 54 | D8 | 34 | TRP | 2.2 |
| 2 | CE | 4 | GLU | 2.2 |
| 4 | AG | 168 | ARG | 2.2 |
| 31 | BH | 27 | LYS | 2.2 |
| 30 | DG | 86 | MET | 2.2 |
| 52 | B6 | 13 | CYS | 2.2 |
| 6 | AI | 55 | ASP | 2.2 |
| 3 | CF | 134 | ILE | 2.2 |
| 44 | DU | 45 | VAL | 2.2 |
| 31 | DH | 33 | LEU | 2.2 |
| 25 | BA | 2794 | C | 2.2 |
| 45 | DV | 95 | PRO | 2.2 |
| 45 | DV | 116 | VAL | 2.2 |
| 3 | CF | 184 | TYR | 2.2 |
| 23 | CD | 39 | A | 2.2 |
| 3 | CF | 78 | GLY | 2.2 |
| 3 | CF | 200 | ALA | 2.2 |
| 25 | BA | 277 | C | 2.2 |
| 42 | BS | 112 | GLY | 2.2 |
| 11 | CN | 31 | THR | 2.2 |
| 3 | CF | 187 | ALA | 2.2 |
| 26 | DB | 1(M) | A | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 2 | CE | 156 | LYS | 2.2 |
| 12 | AO | 20 | LYS | 2.2 |
| 51 | B5 | 52 | TYR | 2.2 |
| 3 | CF | 72 | LYS | 2.2 |
| 7 | CJ | 154 | TYR | 2.2 |
| 50 | B4 | 39 | CYS | 2.2 |
| 31 | DH | 128 | PRO | 2.2 |
| 3 | CF | 201 | TYR | 2.2 |
| 45 | BV | 156 | LYS | 2.2 |
| 45 | DV | 149 | SER | 2.2 |
| 50 | D4 | 45 | GLY | 2.2 |
| 23 | AD | 38 | A | 2.2 |
| 3 | CF | 104 | GLN | 2.2 |
| 30 | BG | 88 | ILE | 2.2 |
| 45 | DV | 118 | GLN | 2.1 |
| 45 | DV | 154 | ASP | 2.1 |
| 45 | BV | 164 | ALA | 2.1 |
| 3 | CF | 85 | ARG | 2.1 |
| 14 | CQ | 34 | TYR | 2.1 |
| 44 | BU | 102 | CYS | 2.1 |
| 31 | DH | 96 | ALA | 2.1 |
| 45 | BV | 153 | SER | 2.1 |
| 50 | D4 | 7 | PRO | 2.1 |
| 45 | BV | 113 | ALA | 2.1 |
| 1 | CA | 1035 | A | 2.1 |
| 18 | CU | 26 | LEU | 2.1 |
| 25 | DA | 1 | G | 2.1 |
| 23 | CD | 16 | C | 2.1 |
| 25 | BA | 654(Q) | C | 2.1 |
| 31 | DH | 150 | ALA | 2.1 |
| 35 | DO | 125 | VAL | 2.1 |
| 30 | DG | 178 | PHE | 2.1 |
| 25 | DA | 654(N) | G | 2.1 |
| 45 | DV | 4 | ARG | 2.1 |
| 3 | AF | 87 | LEU | 2.1 |
| 3 | AF | 90 | GLU | 2.1 |
| 4 | AG | 167 | GLY | 2.1 |
| 31 | DH | 152 | ARG | 2.1 |
| 25 | DA | 1092 | C | 2.1 |
| 36 | DP | 7 | MET | 2.1 |
| 47 | BZ | 94 | LEU | 2.1 |
| 31 | DH | 46 | GLU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 50 | D4 | 46 | GLN | 2.1 |
| 51 | D5 | 54 | GLY | 2.1 |
| 22 | AB | 55 | G | 2.1 |
| 48 | DW | 44 | LEU | 2.1 |
| 45 | DV | 6 | LYS | 2.1 |
| 3 | CF | 41 | GLY | 2.1 |
| 36 | DP | 65 | PHE | 2.1 |
| 51 | B5 | 57 | VAL | 2.1 |
| 27 | DD | 40 | THR | 2.1 |
| 12 | CO | 20 | LYS | 2.1 |
| 50 | B4 | 64 | GLY | 2.1 |
| 50 | D4 | 24 | THR | 2.1 |
| 7 | AJ | 155 | ARG | 2.1 |
| 11 | AN | 62 | GLN | 2.1 |
| 30 | BG | 135 | LEU | 2.1 |
| 30 | DG | 138 | GLN | 2.1 |
| 44 | BU | 2 | ARG | 2.1 |
| 30 | DG | 10 | LYS | 2.0 |
| 44 | DU | 59 | GLY | 2.0 |
| 52 | D6 | 41 | PRO | 2.0 |
| 22 | AB | 87 | A | 2.0 |
| 36 | DP | 86 | GLY | 2.0 |
| 14 | CQ | 49 | HIS | 2.0 |
| 26 | DB | 88 | C | 2.0 |
| 39 | BR | 134 | GLU | 2.0 |
| 43 | BT | 90 | GLU | 2.0 |
| 36 | DP | 103 | MET | 2.0 |
| 36 | BP | 140 | ALA | 2.0 |
| 45 | BV | 154 | ASP | 2.0 |
| 4 | CG | 49 | ARG | 2.0 |
| 12 | CO | 59 | ARG | 2.0 |
| 50 | D4 | 39 | CYS | 2.0 |
| 14 | CQ | 53 | LEU | 2.0 |
| 36 | DP | 37 | LEU | 2.0 |
| 35 | DO | 124 | LYS | 2.0 |
| 52 | D6 | 36 | LEU | 2.0 |
| 45 | BV | 116 | VAL | 2.0 |
| 29 | DF | 207 | GLY | 2.0 |
| 3 | CF | 102 | ASN | 2.0 |
| 31 | BH | 3 | ARG | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55 | MG | BA | 3156 | 1/1 | 0.27 | - | 40,40,40,40 | 0 |
| 55 | MG | CA | 1653 | 1/1 | 0.14 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3079 | 1/1 | 0.41 | - | 55,55,55,55 | 0 |
| 55 | MG | DA | 3218 | 1/1 | 0.46 | - | 62,62,62,62 | 0 |
| 55 | MG | BD | 301 | 1/1 | 0.55 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3115 | 1/1 | 0.33 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3437 | 1/1 | 0.21 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3102 | 1/1 | 0.31 | - | 66,66,66,66 | 0 |
| 55 | MG | DA | 3520 | 1/1 | 0.87 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3061 | 1/1 | 0.57 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3184 | 1/1 | 0.65 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3110 | 1/1 | 0.54 | - | 59,59,59,59 | 0 |
| 55 | MG | BA | 3409 | 1/1 | 0.20 | - | 68,68,68,68 | 0 |
| 55 | MG | AA | 1619 | 1/1 | 0.39 | - | 63,63,63,63 | 0 |
| 55 | MG | AA | 1708 | 1/1 | 0.44 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3113 | 1/1 | 0.57 | - | 43,43,43,43 | 0 |
| 55 | MG | AA | 1669 | 1/1 | 0.43 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3506 | 1/1 | 0.44 | - | 78,78,78,78 | 0 |
| 55 | MG | AA | 1662 | 1/1 | 0.62 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3158 | 1/1 | 0.27 | - | 41,41,41,41 | 0 |
| 55 | MG | BA | 3016 | 1/1 | 0.52 | - | 39,39,39,39 | 0 |
| 55 | MG | DA | 3122 | 1/1 | 0.47 | - | 46,46,46,46 | 0 |
| 55 | MG | CB | 101 | 1/1 | 0.22 | - | 101,101,101,101 | 0 |
| 55 | MG | AA | 1842 | 1/1 | 0.48 | - | 59,59,59,59 | 0 |
| 55 | MG | CA | 1750 | 1/1 | 0.46 | - | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1689 | 1/1 | 0.24 | - | 115,115,115,115 | 0 |
| 55 | MG | DA | 3191 | 1/1 | 0.57 | - | 46,46,46,46 | 0 |
| 55 | MG | DA | 3196 | 1/1 | 0.46 | - | 50,50,50,50 | 0 |
| 55 | MG | AA | 1797 | 1/1 | 0.15 | - | 99,99,99,99 | 0 |
| 55 | MG | DA | 3398 | 1/1 | 0.43 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3491 | 1/1 | 0.53 | - | 42,42,42,42 | 0 |
| 55 | MG | BA | 3045 | 1/1 | 0.39 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3007 | 1/1 | 0.53 | - | 53,53,53,53 | 0 |
| 55 | MG | AA | 1706 | 1/1 | 0.51 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3338 | 1/1 | 0.33 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3313 | 1/1 | 0.32 | - | 85,85,85,85 | 0 |
| 55 | MG | CA | 1608 | 1/1 | 0.33 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1723 | 1/1 | 0.08 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3056 | 1/1 | 0.22 | - | 54,54,54,54 | 0 |
| 55 | MG | BA | 3225 | 1/1 | 0.23 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3262 | 1/1 | 0.45 | - | 48,48,48,48 | 0 |
| 55 | MG | AA | 1687 | 1/1 | 0.38 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3222 | 1/1 | 0.55 | - | 60,60,60,60 | 0 |
| 55 | MG | DA | 3306 | 1/1 | 0.53 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1841 | 1/1 | 0.42 | - | 59,59,59,59 | 0 |
| 55 | MG | BA | 3338 | 1/1 | 0.38 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1612 | 1/1 | 0.14 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3030 | 1/1 | 0.53 | - | 44,44,44,44 | 0 |
| 55 | MG | BA | 3205 | 1/1 | 0.39 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3333 | 1/1 | 0.53 | - | 80,80,80,80 | 0 |
| 55 | MG | AA | 1664 | 1/1 | 0.21 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3324 | 1/1 | 0.56 | - | 73,73,73,73 | 0 |
| 55 | MG | CA | 1632 | 1/1 | 0.33 | - | 95,95,95,95 | 0 |
| 55 | MG | DA | 3308 | 1/1 | 0.40 | - | 97,97,97,97 | 0 |
| 55 | MG | CA | 1768 | 1/1 | 0.56 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3385 | 1/1 | 0.15 | - | 87,87,87,87 | 0 |
| 55 | MG | CA | 1650 | 1/1 | 0.23 | - | 102,102,102,102 | 0 |
| 55 | MG | AA | 1690 | 1/1 | 0.20 | - | 96,96,96,96 | 0 |
| 55 | MG | CA | 1625 | 1/1 | 0.25 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3431 | 1/1 | 0.71 | - | 88,88,88,88 | 0 |
| 55 | MG | BO | 202 | 1/1 | 0.22 | - | 37,37,37,37 | 0 |
| 55 | MG | DA | 3400 | 1/1 | 0.49 | - | 89,89,89,89 | 0 |
| 55 | MG | AA | 1793 | 1/1 | 0.42 | - | 73,73,73,73 | 0 |
| 55 | MG | CS | 101 | 1/1 | 0.31 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3276 | 1/1 | 0.16 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3447 | 1/1 | 0.45 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3050 | 1/1 | 0.47 | - | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1658 | 1/1 | 0.64 | - | 49,49,49,49 | 0 |
| 55 | MG | BA | 3085 | 1/1 | 0.17 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3223 | 1/1 | 0.35 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3168 | 1/1 | 0.31 | - | 49,49,49,49 | 0 |
| 55 | MG | BA | 3398 | 1/1 | 0.49 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3438 | 1/1 | 0.38 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3548 | 1/1 | 0.49 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3219 | 1/1 | 0.30 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3453 | 1/1 | 0.21 | - | 66,66,66,66 | 0 |
| 55 | MG | DA | 3024 | 1/1 | 0.36 | - | 108,108,108,108 | 0 |
| 55 | MG | DA | 3462 | 1/1 | 0.80 | - | 107,107,107,107 | 0 |
| 55 | MG | CA | 1748 | 1/1 | 0.21 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3043 | 1/1 | 0.22 | - | 32,32,32,32 | 0 |
| 55 | MG | DA | 3157 | 1/1 | 0.70 | - | 47,47,47,47 | 0 |
| 55 | MG | CA | 1728 | 1/1 | 0.68 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3394 | 1/1 | 0.20 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3559 | 1/1 | 0.21 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3162 | 1/1 | 0.53 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3512 | 1/1 | 0.33 | - | 69,69,69,69 | 0 |
| 55 | MG | AA | 1671 | 1/1 | 0.16 | - | 67,67,67,67 | 0 |
| 55 | MG | DA | 3390 | 1/1 | 0.38 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3446 | 1/1 | 0.51 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3033 | 1/1 | 0.39 | - | 38,38,38,38 | 0 |
| 55 | MG | DA | 3280 | 1/1 | 0.55 | - | 46,46,46,46 | 0 |
| 55 | MG | BA | 3528 | 1/1 | 0.47 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3329 | 1/1 | 0.42 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3238 | 1/1 | 0.57 | - | 41,41,41,41 | 0 |
| 55 | MG | DA | 3507 | 1/1 | 0.43 | - | 91,91,91,91 | 0 |
| 55 | MG | CA | 1757 | 1/1 | 0.26 | - | 97,97,97,97 | 0 |
| 55 | MG | DA | 3472 | 1/1 | 0.68 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3179 | 1/1 | 0.44 | - | 64,64,64,64 | 0 |
| 55 | MG | CA | 1631 | 1/1 | 0.13 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1777 | 1/1 | 0.33 | - | 88,88,88,88 | 0 |
| 55 | MG | AA | 1692 | 1/1 | 0.17 | - | 115,115,115,115 | 0 |
| 55 | MG | BB | 207 | 1/1 | 0.27 | - | 83,83,83,83 | 0 |
| 55 | MG | AA | 1642 | 1/1 | 0.67 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3522 | 1/1 | 0.48 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3485 | 1/1 | 0.33 | - | 80,80,80,80 | 0 |
| 55 | MG | AA | 1634 | 1/1 | 0.28 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3567 | 1/1 | 0.31 | - | 80,80,80,80 | 0 |
| 55 | MG | CA | 1656 | 1/1 | 0.35 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3584 | 1/1 | 0.24 | - | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1821 | 1/1 | 0.28 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3480 | 1/1 | 0.44 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3246 | 1/1 | 0.43 | - | 53,53,53,53 | 0 |
| 55 | MG | CA | 1660 | 1/1 | 0.18 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3382 | 1/1 | 0.37 | - | 43,43,43,43 | 0 |
| 55 | MG | DA | 3416 | 1/1 | 0.48 | - | 59,59,59,59 | 0 |
| 55 | MG | DA | 3002 | 1/1 | 0.34 | - | 93,93,93,93 | 0 |
| 55 | MG | DA | 3368 | 1/1 | 0.69 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3224 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 55 | MG | DA | 3328 | 1/1 | 0.32 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3002 | 1/1 | 0.47 | - | 43,43,43,43 | 0 |
| 55 | MG | CA | 1772 | 1/1 | 0.30 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3017 | 1/1 | 0.48 | - | 25,25,25,25 | 0 |
| 55 | MG | BA | 3010 | 1/1 | 0.42 | - | 46,46,46,46 | 0 |
| 55 | MG | BA | 3312 | 1/1 | 0.51 | - | 57,57,57,57 | 0 |
| 55 | MG | BA | 3400 | 1/1 | 0.51 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3212 | 1/1 | 0.60 | - | 48,48,48,48 | 0 |
| 55 | MG | BA | 3293 | 1/1 | 0.29 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1780 | 1/1 | 0.31 | - | 86,86,86,86 | 0 |
| 55 | MG | AA | 1654 | 1/1 | 0.46 | - | 75,75,75,75 | 0 |
| 55 | MG | CC | 103 | 1/1 | 0.98 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3127 | 1/1 | 0.43 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3164 | 1/1 | 0.43 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3289 | 1/1 | 0.57 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3336 | 1/1 | 0.45 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1750 | 1/1 | 0.53 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3171 | 1/1 | 0.38 | - | 63,63,63,63 | 0 |
| 55 | MG | AA | 1726 | 1/1 | 0.49 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3495 | 1/1 | 0.17 | - | 63,63,63,63 | 0 |
| 55 | MG | BU | 201 | 1/1 | 0.22 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1677 | 1/1 | 0.47 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3561 | 1/1 | 0.38 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3255 | 1/1 | 0.37 | - | 46,46,46,46 | 0 |
| 55 | MG | CA | 1670 | 1/1 | 0.52 | - | 56,56,56,56 | 0 |
| 55 | MG | CA | 1703 | 1/1 | 0.30 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3254 | 1/1 | 0.32 | - | 43,43,43,43 | 0 |
| 55 | MG | DA | 3117 | 1/1 | 0.42 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3490 | 1/1 | 0.15 | - | 166,166,166,166 | 0 |
| 55 | MG | CA | 1610 | 1/1 | 0.23 | - | 97,97,97,97 | 0 |
| 55 | MG | BA | 3285 | 1/1 | 0.40 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3534 | 1/1 | 0.36 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1740 | 1/1 | 0.18 | - | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3424 | 1/1 | 0.72 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3147 | 1/1 | 0.21 | - | 55,55,55,55 | 0 |
| 55 | MG | DA | 3483 | 1/1 | 0.19 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3301 | 1/1 | 0.34 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3475 | 1/1 | 0.40 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3211 | 1/1 | 0.47 | - | 39,39,39,39 | 0 |
| 55 | MG | BA | 3437 | 1/1 | 0.44 | - | 67,67,67,67 | 0 |
| 55 | MG | DA | 3329 | 1/1 | 0.36 | - | 44,44,44,44 | 0 |
| 55 | MG | CA | 1720 | 1/1 | 0.49 | - | 102,102,102,102 | 0 |
| 55 | MG | BA | 3186 | 1/1 | 0.41 | - | 36,36,36,36 | 0 |
| 55 | MG | BA | 3618 | 1/1 | 0.43 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3419 | 1/1 | 0.48 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3060 | 1/1 | 0.83 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3601 | 1/1 | 0.29 | - | 85,85,85,85 | 0 |
| 55 | MG | CA | 1645 | 1/1 | 0.22 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3521 | 1/1 | 0.62 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3096 | 1/1 | 0.53 | - | 56,56,56,56 | 0 |
| 55 | MG | DA | 3020 | 1/1 | 0.33 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3105 | 1/1 | 0.38 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3013 | 1/1 | 0.51 | - | 56,56,56,56 | 0 |
| 55 | MG | BA | 3101 | 1/1 | 0.65 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3134 | 1/1 | 0.32 | - | 72,72,72,72 | 0 |
| 55 | MG | AA | 1756 | 1/1 | 0.27 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3015 | 1/1 | 0.36 | - | 38,38,38,38 | 0 |
| 55 | MG | BA | 3434 | 1/1 | 0.55 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3243 | 1/1 | 0.55 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3285 | 1/1 | 0.26 | - | 50,50,50,50 | 0 |
| 55 | MG | BA | 3337 | 1/1 | 0.40 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3215 | 1/1 | 0.52 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3082 | 1/1 | 0.39 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3384 | 1/1 | 0.36 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1680 | 1/1 | 0.35 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3454 | 1/1 | 0.40 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3425 | 1/1 | 0.58 | - | 91,91,91,91 | 0 |
| 55 | MG | CC | 106 | 1/1 | 0.67 | - | 96,96,96,96 | 0 |
| 55 | MG | CN | 201 | 1/1 | 0.21 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3112 | 1/1 | 0.29 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3614 | 1/1 | 0.19 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3071 | 1/1 | 0.28 | - | 70,70,70,70 | 0 |
| 55 | MG | AA | 1751 | 1/1 | 0.39 | - | 98,98,98,98 | 0 |
| 55 | MG | CC | 108 | 1/1 | 0.55 | - | 106,106,106,106 | 0 |
| 55 | MG | BA | 3503 | 1/1 | 0.22 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | CA | 1655 | 1/1 | 0.37 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3525 | 1/1 | 0.35 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3540 | 1/1 | 0.29 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3353 | 1/1 | 0.77 | - | 93,93,93,93 | 0 |
| 55 | MG | BA | 3523 | 1/1 | 0.63 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3116 | 1/1 | 0.48 | - | 74,74,74,74 | 0 |
| 55 | MG | CA | 1764 | 1/1 | 0.54 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3233 | 1/1 | 0.42 | - | 52,52,52,52 | 0 |
| 55 | MG | DA | 3478 | 1/1 | 0.33 | - | 80,80,80,80 | 0 |
| 55 | MG | CA | 1796 | 1/1 | 0.48 | - | 102,102,102,102 | 0 |
| 55 | MG | DA | 3186 | 1/1 | 0.33 | - | 60,60,60,60 | 0 |
| 55 | MG | DA | 3514 | 1/1 | 0.64 | - | 59,59,59,59 | 0 |
| 55 | MG | DA | 3155 | 1/1 | 0.44 | - | 46,46,46,46 | 0 |
| 55 | MG | DA | 3056 | 1/1 | 0.40 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3396 | 1/1 | 0.33 | - | 82,82,82,82 | 0 |
| 55 | MG | BB | 215 | 1/1 | 0.33 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3320 | 1/1 | 0.29 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3586 | 1/1 | 0.38 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3510 | 1/1 | 0.27 | - | 108,108,108,108 | 0 |
| 55 | MG | CA | 1604 | 1/1 | 0.20 | - | 81,81,81,81 | 0 |
| 55 | MG | AA | 1716 | 1/1 | 0.24 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3258 | 1/1 | 0.27 | - | 45,45,45,45 | 0 |
| 55 | MG | AA | 1681 | 1/1 | 0.34 | - | 80,80,80,80 | 0 |
| 55 | MG | AB | 105 | 1/1 | 0.33 | - | 110,110,110,110 | 0 |
| 55 | MG | BA | 3369 | 1/1 | 0.37 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3371 | 1/1 | 0.38 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3331 | 1/1 | 0.40 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1636 | 1/1 | 0.31 | - | 87,87,87,87 | 0 |
| 55 | MG | AA | 1805 | 1/1 | 0.34 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3082 | 1/1 | 0.44 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3390 | 1/1 | 0.32 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3150 | 1/1 | 0.44 | - | 36,36,36,36 | 0 |
| 55 | MG | CA | 1724 | 1/1 | 0.51 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3449 | 1/1 | 0.46 | - | 80,80,80,80 | 0 |
| 55 | MG | AA | 1800 | 1/1 | 0.32 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3198 | 1/1 | 0.18 | - | 45,45,45,45 | 0 |
| 55 | MG | CA | 1705 | 1/1 | 0.49 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3461 | 1/1 | 0.27 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3345 | 1/1 | 0.39 | - | 64,64,64,64 | 0 |
| 55 | MG | AA | 1646 | 1/1 | 0.47 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3302 | 1/1 | 0.40 | - | 26,26,26,26 | 0 |
| 55 | MG | BA | 3533 | 1/1 | 0.56 | - | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3008 | 1/1 | 0.22 | - | 70,70,70,70 | 0 |
| 55 | MG | CA | 1800 | 1/1 | 0.36 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3571 | 1/1 | 0.43 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3322 | 1/1 | 0.53 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3222 | 1/1 | 0.41 | - | 89,89,89,89 | 0 |
| 55 | MG | CA | 1702 | 1/1 | 0.43 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3268 | 1/1 | 0.53 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3241 | 1/1 | 0.48 | - | 46,46,46,46 | 0 |
| 55 | MG | A1 | 101 | 1/1 | 0.16 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1609 | 1/1 | 0.41 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3348 | 1/1 | 0.63 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3317 | 1/1 | 0.75 | - | 89,89,89,89 | 0 |
| 55 | MG | CA | 1718 | 1/1 | 0.10 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3551 | 1/1 | 0.45 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3482 | 1/1 | 0.45 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3578 | 1/1 | 0.42 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3422 | 1/1 | 0.34 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3010 | 1/1 | 0.53 | - | 97,97,97,97 | 0 |
| 55 | MG | AA | 1629 | 1/1 | 0.14 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3455 | 1/1 | 0.31 | - | 69,69,69,69 | 0 |
| 55 | MG | CA | 1669 | 1/1 | 0.20 | - | 60,60,60,60 | 0 |
| 55 | MG | AB | 104 | 1/1 | 0.45 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3504 | 1/1 | 0.34 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3546 | 1/1 | 0.24 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3153 | 1/1 | 0.42 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3114 | 1/1 | 0.18 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3563 | 1/1 | 0.26 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3276 | 1/1 | 0.52 | - | 68,68,68,68 | 0 |
| 55 | MG | CA | 1675 | 1/1 | 0.45 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3305 | 1/1 | 0.41 | - | 70,70,70,70 | 0 |
| 55 | MG | CA | 1634 | 1/1 | 0.42 | - | 77,77,77,77 | 0 |
| 55 | MG | DE | 301 | 1/1 | 0.35 | - | 41,41,41,41 | 0 |
| 55 | MG | BA | 3442 | 1/1 | 0.38 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3170 | 1/1 | 0.49 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3140 | 1/1 | 0.38 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3150 | 1/1 | 0.33 | - | 68,68,68,68 | 0 |
| 55 | MG | AA | 1832 | 1/1 | 0.40 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3247 | 1/1 | 0.24 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3025 | 1/1 | 0.37 | - | 42,42,42,42 | 0 |
| 55 | MG | DA | 3110 | 1/1 | 0.32 | - | 58,58,58,58 | 0 |
| 55 | MG | CA | 1792 | 1/1 | 0.60 | - | 70,70,70,70 | 0 |
| 55 | MG | AA | 1738 | 1/1 | 0.59 | - | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3174 | 1/1 | 0.60 | - | 44,44,44,44 | 0 |
| 55 | MG | AA | 1767 | 1/1 | 0.20 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3031 | 1/1 | 0.38 | - | 33,33,33,33 | 0 |
| 55 | MG | DA | 3092 | 1/1 | 0.41 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3247 | 1/1 | 0.48 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3187 | 1/1 | 0.45 | - | 42,42,42,42 | 0 |
| 55 | MG | DA | 3190 | 1/1 | 0.58 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3412 | 1/1 | 0.48 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3253 | 1/1 | 0.24 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3615 | 1/1 | 0.41 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3487 | 1/1 | 0.22 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3119 | 1/1 | 0.39 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3622 | 1/1 | 0.48 | - | 59,59,59,59 | 0 |
| 55 | MG | AA | 1768 | 1/1 | 0.37 | - | 101,101,101,101 | 0 |
| 55 | MG | BU | 202 | 1/1 | 0.13 | - | 55,55,55,55 | 0 |
| 55 | MG | BA | 3274 | 1/1 | 0.16 | - | 46,46,46,46 | 0 |
| 55 | MG | AD | 101 | 1/1 | 0.38 | - | 101,101,101,101 | 0 |
| 55 | MG | CA | 1804 | 1/1 | 0.28 | - | 75,75,75,75 | 0 |
| 55 | MG | CA | 1717 | 1/1 | 0.22 | - | 106,106,106,106 | 0 |
| 55 | MG | BA | 3348 | 1/1 | 0.32 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3028 | 1/1 | 0.43 | - | 46,46,46,46 | 0 |
| 55 | MG | DA | 3457 | 1/1 | 0.80 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3078 | 1/1 | 0.38 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3323 | 1/1 | 0.32 | - | 66,66,66,66 | 0 |
| 55 | MG | CA | 1737 | 1/1 | 0.28 | - | 99,99,99,99 | 0 |
| 55 | MG | DA | 3375 | 1/1 | 0.86 | - | 88,88,88,88 | 0 |
| 55 | MG | D5 | 2001 | 1/1 | 0.37 | - | 46,46,46,46 | 0 |
| 55 | MG | BA | 3168 | 1/1 | 0.37 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3005 | 1/1 | 0.53 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3097 | 1/1 | 0.30 | - | 52,52,52,52 | 0 |
| 55 | MG | DA | 3316 | 1/1 | 0.36 | - | 61,61,61,61 | 0 |
| 55 | MG | AA | 1665 | 1/1 | 0.72 | - | 70,70,70,70 | 0 |
| 55 | MG | AA | 1712 | 1/1 | 0.38 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3166 | 1/1 | 0.44 | - | 58,58,58,58 | 0 |
| 55 | MG | DA | 3234 | 1/1 | 0.43 | - | 52,52,52,52 | 0 |
| 55 | MG | AA | 1702 | 1/1 | 0.23 | - | 93,93,93,93 | 0 |
| 55 | MG | BA | 3460 | 1/1 | 0.25 | - | 83,83,83,83 | 0 |
| 55 | MG | CA | 1686 | 1/1 | 0.43 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3206 | 1/1 | 0.43 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3524 | 1/1 | 0.31 | - | 105,105,105,105 | 0 |
| 55 | MG | AN | 202 | 1/1 | 0.38 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3335 | 1/1 | 0.38 | - | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1655 | 1/1 | 0.47 | - | 88,88,88,88 | 0 |
| 55 | MG | CA | 1700 | 1/1 | 0.53 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3050 | 1/1 | 0.68 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3462 | 1/1 | 0.33 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3290 | 1/1 | 0.45 | - | 97,97,97,97 | 0 |
| 55 | MG | DA | 3303 | 1/1 | 0.42 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3516 | 1/1 | 0.95 | - | 78,78,78,78 | 0 |
| 55 | MG | CA | 1644 | 1/1 | 0.32 | - | 120,120,120,120 | 0 |
| 55 | MG | CA | 1769 | 1/1 | 0.38 | - | 105,105,105,105 | 0 |
| 55 | MG | DA | 3374 | 1/1 | 0.43 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3244 | 1/1 | 0.34 | - | 58,58,58,58 | 0 |
| 55 | MG | AA | 1713 | 1/1 | 0.49 | - | 115,115,115,115 | 0 |
| 55 | MG | DA | 3063 | 1/1 | 0.54 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3519 | 1/1 | 0.30 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3176 | 1/1 | 0.62 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3105 | 1/1 | 0.35 | - | 45,45,45,45 | 0 |
| 55 | MG | DA | 3015 | 1/1 | 0.67 | - | 89,89,89,89 | 0 |
| 55 | MG | BA | 3064 | 1/1 | 0.28 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3473 | 1/1 | 0.51 | - | 96,96,96,96 | 0 |
| 55 | MG | DA | 3380 | 1/1 | 0.15 | - | 139,139,139,139 | 0 |
| 55 | MG | BA | 3526 | 1/1 | 0.45 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3095 | 1/1 | 0.40 | - | 49,49,49,49 | 0 |
| 55 | MG | CA | 1797 | 1/1 | 0.34 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3001 | 1/1 | 0.49 | - | 47,47,47,47 | 0 |
| 55 | MG | DA | 3510 | 1/1 | 0.42 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3355 | 1/1 | 0.60 | - | 46,46,46,46 | 0 |
| 55 | MG | BA | 3620 | 1/1 | 0.31 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3021 | 1/1 | 0.51 | - | 51,51,51,51 | 0 |
| 55 | MG | DA | 3018 | 1/1 | 0.31 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3161 | 1/1 | 0.45 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3300 | 1/1 | 0.45 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3132 | 1/1 | 0.34 | - | 53,53,53,53 | 0 |
| 55 | MG | CA | 1649 | 1/1 | 0.29 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3047 | 1/1 | 0.47 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3436 | 1/1 | 0.28 | - | 59,59,59,59 | 0 |
| 55 | MG | CA | 1651 | 1/1 | 0.38 | - | 90,90,90,90 | 0 |
| 55 | MG | DA | 3204 | 1/1 | 0.36 | - | 51,51,51,51 | 0 |
| 55 | MG | CA | 1693 | 1/1 | 0.52 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3200 | 1/1 | 0.44 | - | 44,44,44,44 | 0 |
| 55 | MG | BA | 3235 | 1/1 | 0.41 | - | 54,54,54,54 | 0 |
| 55 | MG | DA | 3226 | 1/1 | 0.43 | - | 62,62,62,62 | 0 |
| 55 | MG | AA | 1674 | 1/1 | 0.38 | - | 98,98,98,98 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3579 | 1/1 | 0.20 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3054 | 1/1 | 0.34 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3034 | 1/1 | 0.35 | - | 41,41,41,41 | 0 |
| 55 | MG | BA | 3428 | 1/1 | 0.41 | - | 68,68,68,68 | 0 |
| 55 | MG | CA | 1739 | 1/1 | 0.53 | - | 75,75,75,75 | 0 |
| 55 | MG | AA | 1766 | 1/1 | 0.18 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3467 | 1/1 | 0.42 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3195 | 1/1 | 0.81 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3583 | 1/1 | 0.20 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3505 | 1/1 | 0.55 | - | 96,96,96,96 | 0 |
| 55 | MG | AA | 1779 | 1/1 | 0.36 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3429 | 1/1 | 0.11 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3543 | 1/1 | 0.49 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3319 | 1/1 | 0.34 | - | 65,65,65,65 | 0 |
| 55 | MG | AC | 108 | 1/1 | 0.48 | - | 85,85,85,85 | 0 |
| 55 | MG | CA | 1659 | 1/1 | 0.21 | - | 110,110,110,110 | 0 |
| 55 | MG | BA | 3210 | 1/1 | 0.20 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3331 | 1/1 | 0.52 | - | 50,50,50,50 | 0 |
| 55 | MG | BA | 3575 | 1/1 | 0.37 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1697 | 1/1 | 0.27 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3268 | 1/1 | 0.57 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3012 | 1/1 | 0.30 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3482 | 1/1 | 0.48 | - | 57,57,57,57 | 0 |
| 55 | MG | CA | 1806 | 1/1 | 0.53 | - | 96,96,96,96 | 0 |
| 55 | MG | DA | 3383 | 1/1 | 0.51 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3271 | 1/1 | 0.50 | - | 58,58,58,58 | 0 |
| 55 | MG | BA | 3204 | 1/1 | 0.42 | - | 78,78,78,78 | 0 |
| 55 | MG | CA | 1665 | 1/1 | 0.23 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3271 | 1/1 | 0.19 | - | 35,35,35,35 | 0 |
| 55 | MG | CA | 1663 | 1/1 | 0.41 | - | 81,81,81,81 | 0 |
| 55 | MG | AA | 1688 | 1/1 | 0.28 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3354 | 1/1 | 0.26 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3192 | 1/1 | 0.34 | - | 34,34,34,34 | 0 |
| 55 | MG | DB | 208 | 1/1 | 0.27 | - | 90,90,90,90 | 0 |
| 55 | MG | DA | 3290 | 1/1 | 0.31 | - | 79,79,79,79 | 0 |
| 55 | MG | CA | 1664 | 1/1 | 0.29 | - | 99,99,99,99 | 0 |
| 55 | MG | DA | 3444 | 1/1 | 0.16 | - | 73,73,73,73 | 0 |
| 55 | MG | AA | 1645 | 1/1 | 0.48 | - | 50,50,50,50 | 0 |
| 55 | MG | BA | 3202 | 1/1 | 0.42 | - | 51,51,51,51 | 0 |
| 55 | MG | AA | 1614 | 1/1 | 0.26 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3034 | 1/1 | 0.34 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3372 | 1/1 | 0.33 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1648 | 1/1 | 0.53 | - | 78,78,78,78 | 0 |
| 55 | MG | AA | 1635 | 1/1 | 0.21 | - | 86,86,86,86 | 0 |
| 55 | MG | CA | 1617 | 1/1 | 0.28 | - | 93,93,93,93 | 0 |
| 55 | MG | BA | 3304 | 1/1 | 0.29 | - | 56,56,56,56 | 0 |
| 55 | MG | BA | 3474 | 1/1 | 0.48 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3493 | 1/1 | 0.38 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3245 | 1/1 | 0.55 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3019 | 1/1 | 0.46 | - | 66,66,66,66 | 0 |
| 55 | MG | CA | 1654 | 1/1 | 0.26 | - | 99,99,99,99 | 0 |
| 55 | MG | CA | 1775 | 1/1 | 0.39 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3151 | 1/1 | 0.28 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3549 | 1/1 | 0.29 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3527 | 1/1 | 0.59 | - | 93,93,93,93 | 0 |
| 55 | MG | CA | 1674 | 1/1 | 0.11 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3190 | 1/1 | 0.35 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3086 | 1/1 | 0.30 | - | 95,95,95,95 | 0 |
| 55 | MG | CA | 1725 | 1/1 | 0.22 | - | 86,86,86,86 | 0 |
| 55 | MG | AA | 1676 | 1/1 | 0.39 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3279 | 1/1 | 0.30 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3044 | 1/1 | 0.39 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3568 | 1/1 | 0.48 | - | 83,83,83,83 | 0 |
| 55 | MG | DA | 3363 | 1/1 | 0.77 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3324 | 1/1 | 0.27 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3414 | 1/1 | 0.19 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3489 | 1/1 | 0.27 | - | 70,70,70,70 | 0 |
| 55 | MG | AA | 1777 | 1/1 | 0.48 | - | 90,90,90,90 | 0 |
| 55 | MG | DA | 3089 | 1/1 | 0.55 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3461 | 1/1 | 0.27 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3357 | 1/1 | 0.39 | - | 96,96,96,96 | 0 |
| 55 | MG | DA | 3220 | 1/1 | 0.42 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1820 | 1/1 | 0.29 | - | 75,75,75,75 | 0 |
| 55 | MG | CA | 1692 | 1/1 | 0.52 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3182 | 1/1 | 0.79 | - | 44,44,44,44 | 0 |
| 55 | MG | DA | 3469 | 1/1 | 0.61 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3273 | 1/1 | 0.20 | - | 99,99,99,99 | 0 |
| 55 | MG | BA | 3212 | 1/1 | 0.61 | - | 43,43,43,43 | 0 |
| 55 | MG | BA | 3591 | 1/1 | 0.50 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3457 | 1/1 | 0.90 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3141 | 1/1 | 0.53 | - | 38,38,38,38 | 0 |
| 55 | MG | BA | 3481 | 1/1 | 0.60 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3045 | 1/1 | 0.60 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3439 | 1/1 | 0.33 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3466 | 1/1 | 0.51 | - | 97,97,97,97 | 0 |
| 55 | MG | DA | 3202 | 1/1 | 0.45 | - | 47,47,47,47 | 0 |
| 55 | MG | AA | 1667 | 1/1 | 0.32 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3262 | 1/1 | 0.56 | - | 33,33,33,33 | 0 |
| 55 | MG | BA | 3278 | 1/1 | 0.45 | - | 81,81,81,81 | 0 |
| 55 | MG | BE | 305 | 1/1 | 0.42 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3493 | 1/1 | 0.59 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3334 | 1/1 | 0.45 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3409 | 1/1 | 0.60 | - | 76,76,76,76 | 0 |
| 55 | MG | AA | 1719 | 1/1 | 0.57 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1728 | 1/1 | 0.22 | - | 108,108,108,108 | 0 |
| 55 | MG | DA | 3377 | 1/1 | 0.27 | - | 98,98,98,98 | 0 |
| 55 | MG | DA | 3036 | 1/1 | 0.25 | - | 99,99,99,99 | 0 |
| 55 | MG | AA | 1826 | 1/1 | 0.16 | - | 101,101,101,101 | 0 |
| 55 | MG | DA | 3443 | 1/1 | 0.43 | - | 80,80,80,80 | 0 |
| 55 | MG | AA | 1799 | 1/1 | 0.36 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3325 | 1/1 | 0.46 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3123 | 1/1 | 0.34 | - | 83,83,83,83 | 0 |
| 55 | MG | CA | 1698 | 1/1 | 0.09 | - | 107,107,107,107 | 0 |
| 55 | MG | CA | 1716 | 1/1 | 0.22 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3594 | 1/1 | 0.60 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3366 | 1/1 | 1.17 | - | 94,94,94,94 | 0 |
| 55 | MG | DB | 207 | 1/1 | 0.35 | - | 115,115,115,115 | 0 |
| 55 | MG | CA | 1641 | 1/1 | 0.28 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3226 | 1/1 | 0.43 | - | 50,50,50,50 | 0 |
| 55 | MG | BA | 3125 | 1/1 | 0.55 | - | 52,52,52,52 | 0 |
| 55 | MG | DA | 3498 | 1/1 | 0.27 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3434 | 1/1 | 0.13 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3474 | 1/1 | 0.54 | - | 83,83,83,83 | 0 |
| 55 | MG | AA | 1701 | 1/1 | 0.21 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3428 | 1/1 | 0.60 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3280 | 1/1 | 0.54 | - | 50,50,50,50 | 0 |
| 55 | MG | CA | 1784 | 1/1 | 0.20 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3240 | 1/1 | 0.54 | - | 42,42,42,42 | 0 |
| 55 | MG | CA | 1719 | 1/1 | 0.25 | - | 129,129,129,129 | 0 |
| 55 | MG | BA | 3138 | 1/1 | 0.47 | - | 46,46,46,46 | 0 |
| 55 | MG | DA | 3325 | 1/1 | 0.58 | - | 73,73,73,73 | 0 |
| 55 | MG | AA | 1601 | 1/1 | 0.35 | - | 56,56,56,56 | 0 |
| 55 | MG | AA | 1775 | 1/1 | 0.18 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3030 | 1/1 | 0.36 | - | 74,74,74,74 | 0 |
| 55 | MG | CA | 1612 | 1/1 | 0.45 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3577 | 1/1 | 0.19 | - | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3108 | 1/1 | 0.33 | - | 54,54,54,54 | 0 |
| 55 | MG | BA | 3246 | 1/1 | 0.43 | - | 68,68,68,68 | 0 |
| 55 | MG | AA | 1773 | 1/1 | 0.27 | - | 87,87,87,87 | 0 |
| 55 | MG | CA | 1687 | 1/1 | 0.24 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3022 | 1/1 | 0.57 | - | 60,60,60,60 | 0 |
| 55 | MG | AA | 1778 | 1/1 | 0.19 | - | 106,106,106,106 | 0 |
| 55 | MG | DA | 3275 | 1/1 | 0.37 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3121 | 1/1 | 0.20 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3494 | 1/1 | 0.76 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3188 | 1/1 | 0.36 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3589 | 1/1 | 0.33 | - | 41,41,41,41 | 0 |
| 55 | MG | AA | 1782 | 1/1 | 0.17 | - | 96,96,96,96 | 0 |
| 55 | MG | DA | 3355 | 1/1 | 0.54 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3088 | 1/1 | 0.27 | - | 96,96,96,96 | 0 |
| 55 | MG | CA | 1787 | 1/1 | 0.17 | - | 87,87,87,87 | 0 |
| 55 | MG | AA | 1616 | 1/1 | 0.19 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3131 | 1/1 | 0.23 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3587 | 1/1 | 0.33 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3448 | 1/1 | 0.48 | - | 100,100,100,100 | 0 |
| 55 | MG | AA | 1657 | 1/1 | 0.44 | - | 50,50,50,50 | 0 |
| 55 | MG | BA | 3435 | 1/1 | 0.33 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1801 | 1/1 | 0.54 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3158 | 1/1 | 0.62 | - | 44,44,44,44 | 0 |
| 55 | MG | AA | 1684 | 1/1 | 0.22 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3605 | 1/1 | 0.49 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3131 | 1/1 | 0.35 | - | 59,59,59,59 | 0 |
| 55 | MG | AA | 1823 | 1/1 | 0.52 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3042 | 1/1 | 0.57 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3090 | 1/1 | 0.48 | - | 49,49,49,49 | 0 |
| 55 | MG | BA | 3196 | 1/1 | 0.32 | - | 33,33,33,33 | 0 |
| 55 | MG | AA | 1714 | 1/1 | 0.40 | - | 107,107,107,107 | 0 |
| 55 | MG | BA | 3445 | 1/1 | 0.47 | - | 79,79,79,79 | 0 |
| 55 | MG | CA | 1760 | 1/1 | 0.26 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3252 | 1/1 | 0.47 | - | 67,67,67,67 | 0 |
| 55 | MG | DA | 3244 | 1/1 | 0.51 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3327 | 1/1 | 0.28 | - | 70,70,70,70 | 0 |
| 55 | MG | AA | 1741 | 1/1 | 0.32 | - | 67,67,67,67 | 0 |
| 55 | MG | CA | 1766 | 1/1 | 0.32 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3597 | 1/1 | 0.23 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3189 | 1/1 | 0.43 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3485 | 1/1 | 0.20 | - | 81,81,81,81 | 0 |
| 55 | MG | CC | 104 | 1/1 | 0.63 | - | 89,89,89,89 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3072 | 1/1 | 0.44 | - | 112,112,112,112 | 0 |
| 55 | MG | AA | 1695 | 1/1 | 0.27 | - | 90,90,90,90 | 0 |
| 55 | MG | AA | 1737 | 1/1 | 0.59 | - | 83,83,83,83 | 0 |
| 55 | MG | AA | 1678 | 1/1 | 0.38 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3391 | 1/1 | 0.45 | - | 86,86,86,86 | 0 |
| 55 | MG | AA | 1839 | 1/1 | 0.35 | - | 74,74,74,74 | 0 |
| 55 | MG | AA | 1707 | 1/1 | 0.60 | - | 50,50,50,50 | 0 |
| 55 | MG | AA | 1731 | 1/1 | 0.31 | - | 103,103,103,103 | 0 |
| 55 | MG | AA | 1620 | 1/1 | 0.27 | - | 66,66,66,66 | 0 |
| 55 | MG | DA | 3422 | 1/1 | 0.36 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3057 | 1/1 | 0.15 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3379 | 1/1 | 0.49 | - | 82,82,82,82 | 0 |
| 55 | MG | AA | 1781 | 1/1 | 0.44 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3229 | 1/1 | 0.47 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3187 | 1/1 | 0.49 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3288 | 1/1 | 0.49 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3165 | 1/1 | 0.59 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3607 | 1/1 | 0.38 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3277 | 1/1 | 0.31 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3450 | 1/1 | 0.17 | - | 54,54,54,54 | 0 |
| 55 | MG | DA | 3426 | 1/1 | 0.40 | - | 58,58,58,58 | 0 |
| 55 | MG | BA | 3585 | 1/1 | 0.34 | - | 60,60,60,60 | 0 |
| 55 | MG | CA | 1639 | 1/1 | 0.30 | - | 95,95,95,95 | 0 |
| 55 | MG | BA | 3060 | 1/1 | 0.16 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3283 | 1/1 | 0.43 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3368 | 1/1 | 0.34 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3339 | 1/1 | 0.67 | - | 88,88,88,88 | 0 |
| 55 | MG | CA | 1732 | 1/1 | 0.23 | - | 109,109,109,109 | 0 |
| 55 | MG | BA | 3612 | 1/1 | 0.53 | - | 66,66,66,66 | 0 |
| 55 | MG | DA | 3382 | 1/1 | 0.52 | - | 78,78,78,78 | 0 |
| 55 | MG | CA | 1795 | 1/1 | 0.33 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3536 | 1/1 | 0.67 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3028 | 1/1 | 0.30 | - | 101,101,101,101 | 0 |
| 55 | MG | DA | 3165 | 1/1 | 0.58 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3096 | 1/1 | 0.61 | - | 53,53,53,53 | 0 |
| 55 | MG | DA | 3342 | 1/1 | 0.43 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3347 | 1/1 | 0.11 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3569 | 1/1 | 0.59 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3448 | 1/1 | 0.69 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3014 | 1/1 | 0.48 | - | 53,53,53,53 | 0 |
| 55 | MG | DA | 3238 | 1/1 | 0.43 | - | 60,60,60,60 | 0 |
| 55 | MG | DA | 3526 | 1/1 | 0.32 | - | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3035 | 1/1 | 0.24 | - | 62,62,62,62 | 0 |
| 55 | MG | CA | 1742 | 1/1 | 0.18 | - | 97,97,97,97 | 0 |
| 55 | MG | CA | 1609 | 1/1 | 0.18 | - | 115,115,115,115 | 0 |
| 55 | MG | BA | 3350 | 1/1 | 0.27 | - | 55,55,55,55 | 0 |
| 55 | MG | BA | 3026 | 1/1 | 0.31 | - | 47,47,47,47 | 0 |
| 55 | MG | AA | 1606 | 1/1 | 0.08 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3237 | 1/1 | 0.22 | - | 83,83,83,83 | 0 |
| 55 | MG | DA | 3180 | 1/1 | 0.62 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3476 | 1/1 | 0.33 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1691 | 1/1 | 0.34 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3114 | 1/1 | 0.57 | - | 54,54,54,54 | 0 |
| 55 | MG | BA | 3438 | 1/1 | 0.45 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3077 | 1/1 | 0.15 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3243 | 1/1 | 0.49 | - | 48,48,48,48 | 0 |
| 55 | MG | DU | 201 | 1/1 | 0.16 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3402 | 1/1 | 0.40 | - | 101,101,101,101 | 0 |
| 55 | MG | CA | 1779 | 1/1 | 0.37 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3391 | 1/1 | 0.28 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3370 | 1/1 | 0.11 | - | 67,67,67,67 | 0 |
| 55 | MG | B2 | 201 | 1/1 | 0.46 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3144 | 1/1 | 0.31 | - | 48,48,48,48 | 0 |
| 55 | MG | DA | 3433 | 1/1 | 0.55 | - | 57,57,57,57 | 0 |
| 55 | MG | DA | 3252 | 1/1 | 0.36 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3395 | 1/1 | 0.26 | - | 72,72,72,72 | 0 |
| 55 | MG | AA | 1608 | 1/1 | 0.24 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3451 | 1/1 | 0.50 | - | 65,65,65,65 | 0 |
| 55 | MG | CA | 1602 | 1/1 | 0.33 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3447 | 1/1 | 0.48 | - | 71,71,71,71 | 0 |
| 55 | MG | BF | 302 | 1/1 | 0.21 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3463 | 1/1 | 0.26 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3123 | 1/1 | 0.21 | - | 51,51,51,51 | 0 |
| 55 | MG | CA | 1759 | 1/1 | 0.40 | - | 103,103,103,103 | 0 |
| 55 | MG | DA | 3145 | 1/1 | 0.53 | - | 60,60,60,60 | 0 |
| 55 | MG | CA | 1780 | 1/1 | 0.31 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3356 | 1/1 | 0.31 | - | 67,67,67,67 | 0 |
| 55 | MG | DA | 3091 | 1/1 | 0.36 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3208 | 1/1 | 0.10 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3143 | 1/1 | 0.68 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3452 | 1/1 | 0.42 | - | 41,41,41,41 | 0 |
| 55 | MG | CA | 1636 | 1/1 | 0.32 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3175 | 1/1 | 0.49 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3477 | 1/1 | 0.65 | - | 89,89,89,89 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3378 | 1/1 | 0.55 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3151 | 1/1 | 0.25 | - | 85,85,85,85 | 0 |
| 55 | MG | AA | 1723 | 1/1 | 0.33 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3025 | 1/1 | 1.41 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3162 | 1/1 | 0.30 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1729 | 1/1 | 0.44 | - | 113,113,113,113 | 0 |
| 55 | MG | BA | 3408 | 1/1 | 0.48 | - | 87,87,87,87 | 0 |
| 55 | MG | CA | 1626 | 1/1 | 0.19 | - | 93,93,93,93 | 0 |
| 55 | MG | DA | 3078 | 1/1 | 0.42 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3312 | 1/1 | 0.30 | - | 85,85,85,85 | 0 |
| 55 | MG | B8 | 101 | 1/1 | 0.19 | - | 97,97,97,97 | 0 |
| 55 | MG | AA | 1717 | 1/1 | 0.44 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3274 | 1/1 | 0.28 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3211 | 1/1 | 0.49 | - | 42,42,42,42 | 0 |
| 55 | MG | DA | 3142 | 1/1 | 0.52 | - | 40,40,40,40 | 0 |
| 55 | MG | BA | 3236 | 1/1 | 0.44 | - | 52,52,52,52 | 0 |
| 55 | MG | CA | 1763 | 1/1 | 0.50 | - | 91,91,91,91 | 0 |
| 55 | MG | CA | 1615 | 1/1 | 0.27 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3149 | 1/1 | 0.23 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3518 | 1/1 | 0.41 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3593 | 1/1 | 0.35 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3417 | 1/1 | 0.24 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3516 | 1/1 | 0.34 | - | 105,105,105,105 | 0 |
| 55 | MG | DA | 3489 | 1/1 | 0.19 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3304 | 1/1 | 0.39 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3511 | 1/1 | 0.42 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3133 | 1/1 | 0.31 | - | 66,66,66,66 | 0 |
| 55 | MG | CA | 1671 | 1/1 | 0.59 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3249 | 1/1 | 0.42 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3292 | 1/1 | 0.39 | - | 85,85,85,85 | 0 |
| 55 | MG | CA | 1640 | 1/1 | 0.34 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1638 | 1/1 | 0.32 | - | 101,101,101,101 | 0 |
| 55 | MG | AA | 1622 | 1/1 | 0.20 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3464 | 1/1 | 0.52 | - | 98,98,98,98 | 0 |
| 55 | MG | DA | 3152 | 1/1 | 0.13 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3218 | 1/1 | 0.55 | - | 48,48,48,48 | 0 |
| 55 | MG | DA | 3327 | 1/1 | 0.38 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3351 | 1/1 | 1.00 | - | 78,78,78,78 | 0 |
| 55 | MG | CA | 1647 | 1/1 | 0.52 | - | 61,61,61,61 | 0 |
| 55 | MG | AA | 1607 | 1/1 | 0.24 | - | 89,89,89,89 | 0 |
| 55 | MG | CA | 1614 | 1/1 | 0.42 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3146 | 1/1 | 0.38 | - | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3216 | 1/1 | 0.33 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3431 | 1/1 | 0.40 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3484 | 1/1 | 0.42 | - | 83,83,83,83 | 0 |
| 55 | MG | AA | 1630 | 1/1 | 0.15 | - | 101,101,101,101 | 0 |
| 55 | MG | BA | 3380 | 1/1 | 0.23 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3432 | 1/1 | 0.39 | - | 80,80,80,80 | 0 |
| 55 | MG | CA | 1696 | 1/1 | 0.39 | - | 91,91,91,91 | 0 |
| 55 | MG | CA | 1740 | 1/1 | 0.29 | - | 68,68,68,68 | 0 |
| 55 | MG | AA | 1734 | 1/1 | 0.27 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3389 | 1/1 | 0.27 | - | 59,59,59,59 | 0 |
| 55 | MG | BA | 3041 | 1/1 | 0.32 | - | 46,46,46,46 | 0 |
| 55 | MG | BA | 3353 | 1/1 | 0.45 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3364 | 1/1 | 0.47 | - | 82,82,82,82 | 0 |
| 55 | MG | AA | 1670 | 1/1 | 0.43 | - | 63,63,63,63 | 0 |
| 55 | MG | DB | 213 | 1/1 | 0.18 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3213 | 1/1 | 0.55 | - | 49,49,49,49 | 0 |
| 55 | MG | AA | 1816 | 1/1 | 0.23 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3201 | 1/1 | 0.25 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3063 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 55 | MG | BA | 3576 | 1/1 | 0.42 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3300 | 1/1 | 0.31 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3413 | 1/1 | 0.55 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3298 | 1/1 | 0.41 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3221 | 1/1 | 0.73 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3458 | 1/1 | 0.19 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3208 | 1/1 | 0.44 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3210 | 1/1 | 0.44 | - | 63,63,63,63 | 0 |
| 55 | MG | AA | 1611 | 1/1 | 0.23 | - | 92,92,92,92 | 0 |
| 55 | MG | CC | 102 | 1/1 | 0.48 | - | 73,73,73,73 | 0 |
| 55 | MG | CG | 302 | 1/1 | 0.16 | - | 101,101,101,101 | 0 |
| 55 | MG | DA | 3264 | 1/1 | 0.64 | - | 59,59,59,59 | 0 |
| 55 | MG | AA | 1602 | 1/1 | 0.28 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3103 | 1/1 | 0.35 | - | 50,50,50,50 | 0 |
| 55 | MG | BA | 3558 | 1/1 | 0.12 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3515 | 1/1 | 0.65 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3496 | 1/1 | 0.31 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3163 | 1/1 | 0.59 | - | 50,50,50,50 | 0 |
| 55 | MG | DA | 3346 | 1/1 | 0.51 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3386 | 1/1 | 0.52 | - | 61,61,61,61 | 0 |
| 55 | MG | DB | 210 | 1/1 | 0.39 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1838 | 1/1 | 0.36 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3017 | 1/1 | 0.39 | - | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3265 | 1/1 | 0.73 | - | 60,60,60,60 | 0 |
| 55 | MG | DA | 3037 | 1/1 | 0.22 | - | 98,98,98,98 | 0 |
| 55 | MG | DA | 3414 | 1/1 | 0.32 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3491 | 1/1 | 0.60 | - | 103,103,103,103 | 0 |
| 55 | MG | BA | 3117 | 1/1 | 0.49 | - | 60,60,60,60 | 0 |
| 55 | MG | AA | 1627 | 1/1 | 0.31 | - | 53,53,53,53 | 0 |
| 55 | MG | DA | 3064 | 1/1 | 0.58 | - | 101,101,101,101 | 0 |
| 55 | MG | DA | 3487 | 1/1 | 0.45 | - | 95,95,95,95 | 0 |
| 55 | MG | CA | 1652 | 1/1 | 0.34 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1798 | 1/1 | 0.24 | - | 58,58,58,58 | 0 |
| 55 | MG | DA | 3027 | 1/1 | 0.21 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3200 | 1/1 | 0.42 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3069 | 1/1 | 0.40 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3545 | 1/1 | 0.35 | - | 69,69,69,69 | 0 |
| 55 | MG | CA | 1709 | 1/1 | 0.53 | - | 108,108,108,108 | 0 |
| 55 | MG | AA | 1610 | 1/1 | 0.50 | - | 51,51,51,51 | 0 |
| 55 | MG | BA | 3038 | 1/1 | 0.40 | - | 56,56,56,56 | 0 |
| 55 | MG | CA | 1657 | 1/1 | 0.30 | - | 95,95,95,95 | 0 |
| 55 | MG | AC | 105 | 1/1 | 0.48 | - | 93,93,93,93 | 0 |
| 55 | MG | DA | 3407 | 1/1 | 0.45 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3044 | 1/1 | 0.29 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3182 | 1/1 | 0.31 | - | 43,43,43,43 | 0 |
| 55 | MG | BA | 3107 | 1/1 | 0.42 | - | 36,36,36,36 | 0 |
| 55 | MG | BA | 3453 | 1/1 | 0.59 | - | 60,60,60,60 | 0 |
| 55 | MG | AA | 1748 | 1/1 | 0.39 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3352 | 1/1 | 0.66 | - | 64,64,64,64 | 0 |
| 55 | MG | AA | 1818 | 1/1 | 0.60 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3299 | 1/1 | 0.54 | - | 89,89,89,89 | 0 |
| 55 | MG | BA | 3307 | 1/1 | 0.46 | - | 39,39,39,39 | 0 |
| 55 | MG | BA | 3237 | 1/1 | 0.52 | - | 57,57,57,57 | 0 |
| 55 | MG | AA | 1827 | 1/1 | 0.34 | - | 87,87,87,87 | 0 |
| 55 | MG | CA | 1721 | 1/1 | 0.24 | - | 80,80,80,80 | 0 |
| 55 | MG | CA | 1803 | 1/1 | 0.33 | - | 96,96,96,96 | 0 |
| 56 | ZN | CQ | 101 | 1/1 | 0.11 | - | 120,120,120,120 | 0 |
| 55 | MG | BA | 3067 | 1/1 | 0.21 | - | 48,48,48,48 | 0 |
| 55 | MG | DA | 3094 | 1/1 | 0.29 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3467 | 1/1 | 0.35 | - | 78,78,78,78 | 0 |
| 55 | MG | D1 | 201 | 1/1 | 0.44 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3309 | 1/1 | 0.23 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3124 | 1/1 | 0.53 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3517 | 1/1 | 0.55 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3509 | 1/1 | 0.41 | - | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1617 | 1/1 | 0.52 | - | 69,69,69,69 | 0 |
| 55 | MG | BB | 213 | 1/1 | 0.47 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3532 | 1/1 | 0.22 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3177 | 1/1 | 0.52 | - | 57,57,57,57 | 0 |
| 55 | MG | BB | 211 | 1/1 | 0.37 | - | 92,92,92,92 | 0 |
| 55 | MG | D1 | 202 | 1/1 | 0.42 | - | 89,89,89,89 | 0 |
| 55 | MG | AA | 1743 | 1/1 | 0.13 | - | 107,107,107,107 | 0 |
| 55 | MG | BA | 3282 | 1/1 | 0.12 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3209 | 1/1 | 0.49 | - | 39,39,39,39 | 0 |
| 55 | MG | BA | 3242 | 1/1 | 0.45 | - | 50,50,50,50 | 0 |
| 55 | MG | AA | 1783 | 1/1 | 0.61 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3318 | 1/1 | 0.55 | - | 75,75,75,75 | 0 |
| 55 | MG | CA | 1601 | 1/1 | 0.32 | - | 96,96,96,96 | 0 |
| 55 | MG | AC | 109 | 1/1 | 0.39 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3106 | 1/1 | 0.40 | - | 48,48,48,48 | 0 |
| 55 | MG | AA | 1615 | 1/1 | 0.65 | - | 105,105,105,105 | 0 |
| 55 | MG | DA | 3135 | 1/1 | 0.40 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3041 | 1/1 | 0.47 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3421 | 1/1 | 0.37 | - | 62,62,62,62 | 0 |
| 55 | MG | CA | 1799 | 1/1 | 0.34 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3479 | 1/1 | 0.50 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3213 | 1/1 | 0.47 | - | 41,41,41,41 | 0 |
| 55 | MG | BA | 3048 | 1/1 | 0.57 | - | 77,77,77,77 | 0 |
| 55 | MG | CA | 1689 | 1/1 | 0.32 | - | 89,89,89,89 | 0 |
| 55 | MG | AA | 1715 | 1/1 | 0.32 | - | 115,115,115,115 | 0 |
| 55 | MG | CA | 1701 | 1/1 | 0.40 | - | 88,88,88,88 | 0 |
| 55 | MG | AA | 1730 | 1/1 | 0.37 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3259 | 1/1 | 0.26 | - | 40,40,40,40 | 0 |
| 55 | MG | BA | 3424 | 1/1 | 0.64 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3497 | 1/1 | 0.24 | - | 71,71,71,71 | 0 |
| 55 | MG | CA | 1733 | 1/1 | 0.44 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3209 | 1/1 | 0.49 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1746 | 1/1 | 0.47 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3427 | 1/1 | 0.32 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3495 | 1/1 | 0.34 | - | 123,123,123,123 | 0 |
| 55 | MG | AA | 1694 | 1/1 | 0.14 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3456 | 1/1 | 0.43 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3359 | 1/1 | 0.49 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3116 | 1/1 | 0.36 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3004 | 1/1 | 0.51 | - | 99,99,99,99 | 0 |
| 55 | MG | BA | 3161 | 1/1 | 0.25 | - | 56,56,56,56 | 0 |
| 55 | MG | DA | 3296 | 1/1 | 0.64 | - | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3272 | 1/1 | 0.21 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3341 | 1/1 | 0.53 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3330 | 1/1 | 0.33 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3120 | 1/1 | 0.30 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3076 | 1/1 | 0.34 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3205 | 1/1 | 0.52 | - | 67,67,67,67 | 0 |
| 55 | MG | B3 | 101 | 1/1 | 0.55 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3154 | 1/1 | 0.34 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3352 | 1/1 | 0.38 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3228 | 1/1 | 0.63 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3272 | 1/1 | 0.28 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3251 | 1/1 | 0.44 | - | 68,68,68,68 | 0 |
| 55 | MG | DB | 202 | 1/1 | 0.20 | - | 98,98,98,98 | 0 |
| 55 | MG | BA | 3127 | 1/1 | 0.59 | - | 53,53,53,53 | 0 |
| 55 | MG | BA | 3199 | 1/1 | 0.44 | - | 49,49,49,49 | 0 |
| 55 | MG | BA | 3126 | 1/1 | 0.42 | - | 46,46,46,46 | 0 |
| 55 | MG | BA | 3455 | 1/1 | 0.27 | - | 76,76,76,76 | 0 |
| 55 | MG | AA | 1791 | 1/1 | 0.15 | - | 109,109,109,109 | 0 |
| 55 | MG | BA | 3553 | 1/1 | 0.31 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3194 | 1/1 | 0.45 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3283 | 1/1 | 0.37 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3385 | 1/1 | 0.71 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3148 | 1/1 | 0.48 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3311 | 1/1 | 0.42 | - | 83,83,83,83 | 0 |
| 55 | MG | CA | 1668 | 1/1 | 0.42 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3498 | 1/1 | 0.44 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3345 | 1/1 | 0.71 | - | 73,73,73,73 | 0 |
| 55 | MG | D3 | 101 | 1/1 | 0.46 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1696 | 1/1 | 0.26 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3436 | 1/1 | 0.43 | - | 98,98,98,98 | 0 |
| 55 | MG | DA | 3405 | 1/1 | 0.40 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1771 | 1/1 | 0.11 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3502 | 1/1 | 0.23 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3021 | 1/1 | 0.51 | - | 41,41,41,41 | 0 |
| 55 | MG | CA | 1681 | 1/1 | 0.55 | - | 72,72,72,72 | 0 |
| 55 | MG | CA | 1642 | 1/1 | 0.28 | - | 91,91,91,91 | 0 |
| 55 | MG | CA | 1753 | 1/1 | 0.33 | - | 123,123,123,123 | 0 |
| 55 | MG | BA | 3004 | 1/1 | 0.44 | - | 35,35,35,35 | 0 |
| 55 | MG | BA | 3316 | 1/1 | 0.49 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3346 | 1/1 | 0.38 | - | 51,51,51,51 | 0 |
| 55 | MG | DA | 3503 | 1/1 | 0.66 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3468 | 1/1 | 0.34 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | CA | 1743 | 1/1 | 0.50 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3606 | 1/1 | 0.37 | - | 77,77,77,77 | 0 |
| 55 | MG | AA | 1769 | 1/1 | 0.19 | - | 104,104,104,104 | 0 |
| 55 | MG | AA | 1628 | 1/1 | 0.37 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3476 | 1/1 | 0.38 | - | 107,107,107,107 | 0 |
| 55 | MG | DB | 205 | 1/1 | 0.39 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3087 | 1/1 | 0.50 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3358 | 1/1 | 0.36 | - | 74,74,74,74 | 0 |
| 55 | MG | CA | 1715 | 1/1 | 0.30 | - | 104,104,104,104 | 0 |
| 55 | MG | DA | 3230 | 1/1 | 0.17 | - | 59,59,59,59 | 0 |
| 55 | MG | DA | 3048 | 1/1 | 0.54 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3018 | 1/1 | 0.34 | - | 54,54,54,54 | 0 |
| 55 | MG | DA | 3361 | 1/1 | 0.71 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3514 | 1/1 | 0.33 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3073 | 1/1 | 0.43 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3480 | 1/1 | 0.53 | - | 50,50,50,50 | 0 |
| 55 | MG | BF | 303 | 1/1 | 0.41 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3399 | 1/1 | 0.63 | - | 90,90,90,90 | 0 |
| 55 | MG | AA | 1700 | 1/1 | 0.20 | - | 99,99,99,99 | 0 |
| 55 | MG | DA | 3267 | 1/1 | 0.38 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3019 | 1/1 | 0.94 | - | 90,90,90,90 | 0 |
| 55 | MG | CA | 1707 | 1/1 | 0.60 | - | 98,98,98,98 | 0 |
| 55 | MG | DA | 3172 | 1/1 | 0.28 | - | 88,88,88,88 | 0 |
| 55 | MG | CA | 1736 | 1/1 | 0.82 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1641 | 1/1 | 0.37 | - | 57,57,57,57 | 0 |
| 55 | MG | DA | 3012 | 1/1 | 0.48 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1691 | 1/1 | 0.50 | - | 50,50,50,50 | 0 |
| 55 | MG | DA | 3007 | 1/1 | 0.35 | - | 74,74,74,74 | 0 |
| 55 | MG | DB | 214 | 1/1 | 0.17 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3270 | 1/1 | 0.20 | - | 76,76,76,76 | 0 |
| 55 | MG | CA | 1662 | 1/1 | 0.26 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3500 | 1/1 | 0.28 | - | 97,97,97,97 | 0 |
| 55 | MG | DA | 3343 | 1/1 | 0.46 | - | 95,95,95,95 | 0 |
| 55 | MG | AA | 1785 | 1/1 | 0.43 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3486 | 1/1 | 0.48 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3440 | 1/1 | 0.48 | - | 74,74,74,74 | 0 |
| 55 | MG | CA | 1710 | 1/1 | 0.28 | - | 106,106,106,106 | 0 |
| 55 | MG | BA | 3600 | 1/1 | 0.41 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3373 | 1/1 | 0.50 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3104 | 1/1 | 0.41 | - | 43,43,43,43 | 0 |
| 55 | MG | DA | 3101 | 1/1 | 0.34 | - | 43,43,43,43 | 0 |
| 55 | MG | CA | 1734 | 1/1 | 0.24 | - | 93,93,93,93 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3333 | 1/1 | 0.58 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3513 | 1/1 | 0.44 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3349 | 1/1 | 0.44 | - | 97,97,97,97 | 0 |
| 55 | MG | BA | 3170 | 1/1 | 0.50 | - | 55,55,55,55 | 0 |
| 55 | MG | BA | 3184 | 1/1 | 0.23 | - | 39,39,39,39 | 0 |
| 55 | MG | BA | 3397 | 1/1 | 0.30 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3289 | 1/1 | 0.48 | - | 90,90,90,90 | 0 |
| 55 | MG | B0 | 201 | 1/1 | 0.32 | - | 51,51,51,51 | 0 |
| 55 | MG | AA | 1808 | 1/1 | 0.62 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3291 | 1/1 | 0.57 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3023 | 1/1 | 0.36 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3531 | 1/1 | 0.32 | - | 53,53,53,53 | 0 |
| 55 | MG | AA | 1677 | 1/1 | 0.33 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3522 | 1/1 | 0.53 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3420 | 1/1 | 0.33 | - | 67,67,67,67 | 0 |
| 55 | MG | AA | 1837 | 1/1 | 0.50 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3179 | 1/1 | 0.31 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3350 | 1/1 | 0.29 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3001 | 1/1 | 0.48 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3383 | 1/1 | 0.21 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3469 | 1/1 | 0.27 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3191 | 1/1 | 0.21 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3156 | 1/1 | 0.68 | - | 48,48,48,48 | 0 |
| 55 | MG | AA | 1693 | 1/1 | 0.17 | - | 87,87,87,87 | 0 |
| 55 | MG | CA | 1712 | 1/1 | 0.56 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3259 | 1/1 | 0.28 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3281 | 1/1 | 0.84 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3239 | 1/1 | 0.31 | - | 45,45,45,45 | 0 |
| 55 | MG | CA | 1699 | 1/1 | 0.15 | - | 97,97,97,97 | 0 |
| 55 | MG | AA | 1762 | 1/1 | 0.27 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3362 | 1/1 | 0.61 | - | 53,53,53,53 | 0 |
| 55 | MG | DA | 3153 | 1/1 | 0.36 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3130 | 1/1 | 0.46 | - | 44,44,44,44 | 0 |
| 55 | MG | BA | 3217 | 1/1 | 0.29 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3604 | 1/1 | 0.17 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3291 | 1/1 | 0.44 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3515 | 1/1 | 0.21 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3058 | 1/1 | 0.34 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3084 | 1/1 | 0.54 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3423 | 1/1 | 0.91 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3071 | 1/1 | 0.31 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1648 | 1/1 | 0.44 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3370 | 1/1 | 0.46 | - | 56,56,56,56 | 0 |
| 55 | MG | AA | 1811 | 1/1 | 0.51 | - | 67,67,67,67 | 0 |
| 55 | MG | DA | 3286 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3214 | 1/1 | 0.69 | - | 67,67,67,67 | 0 |
| 55 | MG | DA | 3425 | 1/1 | 0.28 | - | 81,81,81,81 | 0 |
| 55 | MG | AA | 1784 | 1/1 | 0.47 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1637 | 1/1 | 0.23 | - | 98,98,98,98 | 0 |
| 55 | MG | AA | 1831 | 1/1 | 0.51 | - | 90,90,90,90 | 0 |
| 55 | MG | DB | 209 | 1/1 | 0.16 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3207 | 1/1 | 0.54 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3072 | 1/1 | 0.35 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3282 | 1/1 | 0.43 | - | 69,69,69,69 | 0 |
| 55 | MG | CA | 1704 | 1/1 | 0.33 | - | 99,99,99,99 | 0 |
| 55 | MG | CA | 1790 | 1/1 | 0.26 | - | 110,110,110,110 | 0 |
| 55 | MG | DA | 3039 | 1/1 | 0.45 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3166 | 1/1 | 0.64 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3189 | 1/1 | 0.49 | - | 41,41,41,41 | 0 |
| 55 | MG | BA | 3566 | 1/1 | 0.37 | - | 88,88,88,88 | 0 |
| 55 | MG | CA | 1683 | 1/1 | 0.34 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3254 | 1/1 | 0.54 | - | 50,50,50,50 | 0 |
| 55 | MG | AA | 1759 | 1/1 | 0.34 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3335 | 1/1 | 0.26 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3142 | 1/1 | 0.39 | - | 51,51,51,51 | 0 |
| 55 | MG | CA | 1611 | 1/1 | 0.87 | - | 93,93,93,93 | 0 |
| 55 | MG | AA | 1788 | 1/1 | 0.51 | - | 77,77,77,77 | 0 |
| 55 | MG | CA | 1622 | 1/1 | 0.33 | - | 95,95,95,95 | 0 |
| 55 | MG | BA | 3239 | 1/1 | 0.31 | - | 74,74,74,74 | 0 |
| 55 | MG | AN | 201 | 1/1 | 0.20 | - | 68,68,68,68 | 0 |
| 55 | MG | B5 | 101 | 1/1 | 0.31 | - | 45,45,45,45 | 0 |
| 55 | MG | DA | 3315 | 1/1 | 0.35 | - | 108,108,108,108 | 0 |
| 55 | MG | DA | 3075 | 1/1 | 0.36 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1817 | 1/1 | 0.22 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3512 | 1/1 | 0.51 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3016 | 1/1 | 0.47 | - | 78,78,78,78 | 0 |
| 55 | MG | CA | 1735 | 1/1 | 0.21 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3003 | 1/1 | 0.36 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3013 | 1/1 | 0.43 | - | 34,34,34,34 | 0 |
| 55 | MG | DA | 3294 | 1/1 | 0.32 | - | 64,64,64,64 | 0 |
| 55 | MG | CA | 1637 | 1/1 | 0.34 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1618 | 1/1 | 0.29 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3419 | 1/1 | 0.53 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3221 | 1/1 | 0.41 | - | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3396 | 1/1 | 0.23 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3535 | 1/1 | 0.46 | - | 80,80,80,80 | 0 |
| 55 | MG | CA | 1629 | 1/1 | 0.19 | - | 98,98,98,98 | 0 |
| 55 | MG | DA | 3093 | 1/1 | 0.38 | - | 80,80,80,80 | 0 |
| 55 | MG | CA | 1676 | 1/1 | 0.46 | - | 55,55,55,55 | 0 |
| 55 | MG | DA | 3051 | 1/1 | 0.27 | - | 85,85,85,85 | 0 |
| 55 | MG | CA | 1643 | 1/1 | 0.58 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3256 | 1/1 | 0.40 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3009 | 1/1 | 0.33 | - | 36,36,36,36 | 0 |
| 55 | MG | BA | 3361 | 1/1 | 0.42 | - | 64,64,64,64 | 0 |
| 55 | MG | CA | 1620 | 1/1 | 0.49 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3181 | 1/1 | 0.34 | - | 39,39,39,39 | 0 |
| 55 | MG | CA | 1771 | 1/1 | 0.43 | - | 76,76,76,76 | 0 |
| 55 | MG | CA | 1793 | 1/1 | 0.41 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3408 | 1/1 | 0.15 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3356 | 1/1 | 0.48 | - | 70,70,70,70 | 0 |
| 55 | MG | AA | 1772 | 1/1 | 0.60 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3281 | 1/1 | 0.56 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3040 | 1/1 | 0.41 | - | 54,54,54,54 | 0 |
| 55 | MG | DA | 3441 | 1/1 | 0.10 | - | 137,137,137,137 | 0 |
| 55 | MG | DA | 3468 | 1/1 | 0.51 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3091 | 1/1 | 0.55 | - | 35,35,35,35 | 0 |
| 55 | MG | AA | 1833 | 1/1 | 0.50 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3137 | 1/1 | 0.37 | - | 47,47,47,47 | 0 |
| 55 | MG | AB | 101 | 1/1 | 0.29 | - | 90,90,90,90 | 0 |
| 55 | MG | AA | 1679 | 1/1 | 0.36 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3070 | 1/1 | 0.12 | - | 63,63,63,63 | 0 |
| 55 | MG | CA | 1738 | 1/1 | 0.43 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3317 | 1/1 | 0.27 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3599 | 1/1 | 0.49 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3465 | 1/1 | 0.37 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3293 | 1/1 | 0.55 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3429 | 1/1 | 0.40 | - | 99,99,99,99 | 0 |
| 55 | MG | CA | 1755 | 1/1 | 0.55 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3517 | 1/1 | 0.49 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3488 | 1/1 | 0.43 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3344 | 1/1 | 0.39 | - | 55,55,55,55 | 0 |
| 55 | MG | BA | 3266 | 1/1 | 0.43 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3417 | 1/1 | 0.30 | - | 99,99,99,99 | 0 |
| 55 | MG | DA | 3379 | 1/1 | 0.39 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3310 | 1/1 | 0.50 | - | 71,71,71,71 | 0 |
| 55 | MG | AC | 102 | 1/1 | 0.67 | - | 93,93,93,93 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BB | 210 | 1/1 | 0.44 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3099 | 1/1 | 0.55 | - | 67,67,67,67 | 0 |
| 55 | MG | AA | 1803 | 1/1 | 0.42 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3197 | 1/1 | 0.52 | - | 46,46,46,46 | 0 |
| 55 | MG | DA | 3169 | 1/1 | 0.32 | - | 69,69,69,69 | 0 |
| 55 | MG | AB | 103 | 1/1 | 0.47 | - | 111,111,111,111 | 0 |
| 55 | MG | BA | 3357 | 1/1 | 0.53 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3169 | 1/1 | 0.63 | - | 63,63,63,63 | 0 |
| 55 | MG | BE | 301 | 1/1 | 0.34 | - | 59,59,59,59 | 0 |
| 55 | MG | AA | 1666 | 1/1 | 0.50 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3308 | 1/1 | 0.35 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3118 | 1/1 | 0.44 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3403 | 1/1 | 0.50 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3402 | 1/1 | 0.38 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3332 | 1/1 | 0.47 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3544 | 1/1 | 0.43 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3520 | 1/1 | 0.48 | - | 44,44,44,44 | 0 |
| 55 | MG | DA | 3319 | 1/1 | 0.42 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3027 | 1/1 | 0.54 | - | 36,36,36,36 | 0 |
| 55 | MG | BA | 3047 | 1/1 | 0.47 | - | 74,74,74,74 | 0 |
| 55 | MG | AA | 1699 | 1/1 | 0.23 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3098 | 1/1 | 0.47 | - | 68,68,68,68 | 0 |
| 55 | MG | CA | 1801 | 1/1 | 0.32 | - | 89,89,89,89 | 0 |
| 55 | MG | AC | 106 | 1/1 | 0.60 | - | 89,89,89,89 | 0 |
| 55 | MG | CA | 1782 | 1/1 | 0.41 | - | 93,93,93,93 | 0 |
| 55 | MG | CA | 1783 | 1/1 | 0.49 | - | 100,100,100,100 | 0 |
| 55 | MG | BA | 3128 | 1/1 | 0.50 | - | 46,46,46,46 | 0 |
| 55 | MG | DA | 3292 | 1/1 | 0.26 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3471 | 1/1 | 0.51 | - | 80,80,80,80 | 0 |
| 55 | MG | AA | 1757 | 1/1 | 0.10 | - | 110,110,110,110 | 0 |
| 55 | MG | DA | 3026 | 1/1 | 0.50 | - | 95,95,95,95 | 0 |
| 55 | MG | BA | 3167 | 1/1 | 0.40 | - | 73,73,73,73 | 0 |
| 55 | MG | CA | 1713 | 1/1 | 0.64 | - | 102,102,102,102 | 0 |
| 55 | MG | CA | 1749 | 1/1 | 0.29 | - | 89,89,89,89 | 0 |
| 55 | MG | BA | 3087 | 1/1 | 0.34 | - | 77,77,77,77 | 0 |
| 55 | MG | AA | 1647 | 1/1 | 0.47 | - | 88,88,88,88 | 0 |
| 55 | MG | AA | 1672 | 1/1 | 0.46 | - | 87,87,87,87 | 0 |
| 55 | MG | AA | 1668 | 1/1 | 0.64 | - | 76,76,76,76 | 0 |
| 55 | MG | AA | 1626 | 1/1 | 0.47 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3596 | 1/1 | 0.57 | - | 55,55,55,55 | 0 |
| 55 | MG | DA | 3040 | 1/1 | 0.20 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1603 | 1/1 | 0.39 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3344 | 1/1 | 0.37 | - | 95,95,95,95 | 0 |
| 55 | MG | DA | 3337 | 1/1 | 0.51 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3288 | 1/1 | 0.37 | - | 47,47,47,47 | 0 |
| 55 | MG | DA | 3389 | 1/1 | 0.79 | - | 64,64,64,64 | 0 |
| 55 | MG | BA | 3573 | 1/1 | 0.55 | - | 83,83,83,83 | 0 |
| 55 | MG | CA | 1754 | 1/1 | 0.34 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3248 | 1/1 | 0.53 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3440 | 1/1 | 0.49 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3386 | 1/1 | 0.53 | - | 59,59,59,59 | 0 |
| 55 | MG | DB | 206 | 1/1 | 0.31 | - | 90,90,90,90 | 0 |
| 55 | MG | DA | 3090 | 1/1 | 0.39 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3094 | 1/1 | 0.60 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3178 | 1/1 | 0.35 | - | 36,36,36,36 | 0 |
| 55 | MG | BA | 3588 | 1/1 | 0.36 | - | 83,83,83,83 | 0 |
| 55 | MG | AA | 1698 | 1/1 | 0.29 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3427 | 1/1 | 0.39 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3465 | 1/1 | 0.47 | - | 93,93,93,93 | 0 |
| 55 | MG | DA | 3043 | 1/1 | 0.28 | - | 82,82,82,82 | 0 |
| 55 | MG | CA | 1695 | 1/1 | 0.51 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3229 | 1/1 | 0.15 | - | 50,50,50,50 | 0 |
| 55 | MG | BA | 3129 | 1/1 | 0.47 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3036 | 1/1 | 0.56 | - | 44,44,44,44 | 0 |
| 55 | MG | BA | 3219 | 1/1 | 0.50 | - | 76,76,76,76 | 0 |
| 55 | MG | AA | 1625 | 1/1 | 0.44 | - | 57,57,57,57 | 0 |
| 55 | MG | AA | 1830 | 1/1 | 0.31 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3049 | 1/1 | 0.42 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3459 | 1/1 | 0.45 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3623 | 1/1 | 0.41 | - | 60,60,60,60 | 0 |
| 55 | MG | AA | 1787 | 1/1 | 0.48 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3557 | 1/1 | 0.47 | - | 77,77,77,77 | 0 |
| 55 | MG | DE | 302 | 1/1 | 0.27 | - | 65,65,65,65 | 0 |
| 55 | MG | CA | 1746 | 1/1 | 0.64 | - | 57,57,57,57 | 0 |
| 55 | MG | BA | 3562 | 1/1 | 0.35 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3441 | 1/1 | 0.15 | - | 86,86,86,86 | 0 |
| 55 | MG | DB | 204 | 1/1 | 0.23 | - | 82,82,82,82 | 0 |
| 55 | MG | BB | 217 | 1/1 | 0.16 | - | 98,98,98,98 | 0 |
| 55 | MG | AA | 1705 | 1/1 | 0.29 | - | 83,83,83,83 | 0 |
| 55 | MG | DA | 3432 | 1/1 | 0.34 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3069 | 1/1 | 0.49 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3264 | 1/1 | 0.22 | - | 30,30,30,30 | 0 |
| 55 | MG | BA | 3286 | 1/1 | 0.34 | - | 66,66,66,66 | 0 |
| 55 | MG | DA | 3406 | 1/1 | 0.78 | - | 86,86,86,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BB | 201 | 1/1 | 0.49 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3227 | 1/1 | 0.41 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3038 | 1/1 | 0.56 | - | 97,97,97,97 | 0 |
| 55 | MG | DA | 3076 | 1/1 | 0.45 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3163 | 1/1 | 0.56 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3494 | 1/1 | 0.28 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3378 | 1/1 | 0.50 | - | 63,63,63,63 | 0 |
| 55 | MG | CA | 1646 | 1/1 | 0.36 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3478 | 1/1 | 0.25 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3206 | 1/1 | 0.49 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1770 | 1/1 | 0.32 | - | 102,102,102,102 | 0 |
| 55 | MG | DB | 203 | 1/1 | 0.35 | - | 66,66,66,66 | 0 |
| 55 | MG | DA | 3305 | 1/1 | 0.34 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3326 | 1/1 | 0.34 | - | 52,52,52,52 | 0 |
| 55 | MG | DA | 3192 | 1/1 | 0.48 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3251 | 1/1 | 0.31 | - | 74,74,74,74 | 0 |
| 55 | MG | BB | 202 | 1/1 | 0.16 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3471 | 1/1 | 0.34 | - | 72,72,72,72 | 0 |
| 55 | MG | CA | 1684 | 1/1 | 0.59 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3621 | 1/1 | 0.17 | - | 63,63,63,63 | 0 |
| 55 | MG | AA | 1727 | 1/1 | 0.91 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3228 | 1/1 | 0.46 | - | 44,44,44,44 | 0 |
| 55 | MG | DA | 3137 | 1/1 | 0.28 | - | 82,82,82,82 | 0 |
| 55 | MG | AA | 1819 | 1/1 | 0.34 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3309 | 1/1 | 0.29 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3062 | 1/1 | 0.27 | - | 56,56,56,56 | 0 |
| 55 | MG | BA | 3176 | 1/1 | 0.49 | - | 48,48,48,48 | 0 |
| 55 | MG | BA | 3496 | 1/1 | 0.30 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3005 | 1/1 | 0.47 | - | 43,43,43,43 | 0 |
| 55 | MG | BA | 3121 | 1/1 | 0.46 | - | 57,57,57,57 | 0 |
| 55 | MG | AA | 1653 | 1/1 | 0.55 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3079 | 1/1 | 0.37 | - | 54,54,54,54 | 0 |
| 55 | MG | BA | 3321 | 1/1 | 0.46 | - | 77,77,77,77 | 0 |
| 55 | MG | CA | 1694 | 1/1 | 0.48 | - | 97,97,97,97 | 0 |
| 55 | MG | AA | 1776 | 1/1 | 0.20 | - | 82,82,82,82 | 0 |
| 55 | MG | AA | 1660 | 1/1 | 0.62 | - | 53,53,53,53 | 0 |
| 55 | MG | BA | 3032 | 1/1 | 0.51 | - | 49,49,49,49 | 0 |
| 55 | MG | AA | 1631 | 1/1 | 0.21 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3524 | 1/1 | 0.20 | - | 66,66,66,66 | 0 |
| 55 | MG | CA | 1791 | 1/1 | 0.31 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1834 | 1/1 | 0.53 | - | 97,97,97,97 | 0 |
| 55 | MG | BA | 3279 | 1/1 | 0.12 | - | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3479 | 1/1 | 0.17 | - | 99,99,99,99 | 0 |
| 55 | MG | BA | 3401 | 1/1 | 0.42 | - | 62,62,62,62 | 0 |
| 55 | MG | AA | 1824 | 1/1 | 0.65 | - | 86,86,86,86 | 0 |
| 55 | MG | CA | 1778 | 1/1 | 0.40 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3294 | 1/1 | 0.32 | - | 72,72,72,72 | 0 |
| 55 | MG | CA | 1685 | 1/1 | 0.37 | - | 93,93,93,93 | 0 |
| 55 | MG | AA | 1604 | 1/1 | 0.30 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3155 | 1/1 | 0.18 | - | 45,45,45,45 | 0 |
| 55 | MG | BA | 3122 | 1/1 | 0.30 | - | 37,37,37,37 | 0 |
| 55 | MG | CA | 1756 | 1/1 | 0.39 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3477 | 1/1 | 0.51 | - | 95,95,95,95 | 0 |
| 55 | MG | AA | 1650 | 1/1 | 0.50 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3126 | 1/1 | 0.22 | - | 41,41,41,41 | 0 |
| 55 | MG | CA | 1605 | 1/1 | 0.41 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3278 | 1/1 | 0.50 | - | 42,42,42,42 | 0 |
| 55 | MG | AA | 1683 | 1/1 | 0.28 | - | 87,87,87,87 | 0 |
| 55 | MG | AA | 1806 | 1/1 | 0.28 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3347 | 1/1 | 0.49 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3490 | 1/1 | 0.10 | - | 126,126,126,126 | 0 |
| 55 | MG | DB | 201 | 1/1 | 0.41 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3381 | 1/1 | 0.54 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3171 | 1/1 | 0.57 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3003 | 1/1 | 0.44 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3377 | 1/1 | 0.74 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3365 | 1/1 | 0.51 | - | 58,58,58,58 | 0 |
| 55 | MG | DA | 3481 | 1/1 | 0.48 | - | 96,96,96,96 | 0 |
| 55 | MG | CA | 1781 | 1/1 | 0.07 | - | 117,117,117,117 | 0 |
| 55 | MG | BA | 3120 | 1/1 | 0.42 | - | 56,56,56,56 | 0 |
| 55 | MG | BB | 205 | 1/1 | 0.40 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3501 | 1/1 | 0.23 | - | 55,55,55,55 | 0 |
| 55 | MG | BA | 3610 | 1/1 | 0.46 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3232 | 1/1 | 0.40 | - | 44,44,44,44 | 0 |
| 55 | MG | AA | 1735 | 1/1 | 0.50 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1686 | 1/1 | 0.41 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3394 | 1/1 | 0.22 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3342 | 1/1 | 0.30 | - | 66,66,66,66 | 0 |
| 55 | MG | DA | 3415 | 1/1 | 0.55 | - | 96,96,96,96 | 0 |
| 55 | MG | AA | 1796 | 1/1 | 0.14 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3322 | 1/1 | 0.66 | - | 64,64,64,64 | 0 |
| 55 | MG | DP | 201 | 1/1 | 0.35 | - | 65,65,65,65 | 0 |
| 55 | MG | CA | 1679 | 1/1 | 0.40 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3077 | 1/1 | 0.41 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3318 | 1/1 | 0.37 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3141 | 1/1 | 0.47 | - | 35,35,35,35 | 0 |
| 55 | MG | CA | 1667 | 1/1 | 0.23 | - | 102,102,102,102 | 0 |
| 55 | MG | CA | 1682 | 1/1 | 0.39 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3109 | 1/1 | 0.26 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3269 | 1/1 | 0.45 | - | 61,61,61,61 | 0 |
| 55 | MG | AA | 1652 | 1/1 | 0.49 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3450 | 1/1 | 0.42 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3248 | 1/1 | 0.40 | - | 53,53,53,53 | 0 |
| 55 | MG | BB | 203 | 1/1 | 0.44 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1829 | 1/1 | 0.54 | - | 77,77,77,77 | 0 |
| 55 | MG | CA | 1635 | 1/1 | 0.77 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3373 | 1/1 | 0.51 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3470 | 1/1 | 0.19 | - | 80,80,80,80 | 0 |
| 55 | MG | AA | 1774 | 1/1 | 0.18 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3188 | 1/1 | 0.60 | - | 56,56,56,56 | 0 |
| 55 | MG | DA | 3297 | 1/1 | 0.26 | - | 83,83,83,83 | 0 |
| 55 | MG | DA | 3130 | 1/1 | 0.20 | - | 60,60,60,60 | 0 |
| 55 | MG | DB | 211 | 1/1 | 0.48 | - | 93,93,93,93 | 0 |
| 55 | MG | DA | 3029 | 1/1 | 0.31 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3430 | 1/1 | 0.57 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3435 | 1/1 | 0.09 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3616 | 1/1 | 0.49 | - | 58,58,58,58 | 0 |
| 55 | MG | BA | 3037 | 1/1 | 0.38 | - | 44,44,44,44 | 0 |
| 55 | MG | DA | 3459 | 1/1 | 0.38 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3295 | 1/1 | 0.34 | - | 50,50,50,50 | 0 |
| 55 | MG | CA | 1607 | 1/1 | 0.43 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3054 | 1/1 | 0.68 | - | 58,58,58,58 | 0 |
| 55 | MG | CA | 1680 | 1/1 | 0.60 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3388 | 1/1 | 0.43 | - | 74,74,74,74 | 0 |
| 55 | MG | AA | 1815 | 1/1 | 0.51 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3393 | 1/1 | 0.52 | - | 69,69,69,69 | 0 |
| 55 | MG | DA | 3074 | 1/1 | 0.21 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3242 | 1/1 | 0.59 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3143 | 1/1 | 0.31 | - | 58,58,58,58 | 0 |
| 55 | MG | AA | 1673 | 1/1 | 0.51 | - | 78,78,78,78 | 0 |
| 55 | MG | AA | 1755 | 1/1 | 0.55 | - | 104,104,104,104 | 0 |
| 55 | MG | DA | 3360 | 1/1 | 0.55 | - | 65,65,65,65 | 0 |
| 55 | MG | CA | 1722 | 1/1 | 0.37 | - | 75,75,75,75 | 0 |
| 55 | MG | AC | 103 | 1/1 | 0.36 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3384 | 1/1 | 0.29 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3031 | 1/1 | 0.25 | - | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1814 | 1/1 | 0.35 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3006 | 1/1 | 0.41 | - | 38,38,38,38 | 0 |
| 55 | MG | BA | 3470 | 1/1 | 0.35 | - | 88,88,88,88 | 0 |
| 55 | MG | AA | 1813 | 1/1 | 0.33 | - | 107,107,107,107 | 0 |
| 55 | MG | CA | 1794 | 1/1 | 0.29 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3538 | 1/1 | 0.52 | - | 66,66,66,66 | 0 |
| 55 | MG | CA | 1630 | 1/1 | 0.46 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3314 | 1/1 | 0.56 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3508 | 1/1 | 0.72 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3178 | 1/1 | 0.77 | - | 59,59,59,59 | 0 |
| 55 | MG | DA | 3442 | 1/1 | 0.25 | - | 91,91,91,91 | 0 |
| 55 | MG | CC | 101 | 1/1 | 0.43 | - | 92,92,92,92 | 0 |
| 55 | MG | BB | 209 | 1/1 | 0.43 | - | 102,102,102,102 | 0 |
| 55 | MG | CA | 1727 | 1/1 | 0.49 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3095 | 1/1 | 0.47 | - | 37,37,37,37 | 0 |
| 55 | MG | BA | 3164 | 1/1 | 0.71 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3404 | 1/1 | 0.17 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3418 | 1/1 | 0.39 | - | 78,78,78,78 | 0 |
| 55 | MG | AA | 1623 | 1/1 | 0.72 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3375 | 1/1 | 0.26 | - | 50,50,50,50 | 0 |
| 55 | MG | DA | 3257 | 1/1 | 0.35 | - | 49,49,49,49 | 0 |
| 55 | MG | BA | 3132 | 1/1 | 0.45 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3603 | 1/1 | 0.57 | - | 63,63,63,63 | 0 |
| 55 | MG | AA | 1632 | 1/1 | 0.25 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3555 | 1/1 | 0.22 | - | 38,38,38,38 | 0 |
| 55 | MG | DA | 3492 | 1/1 | 0.42 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3160 | 1/1 | 0.42 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3223 | 1/1 | 0.48 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3295 | 1/1 | 0.45 | - | 81,81,81,81 | 0 |
| 55 | MG | CA | 1770 | 1/1 | 0.25 | - | 102,102,102,102 | 0 |
| 55 | MG | DA | 3488 | 1/1 | 0.61 | - | 86,86,86,86 | 0 |
| 55 | MG | AC | 101 | 1/1 | 0.48 | - | 53,53,53,53 | 0 |
| 55 | MG | AA | 1763 | 1/1 | 0.57 | - | 53,53,53,53 | 0 |
| 55 | MG | DA | 3387 | 1/1 | 0.32 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3263 | 1/1 | 0.83 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3046 | 1/1 | 0.34 | - | 65,65,65,65 | 0 |
| 55 | MG | AA | 1804 | 1/1 | 0.17 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3303 | 1/1 | 0.38 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3133 | 1/1 | 0.38 | - | 42,42,42,42 | 0 |
| 55 | MG | DA | 3287 | 1/1 | 0.63 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3299 | 1/1 | 0.35 | - | 38,38,38,38 | 0 |
| 55 | MG | BA | 3230 | 1/1 | 0.59 | - | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3173 | 1/1 | 0.29 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3341 | 1/1 | 0.38 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3405 | 1/1 | 0.46 | - | 56,56,56,56 | 0 |
| 55 | MG | CA | 1621 | 1/1 | 0.41 | - | 66,66,66,66 | 0 |
| 55 | MG | CA | 1678 | 1/1 | 0.24 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3108 | 1/1 | 0.50 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3159 | 1/1 | 0.48 | - | 58,58,58,58 | 0 |
| 55 | MG | BA | 3392 | 1/1 | 0.39 | - | 70,70,70,70 | 0 |
| 55 | MG | BB | 214 | 1/1 | 0.29 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3220 | 1/1 | 0.49 | - | 44,44,44,44 | 0 |
| 55 | MG | AA | 1745 | 1/1 | 0.59 | - | 67,67,67,67 | 0 |
| 56 | ZN | CG | 303 | 1/1 | 0.31 | - | 118,118,118,118 | 0 |
| 55 | MG | BA | 3148 | 1/1 | 0.41 | - | 32,32,32,32 | 0 |
| 55 | MG | BA | 3313 | 1/1 | 0.19 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3160 | 1/1 | 0.41 | - | 42,42,42,42 | 0 |
| 55 | MG | BA | 3554 | 1/1 | 0.46 | - | 45,45,45,45 | 0 |
| 55 | MG | DA | 3059 | 1/1 | 0.82 | - | 106,106,106,106 | 0 |
| 55 | MG | DA | 3023 | 1/1 | 0.46 | - | 57,57,57,57 | 0 |
| 55 | MG | BA | 3241 | 1/1 | 0.51 | - | 60,60,60,60 | 0 |
| 55 | MG | AA | 1822 | 1/1 | 0.11 | - | 107,107,107,107 | 0 |
| 55 | MG | DA | 3260 | 1/1 | 0.60 | - | 41,41,41,41 | 0 |
| 55 | MG | AA | 1749 | 1/1 | 0.24 | - | 81,81,81,81 | 0 |
| 55 | MG | AA | 1661 | 1/1 | 0.32 | - | 48,48,48,48 | 0 |
| 55 | MG | BA | 3416 | 1/1 | 0.28 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3418 | 1/1 | 0.46 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3506 | 1/1 | 0.54 | - | 78,78,78,78 | 0 |
| 55 | MG | CA | 1658 | 1/1 | 0.47 | - | 91,91,91,91 | 0 |
| 55 | MG | AA | 1633 | 1/1 | 0.25 | - | 74,74,74,74 | 0 |
| 55 | MG | CA | 1773 | 1/1 | 0.80 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3340 | 1/1 | 0.26 | - | 77,77,77,77 | 0 |
| 55 | MG | CA | 1708 | 1/1 | 0.12 | - | 97,97,97,97 | 0 |
| 55 | MG | BA | 3443 | 1/1 | 0.15 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3084 | 1/1 | 0.34 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3349 | 1/1 | 0.32 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3403 | 1/1 | 0.68 | - | 93,93,93,93 | 0 |
| 55 | MG | DA | 3197 | 1/1 | 0.69 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3083 | 1/1 | 0.13 | - | 62,62,62,62 | 0 |
| 55 | MG | CA | 1627 | 1/1 | 0.35 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3509 | 1/1 | 0.30 | - | 83,83,83,83 | 0 |
| 55 | MG | DA | 3340 | 1/1 | 0.26 | - | 85,85,85,85 | 0 |
| 55 | MG | AC | 104 | 1/1 | 0.47 | - | 56,56,56,56 | 0 |
| 55 | MG | CA | 1807 | 1/1 | 0.30 | - | 126,126,126,126 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DB | 212 | 1/1 | 0.31 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3053 | 1/1 | 0.62 | - | 62,62,62,62 | 0 |
| 55 | MG | AA | 1643 | 1/1 | 0.70 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3413 | 1/1 | 0.36 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3339 | 1/1 | 0.29 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3024 | 1/1 | 0.37 | - | 27,27,27,27 | 0 |
| 55 | MG | DA | 3061 | 1/1 | 0.57 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3232 | 1/1 | 0.32 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3410 | 1/1 | 0.75 | - | 62,62,62,62 | 0 |
| 55 | MG | CA | 1767 | 1/1 | 0.52 | - | 77,77,77,77 | 0 |
| 55 | MG | A1 | 102 | 1/1 | 0.29 | - | 86,86,86,86 | 0 |
| 55 | MG | CA | 1751 | 1/1 | 0.30 | - | 94,94,94,94 | 0 |
| 55 | MG | CA | 1761 | 1/1 | 0.41 | - | 92,92,92,92 | 0 |
| 55 | MG | AA | 1621 | 1/1 | 0.25 | - | 108,108,108,108 | 0 |
| 55 | MG | BA | 3261 | 1/1 | 0.62 | - | 52,52,52,52 | 0 |
| 55 | MG | AA | 1659 | 1/1 | 0.73 | - | 69,69,69,69 | 0 |
| 55 | MG | AA | 1794 | 1/1 | 0.20 | - | 84,84,84,84 | 0 |
| 55 | MG | AA | 1732 | 1/1 | 0.29 | - | 92,92,92,92 | 0 |
| 55 | MG | AA | 1624 | 1/1 | 0.28 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3006 | 1/1 | 0.59 | - | 71,71,71,71 | 0 |
| 55 | MG | CA | 1623 | 1/1 | 0.12 | - | 90,90,90,90 | 0 |
| 55 | MG | AA | 1753 | 1/1 | 0.10 | - | 108,108,108,108 | 0 |
| 55 | MG | CB | 103 | 1/1 | 0.63 | - | 103,103,103,103 | 0 |
| 55 | MG | BA | 3334 | 1/1 | 0.59 | - | 96,96,96,96 | 0 |
| 55 | MG | BA | 3042 | 1/1 | 0.34 | - | 41,41,41,41 | 0 |
| 55 | MG | BA | 3530 | 1/1 | 0.30 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3529 | 1/1 | 0.46 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3613 | 1/1 | 0.32 | - | 93,93,93,93 | 0 |
| 55 | MG | AA | 1640 | 1/1 | 0.33 | - | 90,90,90,90 | 0 |
| 55 | MG | DA | 3505 | 1/1 | 0.52 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3253 | 1/1 | 0.26 | - | 51,51,51,51 | 0 |
| 55 | MG | BA | 3157 | 1/1 | 0.59 | - | 45,45,45,45 | 0 |
| 55 | MG | CA | 1697 | 1/1 | 0.33 | - | 65,65,65,65 | 0 |
| 55 | MG | CA | 1741 | 1/1 | 0.17 | - | 106,106,106,106 | 0 |
| 55 | MG | DA | 3067 | 1/1 | 0.45 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3277 | 1/1 | 0.31 | - | 89,89,89,89 | 0 |
| 55 | MG | BA | 3234 | 1/1 | 0.48 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3552 | 1/1 | 0.39 | - | 102,102,102,102 | 0 |
| 55 | MG | BA | 3245 | 1/1 | 0.56 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3146 | 1/1 | 0.60 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3376 | 1/1 | 0.44 | - | 73,73,73,73 | 0 |
| 55 | MG | AA | 1725 | 1/1 | 0.19 | - | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3193 | 1/1 | 0.70 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3445 | 1/1 | 0.39 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3374 | 1/1 | 0.44 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1709 | 1/1 | 0.23 | - | 70,70,70,70 | 0 |
| 55 | MG | AA | 1744 | 1/1 | 0.15 | - | 117,117,117,117 | 0 |
| 55 | MG | DA | 3499 | 1/1 | 0.26 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3267 | 1/1 | 0.25 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3250 | 1/1 | 0.20 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3542 | 1/1 | 0.51 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3083 | 1/1 | 0.48 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3602 | 1/1 | 0.27 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3068 | 1/1 | 0.35 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3323 | 1/1 | 0.17 | - | 42,42,42,42 | 0 |
| 55 | MG | BA | 3473 | 1/1 | 0.52 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3183 | 1/1 | 0.53 | - | 57,57,57,57 | 0 |
| 55 | MG | BA | 3582 | 1/1 | 0.46 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3369 | 1/1 | 0.30 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3287 | 1/1 | 0.40 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3415 | 1/1 | 0.40 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3619 | 1/1 | 0.36 | - | 69,69,69,69 | 0 |
| 55 | MG | BA | 3183 | 1/1 | 0.28 | - | 47,47,47,47 | 0 |
| 55 | MG | AA | 1711 | 1/1 | 0.32 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3525 | 1/1 | 0.80 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3092 | 1/1 | 0.45 | - | 32,32,32,32 | 0 |
| 55 | MG | CA | 1785 | 1/1 | 0.30 | - | 105,105,105,105 | 0 |
| 55 | MG | BA | 3109 | 1/1 | 0.34 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3358 | 1/1 | 0.55 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3426 | 1/1 | 0.48 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3081 | 1/1 | 0.53 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3052 | 1/1 | 0.41 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3513 | 1/1 | 0.76 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3306 | 1/1 | 0.30 | - | 67,67,67,67 | 0 |
| 55 | MG | CA | 1711 | 1/1 | 0.39 | - | 90,90,90,90 | 0 |
| 55 | MG | BA | 3135 | 1/1 | 0.54 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3407 | 1/1 | 0.31 | - | 59,59,59,59 | 0 |
| 55 | MG | DA | 3099 | 1/1 | 0.27 | - | 40,40,40,40 | 0 |
| 55 | MG | BA | 3430 | 1/1 | 0.28 | - | 57,57,57,57 | 0 |
| 55 | MG | AA | 1638 | 1/1 | 0.29 | - | 104,104,104,104 | 0 |
| 55 | MG | AA | 1810 | 1/1 | 0.49 | - | 67,67,67,67 | 0 |
| 55 | MG | BB | 208 | 1/1 | 0.29 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3608 | 1/1 | 0.39 | - | 39,39,39,39 | 0 |
| 55 | MG | AA | 1710 | 1/1 | 0.34 | - | 92,92,92,92 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3521 | 1/1 | 0.63 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3360 | 1/1 | 0.28 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3194 | 1/1 | 0.42 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3519 | 1/1 | 0.34 | - | 80,80,80,80 | 0 |
| 55 | MG | CA | 1730 | 1/1 | 0.28 | - | 106,106,106,106 | 0 |
| 55 | MG | AA | 1809 | 1/1 | 0.38 | - | 63,63,63,63 | 0 |
| 55 | MG | AH | 201 | 1/1 | 0.44 | - | 99,99,99,99 | 0 |
| 55 | MG | AA | 1840 | 1/1 | 0.51 | - | 87,87,87,87 | 0 |
| 55 | MG | CA | 1789 | 1/1 | 0.57 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1704 | 1/1 | 0.12 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3174 | 1/1 | 0.79 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3180 | 1/1 | 0.39 | - | 37,37,37,37 | 0 |
| 55 | MG | DA | 3065 | 1/1 | 0.46 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3035 | 1/1 | 0.27 | - | 37,37,37,37 | 0 |
| 55 | MG | CA | 1714 | 1/1 | 0.55 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3381 | 1/1 | 0.51 | - | 99,99,99,99 | 0 |
| 55 | MG | BA | 3172 | 1/1 | 0.36 | - | 34,34,34,34 | 0 |
| 55 | MG | AA | 1747 | 1/1 | 0.48 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3240 | 1/1 | 0.69 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3298 | 1/1 | 0.30 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3367 | 1/1 | 0.41 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3167 | 1/1 | 0.42 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3203 | 1/1 | 0.50 | - | 85,85,85,85 | 0 |
| 55 | MG | CA | 1752 | 1/1 | 0.18 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3231 | 1/1 | 0.51 | - | 73,73,73,73 | 0 |
| 55 | MG | CA | 1706 | 1/1 | 0.44 | - | 87,87,87,87 | 0 |
| 55 | MG | AA | 1752 | 1/1 | 0.28 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3022 | 1/1 | 0.44 | - | 30,30,30,30 | 0 |
| 55 | MG | CA | 1758 | 1/1 | 0.44 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3609 | 1/1 | 0.64 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3134 | 1/1 | 0.22 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3195 | 1/1 | 0.48 | - | 47,47,47,47 | 0 |
| 55 | MG | DA | 3086 | 1/1 | 0.25 | - | 114,114,114,114 | 0 |
| 55 | MG | CA | 1606 | 1/1 | 0.41 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3617 | 1/1 | 0.74 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3410 | 1/1 | 0.47 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3068 | 1/1 | 0.20 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3454 | 1/1 | 0.49 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3420 | 1/1 | 0.38 | - | 94,94,94,94 | 0 |
| 55 | MG | AA | 1802 | 1/1 | 0.48 | - | 85,85,85,85 | 0 |
| 55 | MG | BA | 3484 | 1/1 | 0.28 | - | 117,117,117,117 | 0 |
| 55 | MG | BA | 3296 | 1/1 | 0.38 | - | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1703 | 1/1 | 0.33 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3518 | 1/1 | 0.27 | - | 70,70,70,70 | 0 |
| 55 | MG | DA | 3266 | 1/1 | 0.52 | - | 55,55,55,55 | 0 |
| 55 | MG | BA | 3564 | 1/1 | 0.63 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3177 | 1/1 | 0.39 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3125 | 1/1 | 0.41 | - | 45,45,45,45 | 0 |
| 55 | MG | DA | 3107 | 1/1 | 0.34 | - | 53,53,53,53 | 0 |
| 55 | MG | CA | 1690 | 1/1 | 0.38 | - | 68,68,68,68 | 0 |
| 55 | MG | CA | 1765 | 1/1 | 0.30 | - | 101,101,101,101 | 0 |
| 55 | MG | AA | 1685 | 1/1 | 0.38 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3065 | 1/1 | 0.40 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3111 | 1/1 | 0.29 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3423 | 1/1 | 0.56 | - | 61,61,61,61 | 0 |
| 55 | MG | CA | 1666 | 1/1 | 0.30 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3492 | 1/1 | 0.50 | - | 77,77,77,77 | 0 |
| 55 | MG | AA | 1736 | 1/1 | 0.62 | - | 90,90,90,90 | 0 |
| 55 | MG | CA | 1774 | 1/1 | 0.18 | - | 104,104,104,104 | 0 |
| 55 | MG | DA | 3351 | 1/1 | 0.39 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3009 | 1/1 | 0.53 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3070 | 1/1 | 0.34 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3376 | 1/1 | 0.49 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3231 | 1/1 | 0.42 | - | 72,72,72,72 | 0 |
| 55 | MG | AA | 1836 | 1/1 | 0.58 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3214 | 1/1 | 0.42 | - | 40,40,40,40 | 0 |
| 55 | MG | DA | 3354 | 1/1 | 0.48 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3203 | 1/1 | 0.29 | - | 48,48,48,48 | 0 |
| 55 | MG | AA | 1795 | 1/1 | 0.22 | - | 73,73,73,73 | 0 |
| 55 | MG | AA | 1721 | 1/1 | 0.32 | - | 77,77,77,77 | 0 |
| 55 | MG | AA | 1644 | 1/1 | 0.20 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3433 | 1/1 | 0.20 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3483 | 1/1 | 0.37 | - | 68,68,68,68 | 0 |
| 55 | MG | BE | 303 | 1/1 | 0.39 | - | 44,44,44,44 | 0 |
| 55 | MG | DA | 3032 | 1/1 | 0.16 | - | 76,76,76,76 | 0 |
| 55 | MG | CA | 1688 | 1/1 | 0.35 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3464 | 1/1 | 0.51 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3499 | 1/1 | 0.38 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3411 | 1/1 | 0.21 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3598 | 1/1 | 0.30 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3199 | 1/1 | 0.53 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3451 | 1/1 | 0.48 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3263 | 1/1 | 0.64 | - | 54,54,54,54 | 0 |
| 55 | MG | AA | 1761 | 1/1 | 0.42 | - | 113,113,113,113 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3363 | 1/1 | 0.59 | - | 67,67,67,67 | 0 |
| 55 | MG | BA | 3081 | 1/1 | 0.31 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3458 | 1/1 | 0.57 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3256 | 1/1 | 0.42 | - | 49,49,49,49 | 0 |
| 55 | MG | BA | 3104 | 1/1 | 0.23 | - | 57,57,57,57 | 0 |
| 55 | MG | BA | 3201 | 1/1 | 0.65 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1656 | 1/1 | 0.47 | - | 87,87,87,87 | 0 |
| 55 | MG | CA | 1731 | 1/1 | 0.56 | - | 72,72,72,72 | 0 |
| 55 | MG | DA | 3284 | 1/1 | 0.33 | - | 56,56,56,56 | 0 |
| 55 | MG | BA | 3098 | 1/1 | 0.25 | - | 48,48,48,48 | 0 |
| 55 | MG | DA | 3066 | 1/1 | 0.56 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3397 | 1/1 | 0.34 | - | 60,60,60,60 | 0 |
| 55 | MG | DA | 3500 | 1/1 | 0.35 | - | 92,92,92,92 | 0 |
| 55 | MG | DA | 3112 | 1/1 | 0.19 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3387 | 1/1 | 0.42 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3227 | 1/1 | 0.74 | - | 50,50,50,50 | 0 |
| 55 | MG | DA | 3014 | 1/1 | 0.55 | - | 74,74,74,74 | 0 |
| 55 | MG | BE | 304 | 1/1 | 0.36 | - | 80,80,80,80 | 0 |
| 55 | MG | BA | 3145 | 1/1 | 0.39 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3144 | 1/1 | 0.28 | - | 60,60,60,60 | 0 |
| 55 | MG | CA | 1672 | 1/1 | 0.76 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3321 | 1/1 | 0.55 | - | 66,66,66,66 | 0 |
| 55 | MG | AA | 1739 | 1/1 | 0.16 | - | 93,93,93,93 | 0 |
| 55 | MG | BA | 3029 | 1/1 | 0.41 | - | 35,35,35,35 | 0 |
| 55 | MG | BA | 3139 | 1/1 | 0.40 | - | 35,35,35,35 | 0 |
| 55 | MG | BA | 3372 | 1/1 | 0.32 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3152 | 1/1 | 0.51 | - | 40,40,40,40 | 0 |
| 55 | MG | DA | 3404 | 1/1 | 0.28 | - | 61,61,61,61 | 0 |
| 55 | MG | BA | 3080 | 1/1 | 0.17 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3595 | 1/1 | 0.22 | - | 65,65,65,65 | 0 |
| 55 | MG | DA | 3326 | 1/1 | 0.40 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3020 | 1/1 | 0.47 | - | 41,41,41,41 | 0 |
| 55 | MG | BA | 3328 | 1/1 | 0.70 | - | 69,69,69,69 | 0 |
| 55 | MG | AC | 107 | 1/1 | 0.29 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3058 | 1/1 | 0.34 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3401 | 1/1 | 0.20 | - | 71,71,71,71 | 0 |
| 56 | ZN | AQ | 102 | 1/1 | 0.10 | - | 122,122,122,122 | 0 |
| 55 | MG | AA | 1807 | 1/1 | 0.49 | - | 98,98,98,98 | 0 |
| 55 | MG | BA | 3193 | 1/1 | 0.54 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3258 | 1/1 | 0.29 | - | 37,37,37,37 | 0 |
| 55 | MG | BA | 3051 | 1/1 | 0.23 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3088 | 1/1 | 0.17 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1764 | 1/1 | 0.16 | - | 79,79,79,79 | 0 |
| 55 | MG | AA | 1812 | 1/1 | 0.61 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3074 | 1/1 | 0.46 | - | 49,49,49,49 | 0 |
| 55 | MG | DA | 3102 | 1/1 | 0.34 | - | 51,51,51,51 | 0 |
| 55 | MG | AA | 1720 | 1/1 | 0.24 | - | 93,93,93,93 | 0 |
| 55 | MG | DA | 3371 | 1/1 | 0.51 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3093 | 1/1 | 0.30 | - | 57,57,57,57 | 0 |
| 55 | MG | AA | 1825 | 1/1 | 0.23 | - | 93,93,93,93 | 0 |
| 55 | MG | BA | 3547 | 1/1 | 0.43 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3136 | 1/1 | 0.39 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3511 | 1/1 | 0.18 | - | 89,89,89,89 | 0 |
| 55 | MG | BE | 302 | 1/1 | 0.22 | - | 56,56,56,56 | 0 |
| 55 | MG | CA | 1776 | 1/1 | 0.55 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3250 | 1/1 | 0.42 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3257 | 1/1 | 0.25 | - | 64,64,64,64 | 0 |
| 55 | MG | BB | 204 | 1/1 | 0.33 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3136 | 1/1 | 0.10 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3080 | 1/1 | 0.56 | - | 75,75,75,75 | 0 |
| 55 | MG | DA | 3261 | 1/1 | 0.49 | - | 58,58,58,58 | 0 |
| 55 | MG | DA | 3501 | 1/1 | 0.92 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3310 | 1/1 | 0.37 | - | 57,57,57,57 | 0 |
| 55 | MG | CA | 1802 | 1/1 | 0.50 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3011 | 1/1 | 0.31 | - | 42,42,42,42 | 0 |
| 55 | MG | BA | 3008 | 1/1 | 0.47 | - | 37,37,37,37 | 0 |
| 55 | MG | BA | 3362 | 1/1 | 0.26 | - | 48,48,48,48 | 0 |
| 55 | MG | DA | 3311 | 1/1 | 0.42 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3406 | 1/1 | 0.64 | - | 82,82,82,82 | 0 |
| 55 | MG | AA | 1675 | 1/1 | 0.43 | - | 80,80,80,80 | 0 |
| 55 | MG | AA | 1742 | 1/1 | 0.17 | - | 78,78,78,78 | 0 |
| 55 | MG | B7 | 101 | 1/1 | 0.45 | - | 67,67,67,67 | 0 |
| 55 | MG | AA | 1754 | 1/1 | 0.22 | - | 95,95,95,95 | 0 |
| 55 | MG | BA | 3233 | 1/1 | 0.39 | - | 48,48,48,48 | 0 |
| 55 | MG | CA | 1805 | 1/1 | 0.32 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3502 | 1/1 | 0.52 | - | 97,97,97,97 | 0 |
| 55 | MG | DA | 3139 | 1/1 | 0.47 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3185 | 1/1 | 0.35 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3128 | 1/1 | 0.38 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3592 | 1/1 | 0.46 | - | 89,89,89,89 | 0 |
| 55 | MG | CA | 1747 | 1/1 | 0.30 | - | 94,94,94,94 | 0 |
| 55 | MG | BA | 3444 | 1/1 | 0.54 | - | 78,78,78,78 | 0 |
| 55 | MG | CA | 1619 | 1/1 | 0.47 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3062 | 1/1 | 0.25 | - | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3011 | 1/1 | 0.23 | - | 65,65,65,65 | 0 |
| 55 | MG | BA | 3446 | 1/1 | 0.24 | - | 92,92,92,92 | 0 |
| 55 | MG | BA | 3103 | 1/1 | 0.52 | - | 52,52,52,52 | 0 |
| 55 | MG | DA | 3236 | 1/1 | 0.33 | - | 55,55,55,55 | 0 |
| 55 | MG | CA | 1798 | 1/1 | 0.25 | - | 85,85,85,85 | 0 |
| 55 | MG | DA | 3270 | 1/1 | 0.35 | - | 83,83,83,83 | 0 |
| 55 | MG | CA | 1628 | 1/1 | 0.23 | - | 101,101,101,101 | 0 |
| 55 | MG | CA | 1661 | 1/1 | 0.19 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3075 | 1/1 | 0.31 | - | 110,110,110,110 | 0 |
| 55 | MG | CC | 105 | 1/1 | 0.58 | - | 82,82,82,82 | 0 |
| 55 | MG | CA | 1616 | 1/1 | 0.31 | - | 88,88,88,88 | 0 |
| 55 | MG | AA | 1724 | 1/1 | 0.22 | - | 84,84,84,84 | 0 |
| 55 | MG | DA | 3449 | 1/1 | 0.47 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3343 | 1/1 | 0.30 | - | 60,60,60,60 | 0 |
| 55 | MG | BA | 3059 | 1/1 | 0.39 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3580 | 1/1 | 0.19 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3235 | 1/1 | 0.43 | - | 48,48,48,48 | 0 |
| 55 | MG | DA | 3198 | 1/1 | 0.30 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3100 | 1/1 | 0.35 | - | 42,42,42,42 | 0 |
| 55 | MG | BA | 3140 | 1/1 | 0.25 | - | 58,58,58,58 | 0 |
| 55 | MG | DA | 3412 | 1/1 | 0.38 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3073 | 1/1 | 0.52 | - | 80,80,80,80 | 0 |
| 55 | MG | DA | 3504 | 1/1 | 0.42 | - | 65,65,65,65 | 0 |
| 55 | MG | DR | 201 | 1/1 | 0.17 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3033 | 1/1 | 0.29 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3111 | 1/1 | 0.37 | - | 59,59,59,59 | 0 |
| 55 | MG | BA | 3411 | 1/1 | 0.37 | - | 68,68,68,68 | 0 |
| 55 | MG | BA | 3046 | 1/1 | 0.37 | - | 39,39,39,39 | 0 |
| 55 | MG | DA | 3497 | 1/1 | 0.32 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3113 | 1/1 | 0.53 | - | 57,57,57,57 | 0 |
| 55 | MG | DA | 3364 | 1/1 | 0.35 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1613 | 1/1 | 0.07 | - | 85,85,85,85 | 0 |
| 55 | MG | CA | 1613 | 1/1 | 0.28 | - | 68,68,68,68 | 0 |
| 55 | MG | AB | 102 | 1/1 | 0.24 | - | 86,86,86,86 | 0 |
| 55 | MG | DA | 3149 | 1/1 | 0.65 | - | 57,57,57,57 | 0 |
| 55 | MG | BA | 3508 | 1/1 | 0.41 | - | 59,59,59,59 | 0 |
| 55 | MG | CB | 102 | 1/1 | 0.30 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3265 | 1/1 | 0.39 | - | 50,50,50,50 | 0 |
| 55 | MG | BB | 206 | 1/1 | 0.42 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3365 | 1/1 | 0.31 | - | 50,50,50,50 | 0 |
| 55 | MG | AQ | 101 | 1/1 | 0.16 | - | 88,88,88,88 | 0 |
| 55 | MG | BA | 3297 | 1/1 | 0.24 | - | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3217 | 1/1 | 0.44 | - | 55,55,55,55 | 0 |
| 55 | MG | DA | 3466 | 1/1 | 0.64 | - | 78,78,78,78 | 0 |
| 55 | MG | CG | 301 | 1/1 | 0.38 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3550 | 1/1 | 0.34 | - | 93,93,93,93 | 0 |
| 55 | MG | AA | 1722 | 1/1 | 0.49 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3421 | 1/1 | 0.32 | - | 62,62,62,62 | 0 |
| 55 | MG | DA | 3175 | 1/1 | 0.39 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3456 | 1/1 | 0.53 | - | 78,78,78,78 | 0 |
| 55 | MG | AA | 1835 | 1/1 | 0.23 | - | 87,87,87,87 | 0 |
| 55 | MG | CC | 107 | 1/1 | 0.60 | - | 99,99,99,99 | 0 |
| 55 | MG | AA | 1760 | 1/1 | 0.68 | - | 78,78,78,78 | 0 |
| 55 | MG | AA | 1663 | 1/1 | 0.27 | - | 47,47,47,47 | 0 |
| 55 | MG | BA | 3106 | 1/1 | 0.37 | - | 75,75,75,75 | 0 |
| 55 | MG | DE | 303 | 1/1 | 0.34 | - | 56,56,56,56 | 0 |
| 55 | MG | BA | 3284 | 1/1 | 0.47 | - | 56,56,56,56 | 0 |
| 55 | MG | BA | 3097 | 1/1 | 0.41 | - | 59,59,59,59 | 0 |
| 55 | MG | BA | 3216 | 1/1 | 0.34 | - | 33,33,33,33 | 0 |
| 55 | MG | CA | 1673 | 1/1 | 0.56 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3359 | 1/1 | 0.30 | - | 76,76,76,76 | 0 |
| 55 | MG | BA | 3039 | 1/1 | 0.30 | - | 42,42,42,42 | 0 |
| 55 | MG | BO | 201 | 1/1 | 0.37 | - | 62,62,62,62 | 0 |
| 56 | ZN | AG | 302 | 1/1 | 0.34 | - | 95,95,95,95 | 0 |
| 55 | MG | BA | 3574 | 1/1 | 0.49 | - | 78,78,78,78 | 0 |
| 55 | MG | BA | 3154 | 1/1 | 0.27 | - | 55,55,55,55 | 0 |
| 55 | MG | BA | 3570 | 1/1 | 0.44 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3055 | 1/1 | 0.61 | - | 68,68,68,68 | 0 |
| 55 | MG | CA | 1762 | 1/1 | 0.35 | - | 96,96,96,96 | 0 |
| 55 | MG | AA | 1639 | 1/1 | 0.33 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3556 | 1/1 | 0.49 | - | 58,58,58,58 | 0 |
| 55 | MG | BF | 301 | 1/1 | 0.07 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3330 | 1/1 | 0.22 | - | 81,81,81,81 | 0 |
| 55 | MG | AG | 301 | 1/1 | 0.62 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3089 | 1/1 | 0.29 | - | 88,88,88,88 | 0 |
| 55 | MG | CA | 1618 | 1/1 | 0.19 | - | 93,93,93,93 | 0 |
| 55 | MG | AA | 1786 | 1/1 | 0.17 | - | 86,86,86,86 | 0 |
| 55 | MG | BA | 3052 | 1/1 | 0.25 | - | 64,64,64,64 | 0 |
| 55 | MG | DA | 3129 | 1/1 | 0.27 | - | 82,82,82,82 | 0 |
| 55 | MG | DA | 3314 | 1/1 | 0.49 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3452 | 1/1 | 0.21 | - | 83,83,83,83 | 0 |
| 55 | MG | BA | 3332 | 1/1 | 0.37 | - | 61,61,61,61 | 0 |
| 55 | MG | DA | 3255 | 1/1 | 0.30 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3539 | 1/1 | 0.20 | - | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3486 | 1/1 | 0.34 | - | 68,68,68,68 | 0 |
| 55 | MG | DA | 3302 | 1/1 | 0.59 | - | 95,95,95,95 | 0 |
| 55 | MG | BA | 3463 | 1/1 | 0.27 | - | 72,72,72,72 | 0 |
| 55 | MG | BA | 3541 | 1/1 | 0.32 | - | 96,96,96,96 | 0 |
| 55 | MG | DA | 3395 | 1/1 | 0.49 | - | 69,69,69,69 | 0 |
| 55 | MG | CA | 1786 | 1/1 | 0.30 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3269 | 1/1 | 0.48 | - | 84,84,84,84 | 0 |
| 55 | MG | CA | 1624 | 1/1 | 0.37 | - | 88,88,88,88 | 0 |
| 55 | MG | DA | 3118 | 1/1 | 0.38 | - | 71,71,71,71 | 0 |
| 55 | MG | AA | 1790 | 1/1 | 0.25 | - | 98,98,98,98 | 0 |
| 55 | MG | AA | 1605 | 1/1 | 0.38 | - | 82,82,82,82 | 0 |
| 55 | MG | CA | 1744 | 1/1 | 0.30 | - | 79,79,79,79 | 0 |
| 55 | MG | BA | 3590 | 1/1 | 0.38 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3119 | 1/1 | 0.46 | - | 98,98,98,98 | 0 |
| 55 | MG | DA | 3225 | 1/1 | 0.54 | - | 73,73,73,73 | 0 |
| 55 | MG | DA | 3159 | 1/1 | 0.28 | - | 37,37,37,37 | 0 |
| 55 | MG | BA | 3439 | 1/1 | 0.39 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3275 | 1/1 | 0.25 | - | 73,73,73,73 | 0 |
| 55 | MG | BA | 3537 | 1/1 | 0.49 | - | 89,89,89,89 | 0 |
| 55 | MG | BA | 3173 | 1/1 | 0.59 | - | 52,52,52,52 | 0 |
| 55 | MG | BA | 3066 | 1/1 | 0.31 | - | 62,62,62,62 | 0 |
| 55 | MG | BA | 3611 | 1/1 | 0.51 | - | 87,87,87,87 | 0 |
| 55 | MG | DA | 3523 | 1/1 | 0.92 | - | 81,81,81,81 | 0 |
| 55 | MG | BA | 3207 | 1/1 | 0.59 | - | 41,41,41,41 | 0 |
| 55 | MG | AA | 1718 | 1/1 | 0.48 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3185 | 1/1 | 0.38 | - | 76,76,76,76 | 0 |
| 55 | MG | AA | 1603 | 1/1 | 0.32 | - | 63,63,63,63 | 0 |
| 55 | MG | BA | 3388 | 1/1 | 0.53 | - | 88,88,88,88 | 0 |
| 55 | MG | CA | 1729 | 1/1 | 0.85 | - | 77,77,77,77 | 0 |
| 55 | MG | BA | 3507 | 1/1 | 0.30 | - | 89,89,89,89 | 0 |
| 55 | MG | AA | 1682 | 1/1 | 0.17 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3085 | 1/1 | 0.45 | - | 91,91,91,91 | 0 |
| 55 | MG | DA | 3057 | 1/1 | 0.45 | - | 83,83,83,83 | 0 |
| 55 | MG | DA | 3100 | 1/1 | 0.45 | - | 44,44,44,44 | 0 |
| 55 | MG | AA | 1765 | 1/1 | 0.60 | - | 84,84,84,84 | 0 |
| 55 | MG | BA | 3053 | 1/1 | 0.33 | - | 95,95,95,95 | 0 |
| 55 | MG | AA | 1792 | 1/1 | 0.22 | - | 55,55,55,55 | 0 |
| 55 | MG | CA | 1726 | 1/1 | 0.59 | - | 75,75,75,75 | 0 |
| 55 | MG | BA | 3055 | 1/1 | 0.44 | - | 57,57,57,57 | 0 |
| 55 | MG | CA | 1633 | 1/1 | 0.30 | - | 91,91,91,91 | 0 |
| 55 | MG | BA | 3393 | 1/1 | 0.57 | - | 81,81,81,81 | 0 |
| 55 | MG | B1 | 201 | 1/1 | 0.31 | - | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3560 | 1/1 | 0.61 | - | 78,78,78,78 | 0 |
| 55 | MG | DA | 3215 | 1/1 | 0.44 | - | 42,42,42,42 | 0 |
| 55 | MG | BA | 3565 | 1/1 | 0.39 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3307 | 1/1 | 0.25 | - | 77,77,77,77 | 0 |
| 55 | MG | DA | 3366 | 1/1 | 0.47 | - | 83,83,83,83 | 0 |
| 55 | MG | DA | 3124 | 1/1 | 0.55 | - | 54,54,54,54 | 0 |
| 55 | MG | DA | 3181 | 1/1 | 0.48 | - | 50,50,50,50 | 0 |
| 55 | MG | DA | 3301 | 1/1 | 0.41 | - | 63,63,63,63 | 0 |
| 55 | MG | DA | 3224 | 1/1 | 0.51 | - | 66,66,66,66 | 0 |
| 55 | MG | BA | 3581 | 1/1 | 0.37 | - | 69,69,69,69 | 0 |
| 55 | MG | BB | 212 | 1/1 | 0.48 | - | 81,81,81,81 | 0 |
| 55 | MG | DA | 3392 | 1/1 | 0.47 | - | 68,68,68,68 | 0 |
| 55 | MG | AA | 1733 | 1/1 | 0.60 | - | 71,71,71,71 | 0 |
| 55 | MG | DA | 3320 | 1/1 | 0.16 | - | 76,76,76,76 | 0 |
| 55 | MG | DA | 3460 | 1/1 | 0.45 | - | 72,72,72,72 | 0 |
| 55 | MG | AA | 1649 | 1/1 | 0.37 | - | 79,79,79,79 | 0 |
| 55 | MG | DA | 3399 | 1/1 | 0.51 | - | 76,76,76,76 | 0 |
| 55 | MG | CA | 1788 | 1/1 | 0.30 | - | 84,84,84,84 | 0 |
| 55 | MG | AA | 1651 | 1/1 | 0.57 | - | 71,71,71,71 | 0 |
| 55 | MG | BA | 3367 | 1/1 | 0.36 | - | 82,82,82,82 | 0 |
| 55 | MG | BA | 3475 | 1/1 | 0.33 | - | 83,83,83,83 | 0 |
| 55 | MG | AA | 1758 | 1/1 | 0.36 | - | 85,85,85,85 | 0 |
| 55 | MG | AA | 1789 | 1/1 | 0.35 | - | 74,74,74,74 | 0 |
| 55 | MG | DA | 3115 | 1/1 | 0.54 | - | 49,49,49,49 | 0 |
| 55 | MG | BA | 3273 | 1/1 | 0.34 | - | 94,94,94,94 | 0 |
| 55 | MG | CA | 1745 | 1/1 | 0.14 | - | 91,91,91,91 | 0 |
| 55 | MG | BB | 216 | 1/1 | 0.28 | - | 94,94,94,94 | 0 |
| 55 | MG | DA | 3147 | 1/1 | 0.42 | - | 53,53,53,53 | 0 |
| 55 | MG | BA | 3472 | 1/1 | 0.57 | - | 89,89,89,89 | 0 |
| 55 | MG | DA | 3138 | 1/1 | 0.27 | - | 70,70,70,70 | 0 |
| 55 | MG | BA | 3260 | 1/1 | 0.41 | - | 47,47,47,47 | 0 |
| 55 | MG | DA | 3336 | 1/1 | 0.49 | - | 87,87,87,87 | 0 |
| 55 | MG | BA | 3249 | 1/1 | 0.25 | - | 30,30,30,30 | 0 |
| 55 | MG | DA | 3049 | 1/1 | 0.37 | - | 74,74,74,74 | 0 |
| 55 | MG | BA | 3572 | 1/1 | 0.38 | - | 87,87,87,87 | 0 |
| 55 | MG | AA | 1828 | 1/1 | 0.14 | - | 105,105,105,105 | 0 |
| 55 | MG | BA | 3315 | 1/1 | 0.34 | - | 78,78,78,78 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.