



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:33 am BST

PDB ID : 4V5L
Title : The structure of EF-Tu and aminoacyl-tRNA bound to the 70S ribosome with a GTP analog
Authors : Voorhees, R.M.; Schmeing, T.M.; Ramakrishnan, V.
Deposited on : 2010-09-02
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

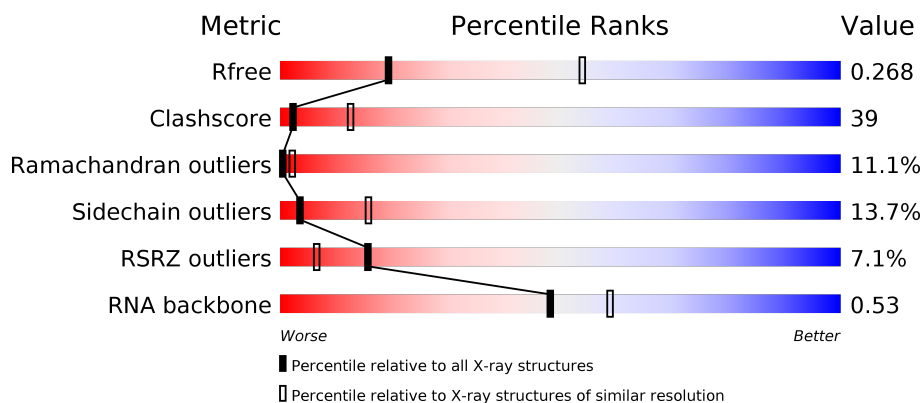
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



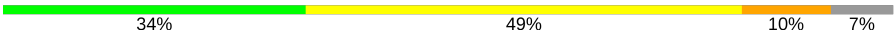

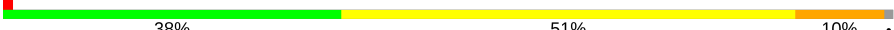
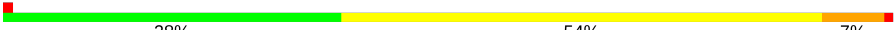
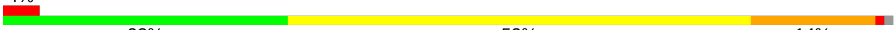
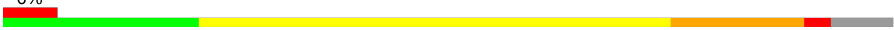










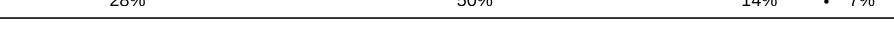
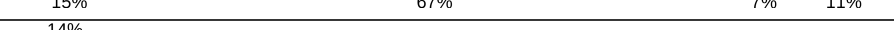


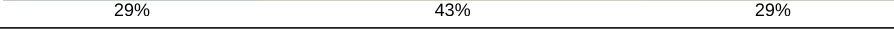
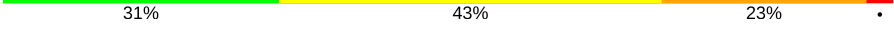


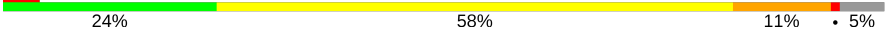
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1094 (3.10-3.10) |
| Clashscore | 141614 | 1184 (3.10-3.10) |
| Ramachandran outliers | 138981 | 1141 (3.10-3.10) |
| Sidechain outliers | 138945 | 1141 (3.10-3.10) |
| RSRZ outliers | 127900 | 1067 (3.10-3.10) |
| RNA backbone | 3102 | 1116 (3.40-2.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | AA | 1522 | <div> <div>2%</div> <div>33% 52% 11%</div> </div> |
| 2 | AB | 256 | <div> <div>5%</div> <div>20% 54% 15% 9%</div> </div> |
| 3 | AC | 239 | <div> <div>29% 48% 9% 14%</div> </div> |
| 4 | AD | 209 | <div> <div>% 38% 47% 14%</div> </div> |

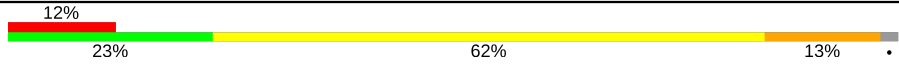
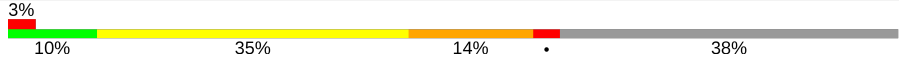
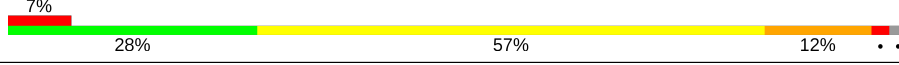

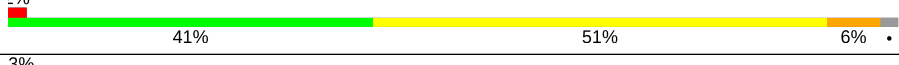
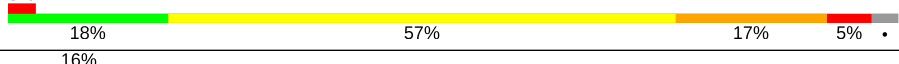
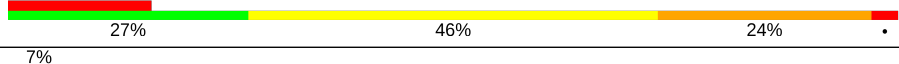

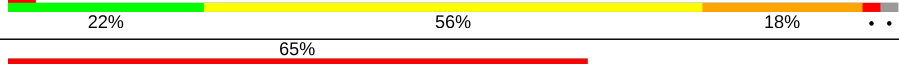
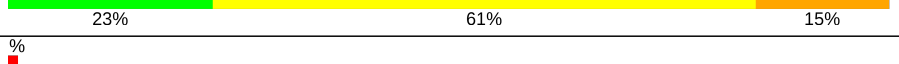
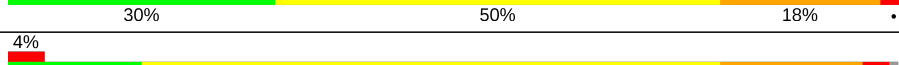
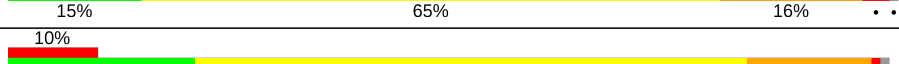
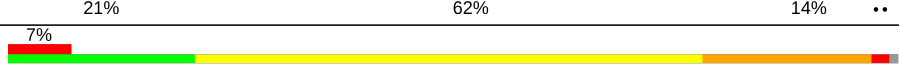
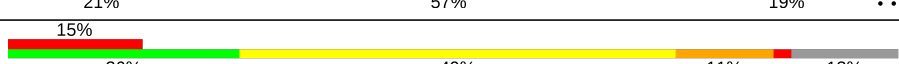
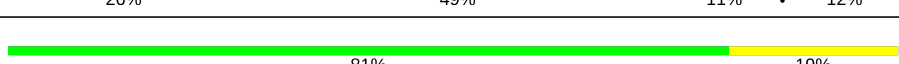
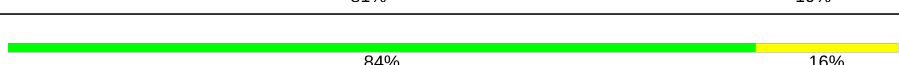
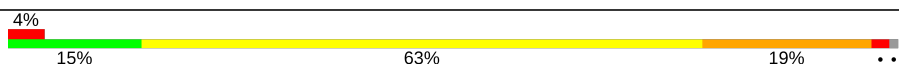
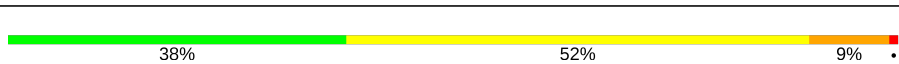
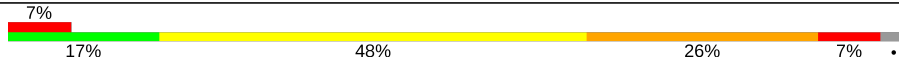

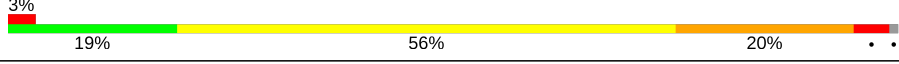
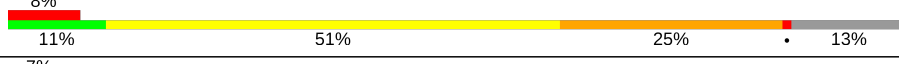

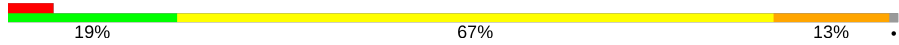

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | AE | 162 |  |
| 6 | AF | 101 |  |
| 7 | AG | 156 |  |
| 8 | AH | 138 |  |
| 9 | AI | 128 |  |
| 10 | AJ | 105 |  |
| 11 | AK | 129 |  |
| 12 | AL | 135 |  |
| 13 | AM | 126 |  |
| 14 | AN | 61 |  |
| 15 | AO | 89 |  |
| 16 | AP | 88 |  |
| 17 | AQ | 105 |  |
| 18 | AR | 88 |  |
| 19 | AS | 93 |  |
| 20 | AT | 106 |  |
| 21 | AU | 27 |  |
| 22 | AV | 76 |  |
| 22 | AW | 76 |  |
| 23 | AX | 14 |  |
| 24 | AY | 77 |  |
| 25 | AZ | 405 |  |
| 26 | B0 | 85 |  |
| 27 | B1 | 98 |  |
| 28 | B2 | 72 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 29 | B3 | 60 |  |
| 30 | B4 | 71 |  |
| 31 | B5 | 60 |  |
| 32 | B6 | 54 |  |
| 33 | B7 | 49 |  |
| 34 | B8 | 65 |  |
| 35 | B9 | 37 |  |
| 36 | BA | 2915 |  |
| 37 | BB | 122 |  |
| 38 | BC | 229 |  |
| 39 | BD | 276 |  |
| 40 | BE | 206 |  |
| 41 | BF | 210 |  |
| 42 | BG | 182 |  |
| 43 | BH | 180 |  |
| 44 | BJ | 130 |  |
| 45 | BK | 140 |  |
| 46 | BN | 140 |  |
| 47 | BO | 122 |  |
| 48 | BP | 150 |  |
| 49 | BQ | 141 |  |
| 50 | BR | 118 |  |
| 51 | BS | 112 |  |
| 52 | BT | 146 |  |
| 53 | BU | 118 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54 | BV | 101 | |
| 55 | BW | 113 | |
| 56 | BX | 96 | |
| 57 | BY | 110 | |
| 58 | BZ | 206 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | H2U | AY | 16 | - | - | - | X |
| 24 | H2U | AY | 17 | - | - | - | X |

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 153628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1504 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32329 | 14390 | 5992 | 10444 | 1503 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 234 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1900 | 1213 | 341 | 341 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AC | 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 | AD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1146 | 724 | 217 | 201 | 4 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | AI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1011 | 639 | 198 | 174 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 794 | 499 | 156 | 138 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 970 | 611 | 195 | 163 | 1 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| AL | 1 | MET | - | expression tag | UNP P17293 |
| AL | 2 | VAL | - | expression tag | UNP P17293 |
| AL | 3 | ALA | - | expression tag | UNP P17293 |
| AL | 4 | LEU | - | expression tag | UNP P17293 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 987 | 611 | 205 | 169 | 2 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 700 | 443 | 139 | 117 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 629 | 403 | 114 | 110 | 2 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 24 | Total | C | N | O | 0 | 0 | 0 |
| | | | 208 | 128 | 50 | 30 | | | |

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | AV | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1619 | 723 | 290 | 531 | 75 | | | |
| 22 | AW | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1619 | 723 | 290 | 531 | 75 | | | |

- Molecule 23 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 23 | AX | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 298 | 135 | 56 | 94 | 13 | | | |

- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 24 | AY | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1644 | 742 | 289 | 535 | 76 | 2 | | |

- Molecule 25 is a protein called ELONGATION FACTOR TU.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 25 | AZ | 405 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3142 | 1983 | 550 | 597 | 12 | | | |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | B0 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 410 | 140 | 111 | 1 | | | |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | B1 | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 731 | 460 | 145 | 125 | 1 | | | |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | B2 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 598 | 370 | 121 | 106 | 1 | | | |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | B3 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 467 | 298 | 90 | 78 | 1 | | | |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | B4 | 44 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 340 | 218 | 57 | 61 | 4 | | | |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32 | B6 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 433 | 270 | 88 | 71 | 4 | | | |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33 | B7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 34 | B8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 507 | 326 | 101 | 78 | 2 | | | |

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 35 | B9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 36 | BA | 2901 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62477 | 27807 | 11683 | 20087 | 2900 | | | |

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 37 | BB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 38 | BC | 228 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1742 | 1101 | 319 | 319 | 3 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| BC | 27 | ARG | LEU | conflict | UNP Q5SLP7 |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2145 | 1353 | 428 | 361 | 3 | | | |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1563 | 988 | 299 | 270 | 6 | | | |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 41 | BF | 207 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1623 | 1035 | 303 | 282 | 3 | | | |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BH | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1222 | 773 | 228 | 220 | 1 | | | |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44 | BJ | 130 | Total | C | N | O | 0 | 0 | 0 |
| | | | 651 | 391 | 130 | 130 | | | |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 45 | BK | 140 | Total | C | N | O | 0 | 0 | 0 |
| | | | 700 | 420 | 140 | 140 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 51 | BS | 98 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 770 | 486 | 154 | 130 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | BT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56 | BX | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | | |

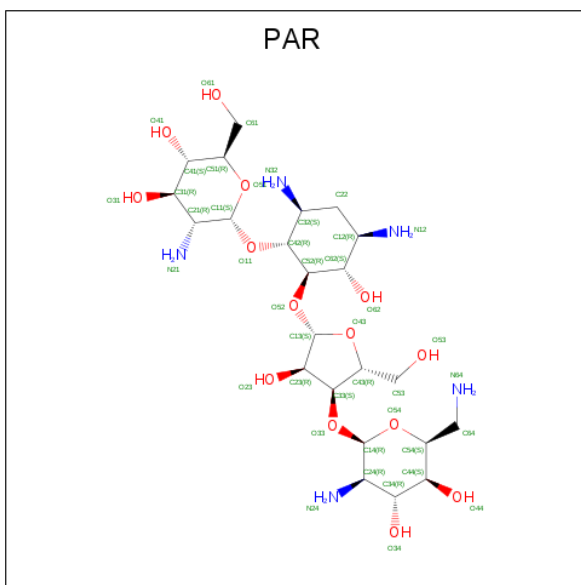
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57 | BY | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 775 | 500 | 148 | 123 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58 | BZ | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1403 | 897 | 252 | 252 | 2 | | | |

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).

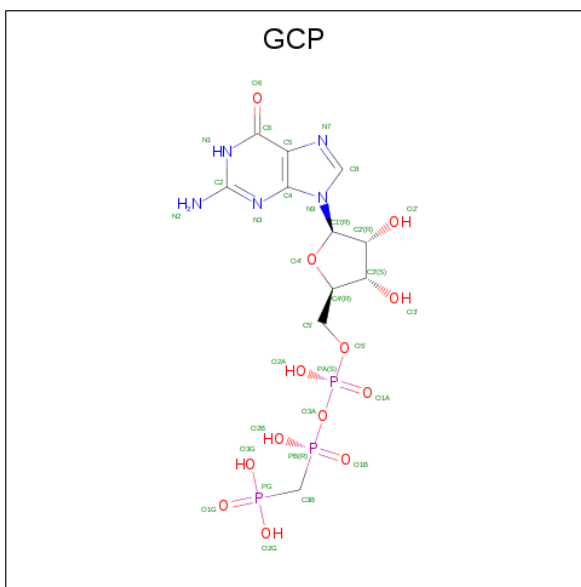


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 59 | AA | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60 | B9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | AD | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | AN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



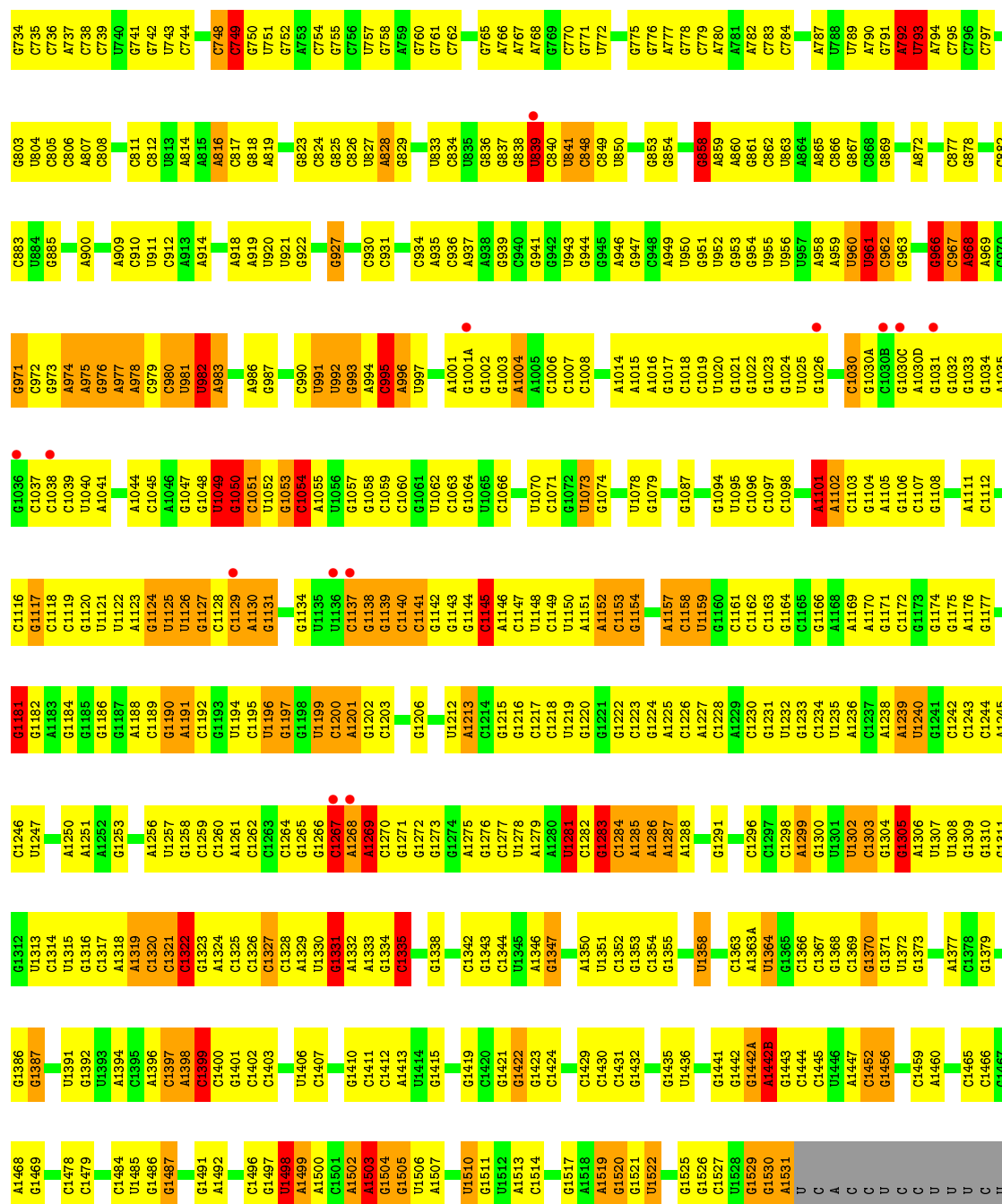
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 61 | AZ | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 32 | 11 | 5 | 13 | 3 | | |

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 62 | AZ | 1 | Total Mg 1 1 | 0 | 0 |

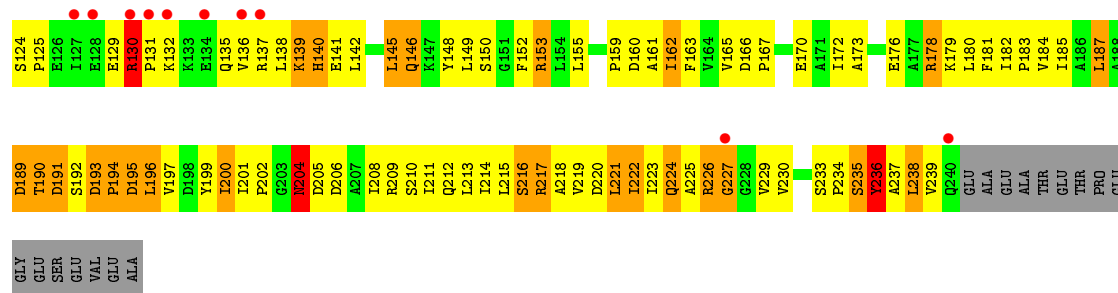
- Molecule 63 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 63 | AZ | 1 | Total O 1 1 | 0 | 0 |

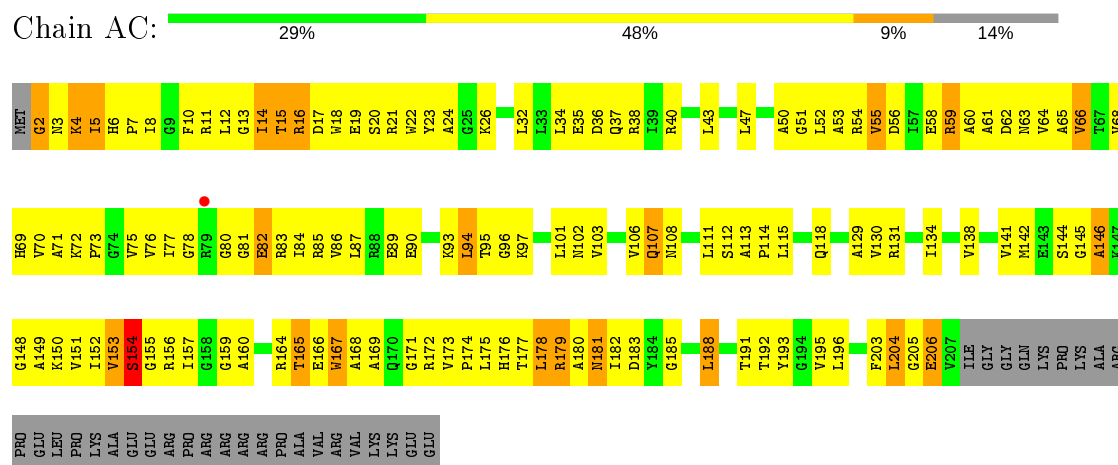


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

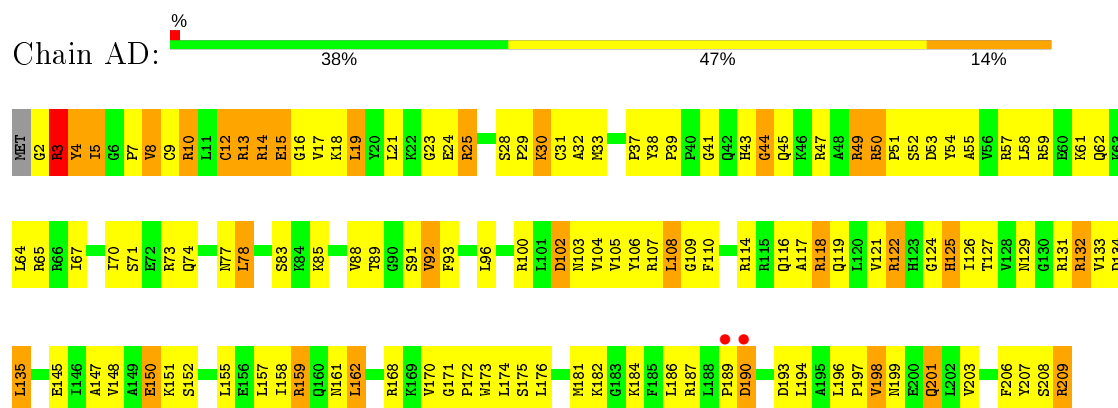




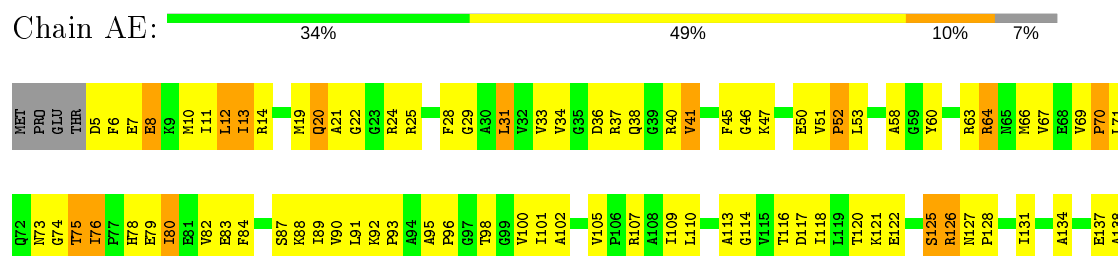
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

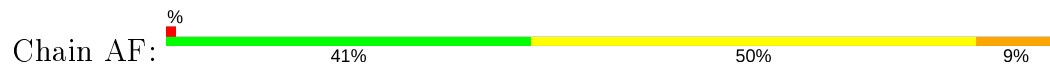


- Molecule 5: 30S RIBOSOMAL PROTEIN S5

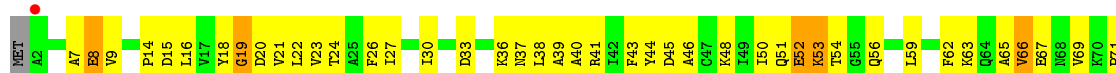




• Molecule 6: 30S RIBOSOMAL PROTEIN S6



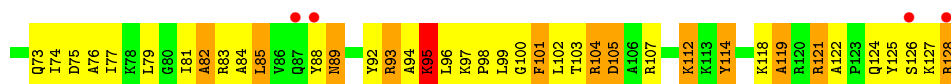
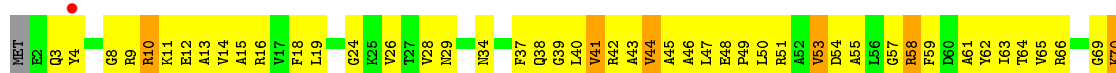
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

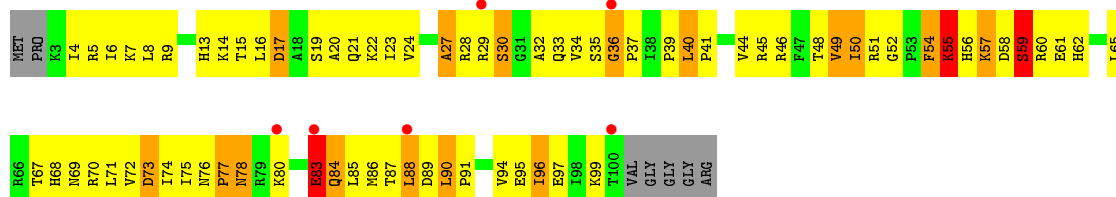


• Molecule 9: 30S RIBOSOMAL PROTEIN S9




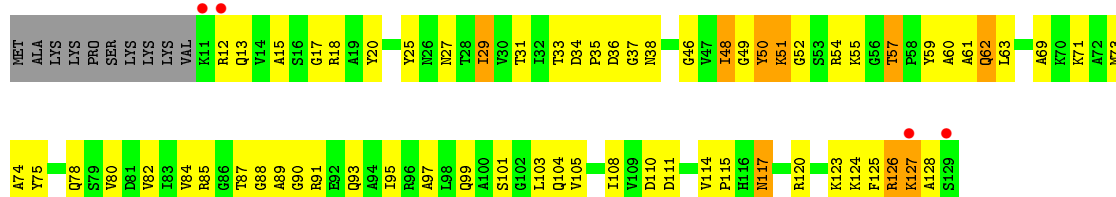
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ: 



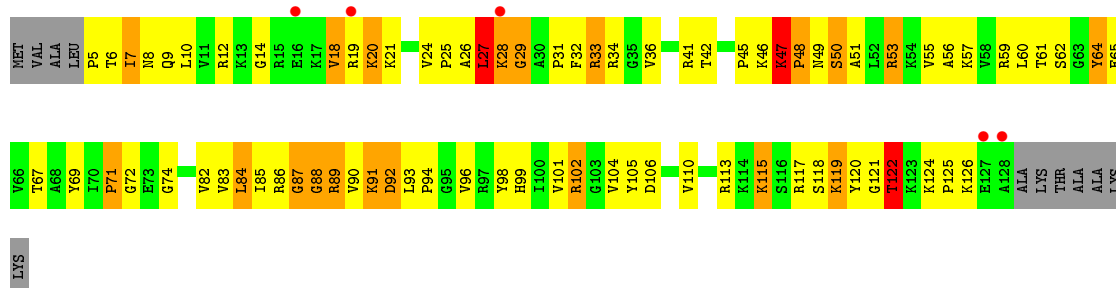
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK: 

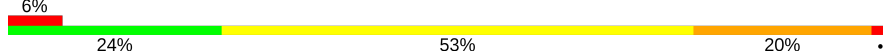


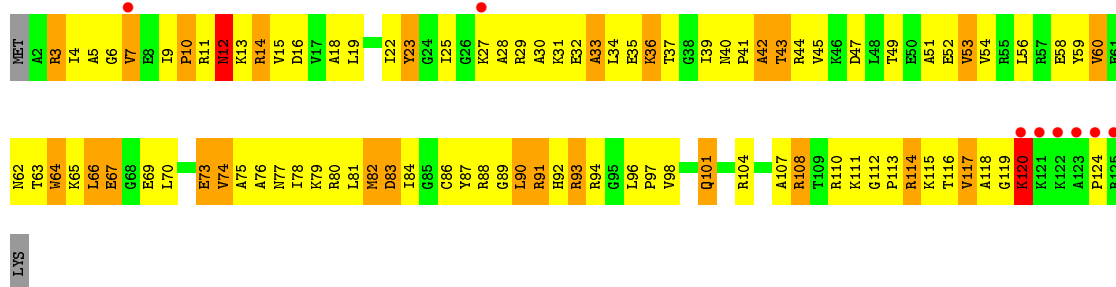
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL: 



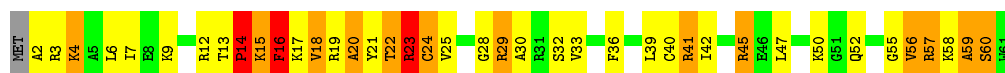
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM: 



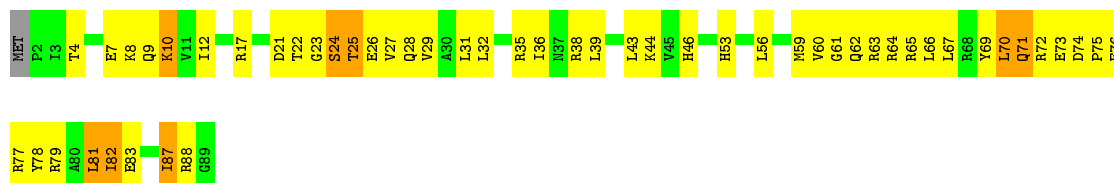
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN: 



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 40% 49% 9%



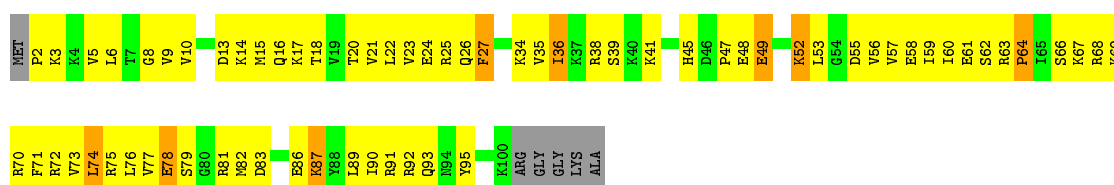
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 33% 51% 10% 6%



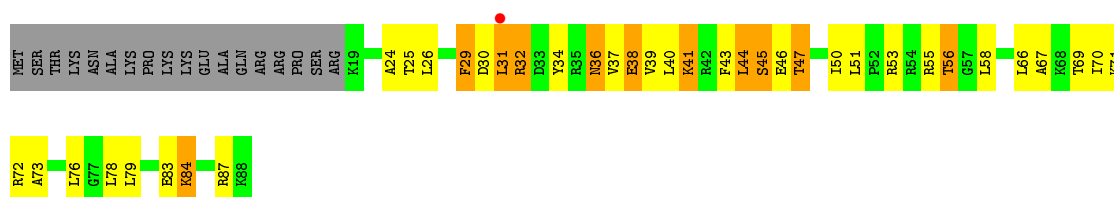
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 30% 57% 8% 6%



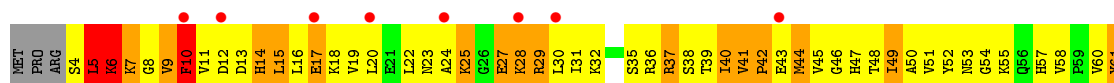
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

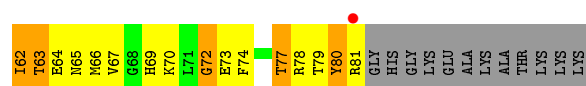
Chain AR: 36% 31% 13% 20%



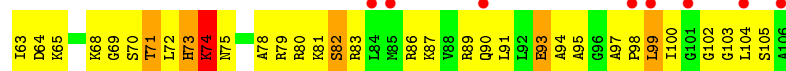
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 10% 11% 47% 23% 16%





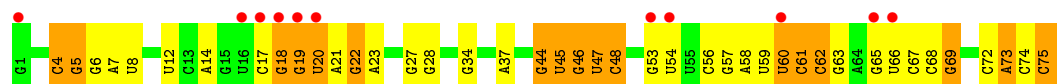
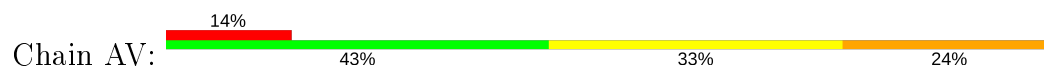
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



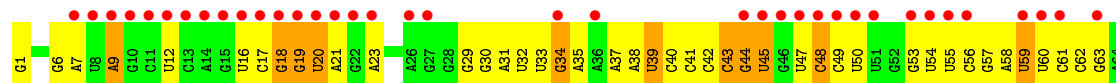
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

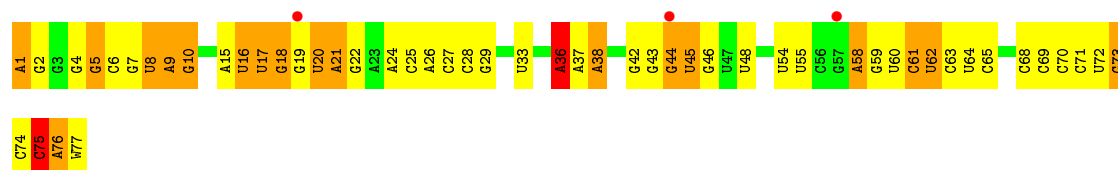


• Molecule 23: MRNA

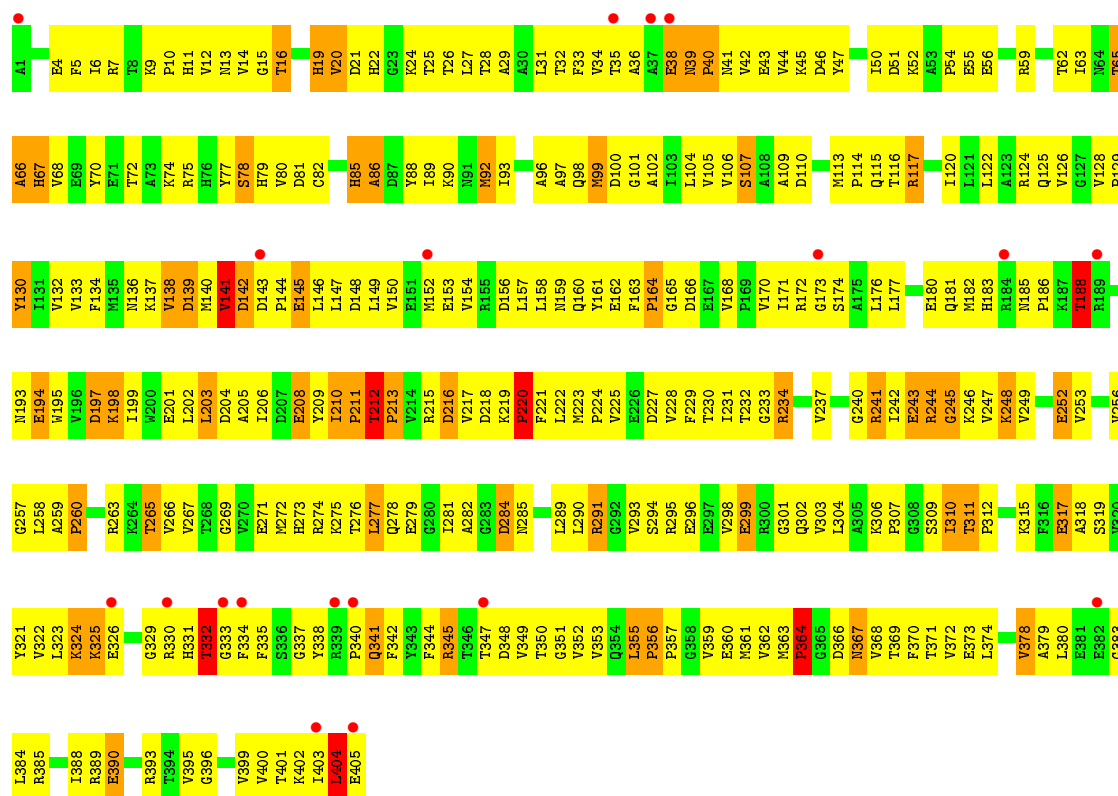


• Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

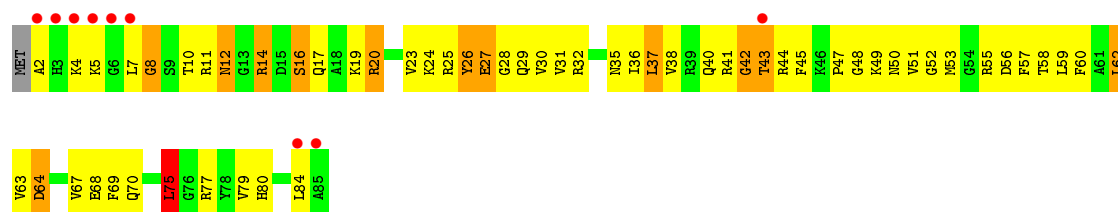


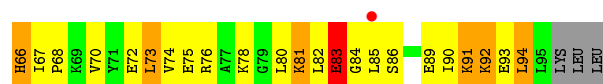


• Molecule 25: ELONGATION FACTOR TU

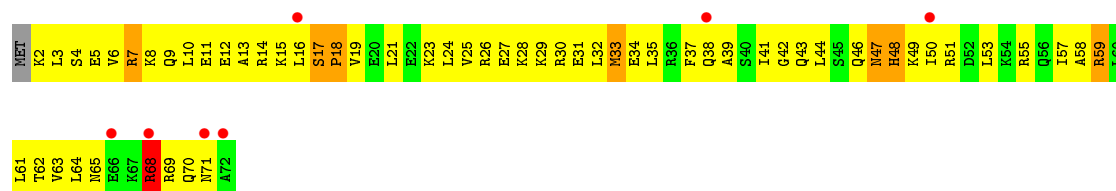


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

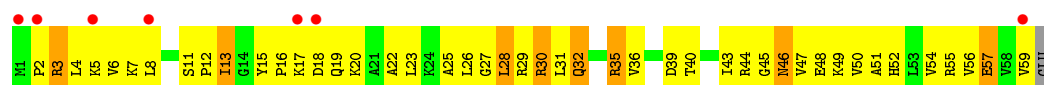




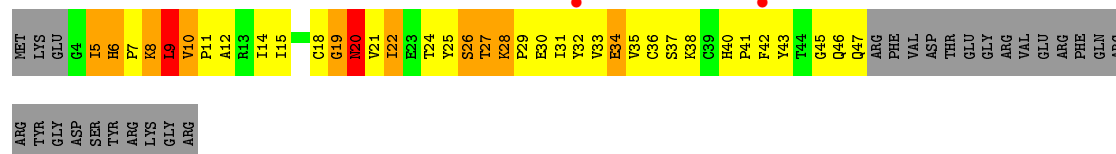
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



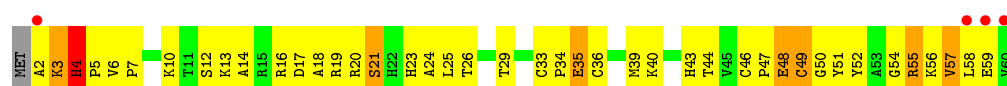
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



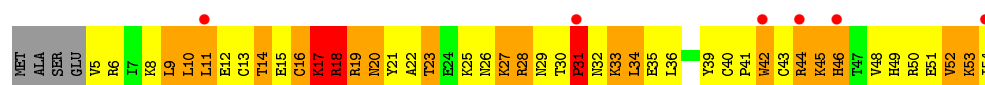
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 31: 50S RIBOSOMAL PROTEIN L32

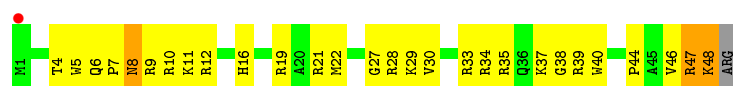


• Molecule 32: 50S RIBOSOMAL PROTEIN L33



• Molecule 33: 50S RIBOSOMAL PROTEIN L34

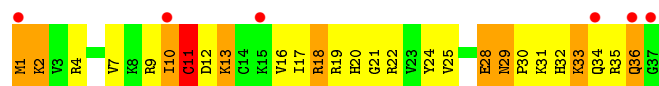




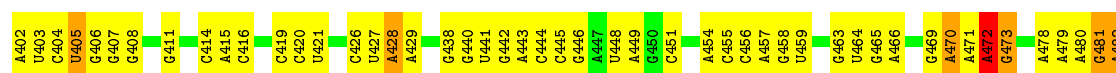
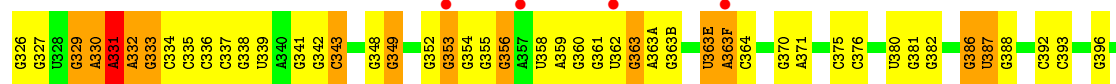
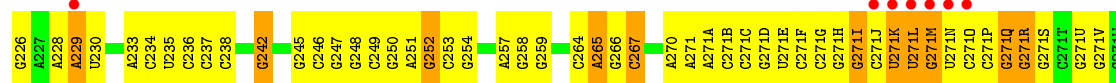
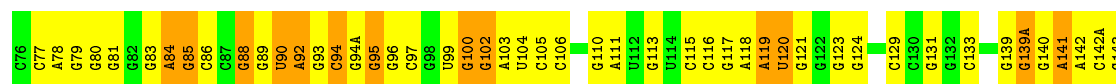
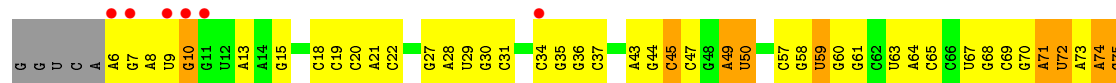
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



• Molecule 35: 50S RIBOSOMAL PROTEIN L36

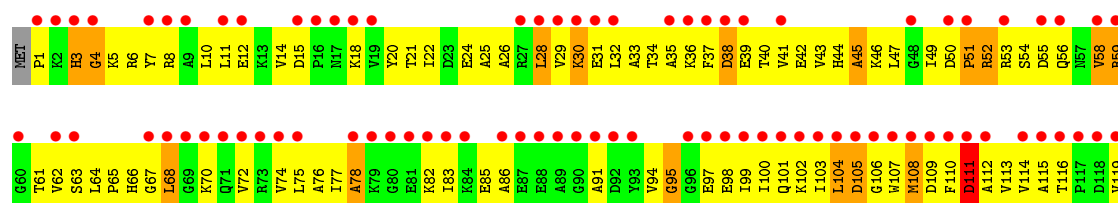


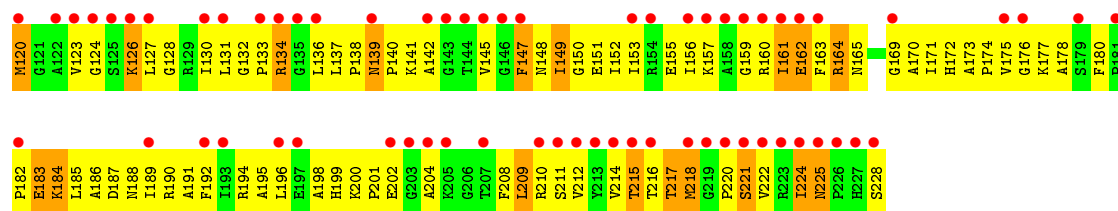
• Molecule 36: 23S RIBOSOMAL RNA



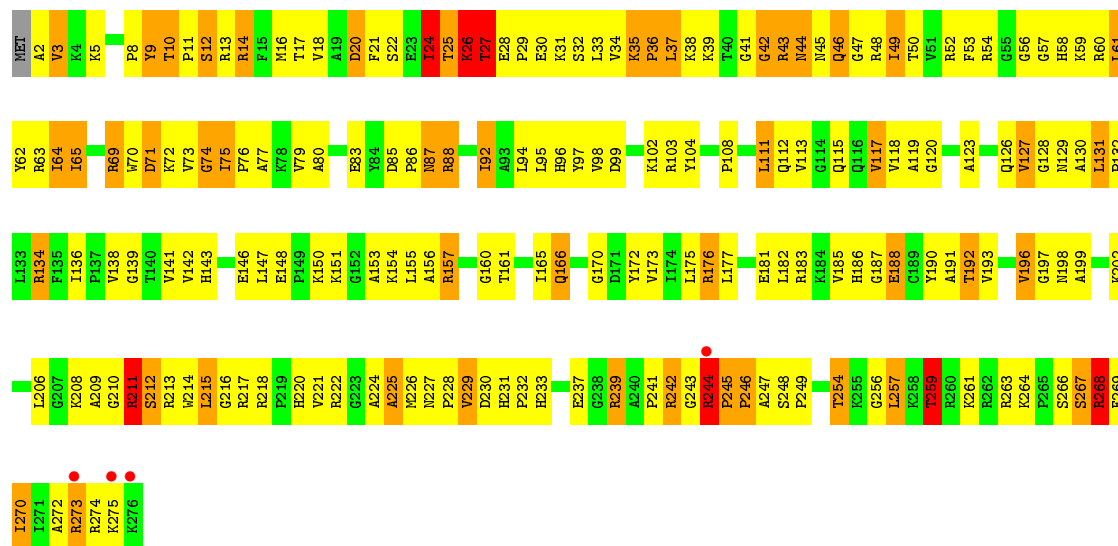
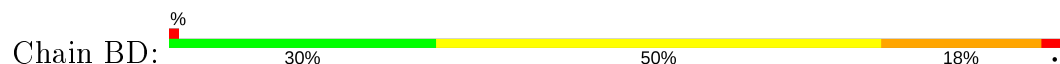
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
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| U1205 | G1206 | C1207 | C1208 | G1209 | A1210 | U1211 | G1212 | A1213 | A1214 | G1215 | G1216 | G1217 | C1218 | G1219 | A1220 | C1221 | C1221A | C1222 | G1223 | C1224 | G1225 | A1226 | G1227 | G1228 | G1229 | G1230 | U1231 | G1232 | C1233 | U1234 | G1235 | | G1238 | G1239 | U1240 | A1241 | A1242 | G1243 | G1244 | G1245 | A1246 | A1247 | G1248 | C1251 | G1252 | A1253 | A1254 | U1255 | G1256 | C1257 | G1258 | U1259 | G1260 | U1198 | U1199 | G1202 | G1203 | A1204 | U1263 | G1264 | A1265 | G1266 | | |
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| C1140 | U1141 | A1142 | A1143 | G1144 | C1145 | | | A1148 | G1149 | C1150 | G1151 | C1152 | C1153 | G1154 | A1155 | A1156 | G1157 | C1158 | U1159 | G1160 | G1161 | G1162 | G1163 | G1164 | U1165 | G1166 | U1167 | G1168 | G1169 | G1170 | G1171 | G1172 | A1173 | A1174 | U1175 | G1176 | A1177 | C1178 | C1179 | C1180 | G1184 | C1185 | G1186 | U1187 | U1188 | A1189 | G1190 | G1191 | G1192 | G1193 | A1194 | G1195 | U1198 | U1199 | G1202 | G1203 | A1204 | U1263 | G1264 | A1265 | G1266 | | | |
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2349 | G2350 | G2351 | G2354 | G2355 | G2356 | G2357 | A2360 | G2361 | G2362 | G2363 | G2364 | G2365 | G2366 | G2367 | G2368 | G2369 | G2370 | G2371 | G2372 | G2373 | G2374 | G2375 | A2376 | A2377 | A2378 | G2379 | G2383 | G2384 | G2385 | G2386 | G2387 | G2391 | A2392 | G2393 | G2394 | G2395 | G2396 | G2397 | G2398 | G2399 | G2400 | U2401 | G2402 | G2405 | U2406 | U2407 | U2408 | G2409 | G2410 | G2411 | A2412 | G2413 | G2414 | G2415 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2279 | G2280 | G2282 | G2283 | G2284 | G2285 | A2286 | G2287 | A2288 | G2289 | G2290 | G2291 | G2292 | G2293 | A2294 | G2295 | G2296 | G2297 | G2298 | G2299 | G2303 | G2304 | A2305 | G2306 | G2307 | G2308 | A2309 | A2310 | A2311 | G2312 | G2313 | G2314 | G2315 | G2316 | G2317 | G2318 | A2319 | A2320 | A2327 | A2328 | G2329 | G2330 | G2331 | U2332 | A2333 | A2336 | G2339 | G2340 | G2341 | G2342 | G2343 | U2344 | G2345 | A2346 | G2347 | U2348 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| G2141 | G2142 | G2143 | U2144 | G2145 | G2146 | G2147 | G2148 | G2149 | G2150 | G2151 | G2152 | G2153 | G2154 | G2155 | G2156 | G2157 | G2158 | G2159 | G2160 | G2161 | G2162 | G2163 | G2164 | G2165 | G2166 | G2167 | G2168 | A2169 | A2170 | G2171 | G2172 | G2173 | U2174 | G2175 | G2176 | G2177 | G2178 | G2179 | U2180 | G2181 | G2182 | G2183 | G2184 | G2185 | G2186 | G2187 | G2188 | G2189 | G2190 | G2191 | G2192 | G2193 | G2194 | G2195 | G2196 | U2197 | A2198 | A2199 | G2200 | G2201 | G2202 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2078 | U2079 | G2080 | G2085 | G2086 | G2087 | G2088 | U2089 | G2090 | U2091 | G2092 | G2093 | G2094 | G2095 | U2096 | G2097 | U2098 | G2099 | G2100 | G2101 | U2102 | G2103 | G2104 | G2105 | G2106 | G2107 | G2108 | G2109 | G2110 | G2111 | G2112 | U2113 | A2114 | G2115 | G2116 | G2117 | G2118 | G2119 | G2120 | G2121 | U2122 | G2123 | G2124 | G2125 | A2126 | G2127 | G2128 | G2129 | U2130 | G2131 | G2132 | U2133 | G2134 | G2135 | G2136 | G2137 | G2138 | G2139 | G2140 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| A1936 | A1937 | A1938 | U1939 | U1940 | U1943 | U1946 | U1947 | G1948 | U1949 | U1950 | U1951 | U1952 | U1953 | U1954 | U1955 | U1956 | U1957 | U1958 | U1959 | U1960 | U1961 | U1962 | U1963 | U1964 | U1965 | U1966 | U1967 | U1968 | U1969 | U1970 | U1971 | U1972 | G1973 | G1974 | U1975 | U1976 | U1977 | U1978 | U1979 | U1980 | U1981 | U1982 | U1983 | U1984 | U1985 | U1986 | U1987 | U1988 | U1989 | U1990 | U1991 | U1992 | U1993 | U1994 | U1995 | U1996 | U1997 | U1998 | U1999 | G2000 | A2001 | G2002 | G2003 | G2004 | G2005 | G2006 | G2007 | G2008 | G2009 | G2010 | U2011 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U1851 | U1852 | A1853 | A1854 | G1855 | G1856 | G1857 | G1858 | A1859 | G1860 | G1861 | G1862 | G1863 | G1864 | G1865 | G1866 | U1867 | G1868 | G1869 | G1870 | G1871 | G1872 | G1873 | G1874 | G1875 | G1876 | G1877 | G1878 | G1879 | G1880 | G1881 | G1882 | G1883 | G1884 | G1885 | G1886 | G1887 | G1888 | A1889 | A1890 | G1891 | G1892 | G1893 | G1894 | G1895 | G1896 | G1897 | G1898 | G1899 | G1900 | A1901 | A1902 | G1903 | G1904 | G1905 | G1906 | G1907 | G1908 | G1909 | G1910 | G1911 | G1912 | A1913 | G1914 | G1915 | A1916 | U1917 | G1918 | G1919 | G1920 | G1921 | G1922 | G1923 | G1924 | G1925 | G1926 | G1927 | G1928 | G1929 | G1930 | U1931 | A1932 | A1933 | G1934 | A1935 | U1936 | U1937 | U1938 | U1939 | U1940 | U1941 | U1942 | U1943 | U1944 | U1945 | U1946 | U1947 | U1948 | U1949 | U1950 | U1951 | U1952 | U1953 | U1954 | U1955 | U1956 | U1957 | U1958 | U1959 | U1960 | U1961 | U1962 | U1963 | U1964 | U1965 | U1966 | U1967 | U1968 | U1969 | U1970 | U1971 | U1972 | U1973 | U1974 | U1975 | U1976 | U1977 | U1978 | U1979 | U1980 | U1981 | U1982 | U1983 | U1984 | U1985 | U1986 | U1987 | U1988 | U1989 | U1990 | U1991 | U1992 | U1993 | U1994 | U1995 | U1996 | U1997 | U1998 | U1999 | G2000 | A2001 | G2002 | G2003 | G2004 | G2005 | G2006 | G2007 | G2008 | G2009 | G2010 | U2011 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C1781 | C1782 | A1783 | A1784 | A1785 | A1786 | A1787 | C1788 | A1789 | C1790 | A1791 | U1794 | C1795 | U1796 | C1797 | U1798 | G1799 | C1800 | C1801 | A1802 | C1803 | A1804 | U1805 | G1806 | G1807 | C1808 | U1809 | A1810 | G1811 | A1812 | G1813 | G1816 | U1817 | U1818 | A1819 | U1820 | G1824 | A1825 | G1826 | C1827 | G1828 | A1829 | C1830 | G1831 | G1832 | G1833 | G1834 | C1835 | C1836 | C1837 | A1838 | C1839 | C1840 | C1841 | C1842 | C1843 | C1844 | G1845 | C1846 | C1847 | C1848 | C1849 | C1850 | C1851 | C1852 | C1853 | C1854 | C1855 | C1856 | C1857 | C1858 | C1859 | C1860 | C1861 | C1862 | C1863 | C1864 | C1865 | C1866 | C1867 | C1868 | C1869 | C1870 | C1871 | C1872 | C1873 | C1874 | C1875 | C1876 | C1877 | C1878 | C1879 | C1880 | C1881 | C1882 | C1883 | C1884 | C1885 | C1886 | C1887 | C1888 | C1889 | C1890 | C1891 | C1892 | C1893 | C1894 | C1895 | C1896 | C1897 | C1898 | C1899 | C1900 | C1901 | C1902 | C1903 | C1904 | C1905 | C1906 | C1907 | C1908 | C1909 | C1910 | C1911 | C1912 | C1913 | C1914 | C1915 | C1916 | C1917 | C1918 | C1919 | C1920 | C1921 | C1922 | C1923 | C1924 | C1925 | C1926 | C1927 | C1928 | C1929 | C1930 | C1931 | C1932 | C1933 | C1934 | C1935 | C1936 | C1937 | C1938 | C1939 | C1940 | C1941 | C1942 | C1943 | C1944 | C1945 | C1946 | C1947 | C1948 | C1949 | C1950 | C1951 | C1952 | C1953 | C1954 | C1955 | C1956 | C1957 | C1958 | C1959 | C1960 | C1961 | C1962 | C1963 | C1964 | C1965 | C1966 | C1967 | C1968 | C1969 | C1970 | C1971 | C1972 | C1973 | C1974 | C1975 | C1976 | C1977 | C1978 | C1979 | C1980 | C1981 | C1982 | C1983 | C1984 | C1985 | C1986 | C1987 | C1988 | C1989 | C1990 | C1991 | C1992 | C1993 | C1994 | C1995 | C1996 | C1997 | C1998 | C1999 | G2000 | A2001 | G2002 | G2003 | G2004 | G2005 | G2006 | G2007 | G2008 | G2009 | G2010 | U2011 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U1692 | G1696 | G1697 | A1698 | A1701 | G1702 | C1708 | U1709 | C1710 | G1714 | G1717 | G1718 | G1719 | U1720 | G1721 | A1722 | U1723 | U1724 | U1725 | U1726 | U1727 | U1728 | U1729 | U1730 | U1731 | U1732 | U1733 | U1734 | U1735 | U1736 | U1737 | U1738 | U1739 | U1740 | A1741 | G1742 | C1743 | C1744 | C1745 | G1747 | G1748 | A1749 | G1750 | C1751 | U1752 | U1753 | U1754 | U1755 | U1756 | U1757 | U1758 | U1759 | U1760 | U1761 | U1762 | G1763 | G1764 | C1765 | G1766 | C1767 | U1768 | U1769 | C1770 | C1771 | U1772 | A1773 | C1774 | U1775 | U1776 | U1777 | U1778 | U1779 | U1780 | U1781 | U1782 | U1783 | U1784 | U1785 | U1786 | U1787 | U1788 | U1789 | U1790 | U1791 | U1792 | U1793 | U1794 | U1795 | U1796 | U1797 | U1798 | U1799 | U1800 | U1801 | U1802 | U1803 | U1804 | U1805 | U1806 | U1807 | U1808 | U1809 | U1810 | U1811 | U1812 | U1813 | U1814 | U1815 | U1816 | U1817 | U1818 | U1819 | U1820 | U1821 | U1822 | U1823 | U1824 | U1825 | U1826 | U1827 | U1828 | U1829 | U1830 | U1831 | U1832 | U1833 | U1834 | U1835 | U1836 | U1837 | U1838 | U1839 | U1840 | U1841 | U1842 | U1843 | U1844 | U1845 | U1846 | U1847 | U1848 | U1849 | U1850 | U1851 | U1852 | U1853 | U1854 | U1855 | U1856 | U1857 | U1858 | U1859 | U1860 | U1861 | U1862 | U1863 | U1864 | U1865 | U1866 | U1867 | U1868 | U1869 | U1870 | U1871 | U1872 | U1873 | U1874 | U1875 | U1876 | U1877 | U1878 | U1879 | U1880 | U1881 | U1882 | U1883 | U1884 | U1885 | U1886 | U1887 | U1888 | U1889 | U1890 | U1891 | U1892 | U1893 | U1894 | U1895 | U1896 | U1897 | U1898 | U1899 | U1900 | U1901 | U1902 | U1903 | U1904 | U1905 | U1906 | U1907 | U1908 | U1909 | U1910 | U1911 | U1912 | U1913 | U1914 | U1915 | U1916 | U1917 | U1918 | U1919 | U1920 | U1921 | U1922 | U1923 | U1924 | U1925 | U1926 | U1927 | U1928 | U1929 | U1930 | U1931 | U1932 | U1933 | U1934 | U1935 | U1936 | U1937 | U1938 | U1939 | U1940 | U1941 | U1942 | U1943 | U1944 | U1945 | U1946 | U1947 | U1948 | U1949 | U1950 | U1951 | U1952 | U1953 | U1954 | U1955 | U1956 | U1957 | U1958 | U1959 | U1960 | U1961 | U1962 | U1963 | U1964 | U1965 | U1966 | U1967 | U1968 | U1969 | U1970 | U1971 | U1972 | U1973 | U1974 | U1975 | U1976 | U1977 | U1978 | U1979 | U1980 | U1981 | U1982 | U1983 | U1984 | U1985 | U1986 | U1987 | U1988 | U1989 | U1990 | U1991 | U1992 | U1993 | U1994 | U1995 | U1996 | U1997 | U1998 | U1999 | G2000 | A2001 | G2002 | G2003 | G2004 | G2005 | G2006 | G2007 | G2008 | G2009 | G2010 | U2011 |
| A1542 | C1543 | A1544 | C1547 | C1548 | C1549 | C1550 | C1551 | G1552 | A1553 | A1554 | C1555 | C1556 | C1557 | A1558 | G1559 | A1566 | A1567 | C1568 | C1569 | C1570 | C1571 | C1572 | C1573 | C1574 | C1575 | U1576 | U1577 | C1578 | U1579 | A1580 | C1581 | C1582 | A1583 | C1584 | C1585 | C1586 | A1587 | C1588 | C1589 | U1590 | C1591 | C1592 | G1593 | C1594 | A1595 | A1596 | C1597 | C1598 | C1599 | U1602 | A1603 | C1604 | C1605 | C1606 | C1607 | A1608 | A1609 | U1610 | C1611 | C1612 | C1613 | C1614 | C1615 | A1616 | A1617 | A1618 | C1625 | G1626 | C1636 | A1637 | C1638 | U1639 | U1640 | A1641 | A1642 | G1643 | C1644 | A1645 | C1646 | C1647 | C1648 | C1649 | C1650 | A1651 | A1652 | C1653 | C1654 | C1655 | C1656 | C1657 | C1658 | U1659 | C1664 | A1665 | C1666 | C1667 | A1668 | A1669 | C1670 | C1671 | C1672 | C1673 | C1674 | C1675 | C1676 | C1677 | C1678 | C1679 | C1680 | C1681 | C1682 | C1683 | C1684 | C1685 | C1686 | C1687 | C1688 | C1689 | C1690 | C1691 | C1692 | C1693 | C1694 | C1695 | C1696 | C1697 | C1698 | C1699 | C1700 | C1701 | C1702 | C1703 | C1704 | C1705 | C1706 | C1707 | C1708 | C1709 | C1710 | C1711 | C1712 | C1713 | C1714 | C1715 | C1716 | C1717 | C1718 | C1719 | C1720 | C1721 | C1722 | C1723 | C1724 | C1725 | C1726 | C1727 | C1728 | C1729 | C1730 | C1731 | C1732 | C1733 | C1734 | C1735 | C1736 | C1737 | C1738 | C1739 | C1740 | C1741 | C1742 | C1743 | C1744 | C1745 | C1746 | C1747 | C1748 | C1749 | C1750 | C1751 | C1752 | C1753 | C1754 | C1755 | C1756 | C1757 | C1758 | C1759 | C1760 | C1761 | C1762 | C1763 | C1764 | C1765 | C1766 | C1767 | C1768 | C1769 | C1770 | C1771 | C1772 | C1773 | C1774 | C1775 | C1776 | C177 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

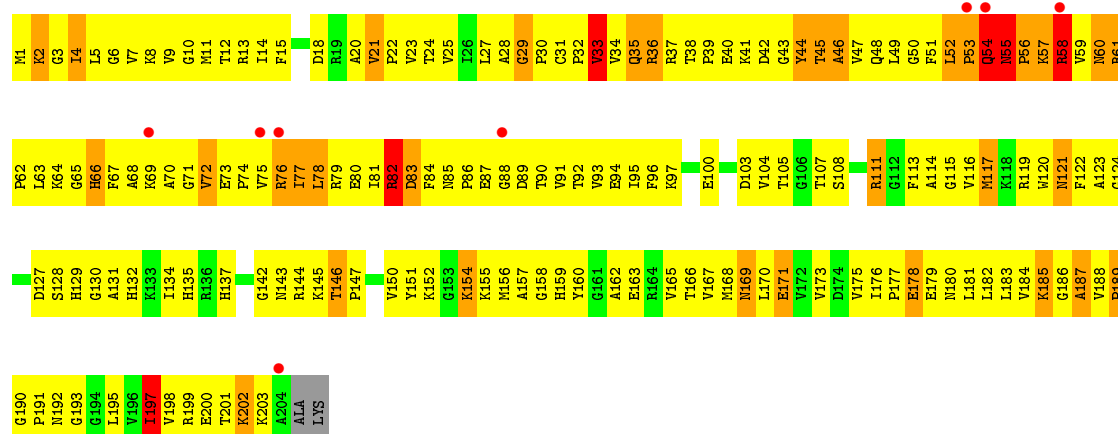




• Molecule 39: 50S RIBOSOMAL PROTEIN L2

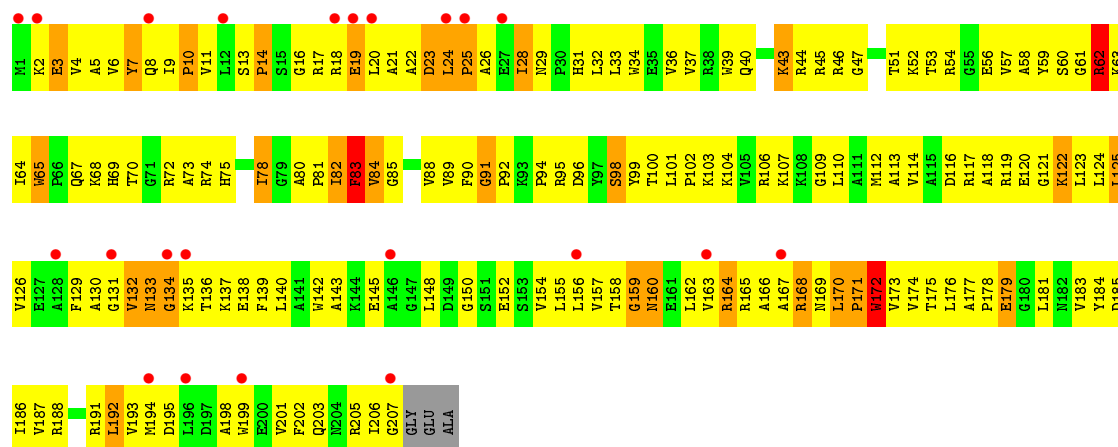


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

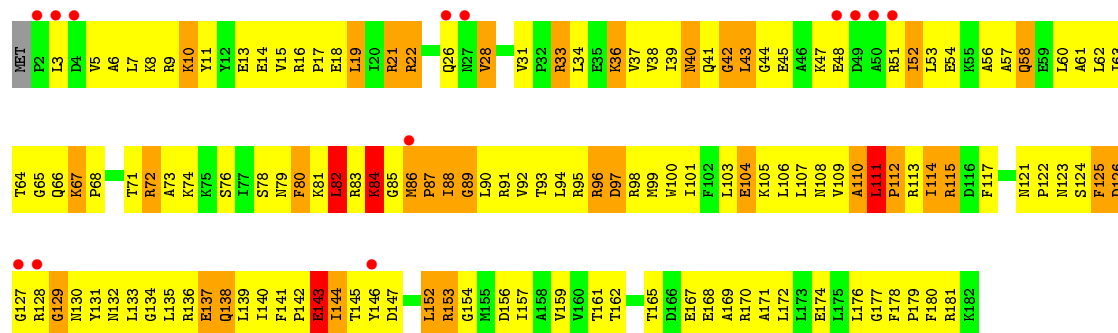


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

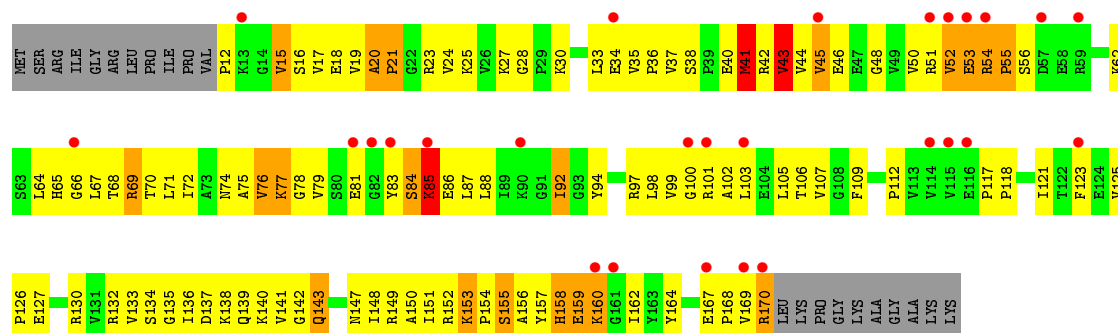




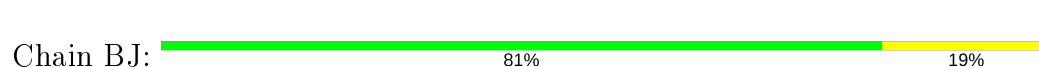
• Molecule 42: 50S RIBOSOMAL PROTEIN L5




• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 44: 50S RIBOSOMAL PROTEIN L10



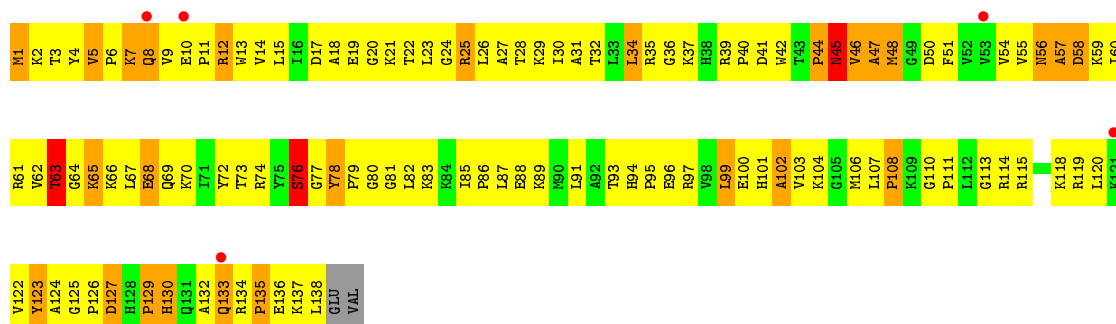
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:  84% 16%



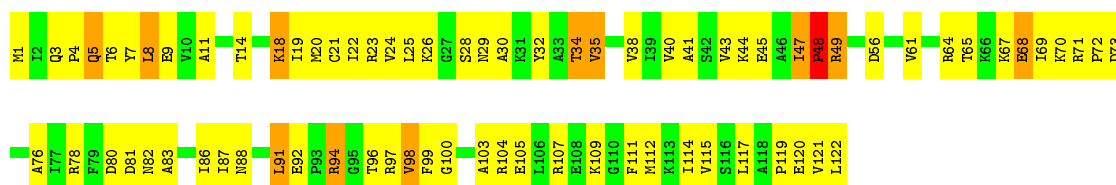
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:  4% 15% 63% 19%




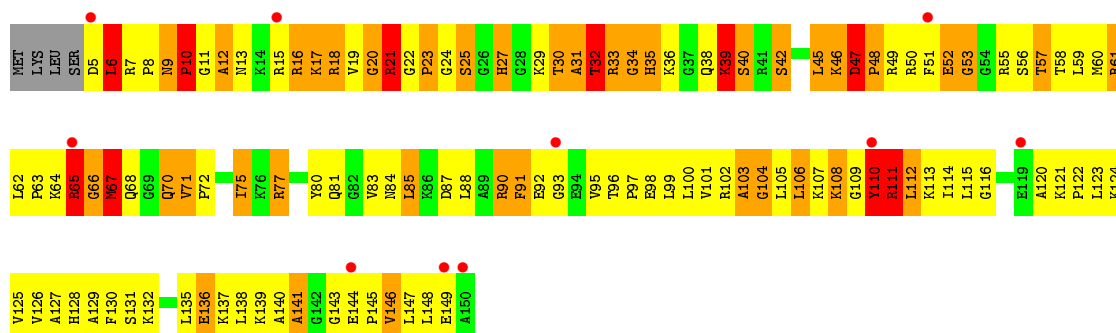
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:  38% 52% 9%



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

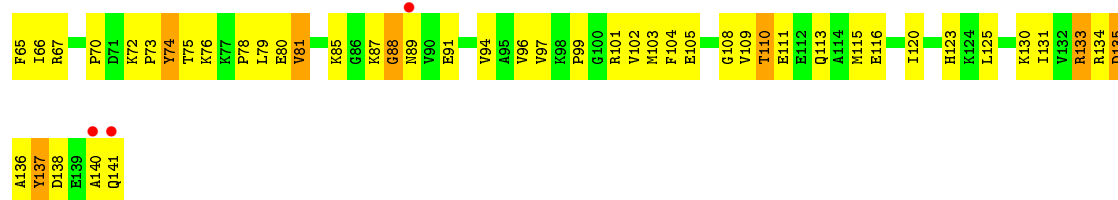
Chain BP:  7% 17% 48% 26% 7%



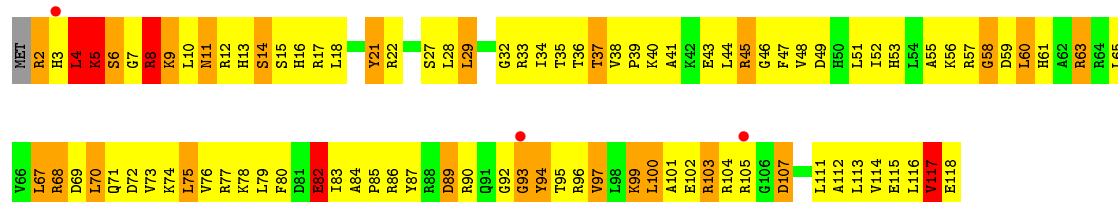
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:  4% 34% 54% 12%

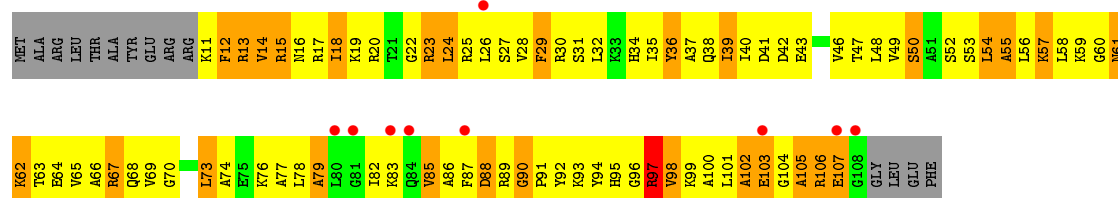
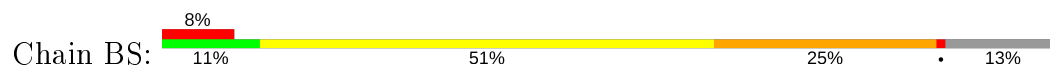




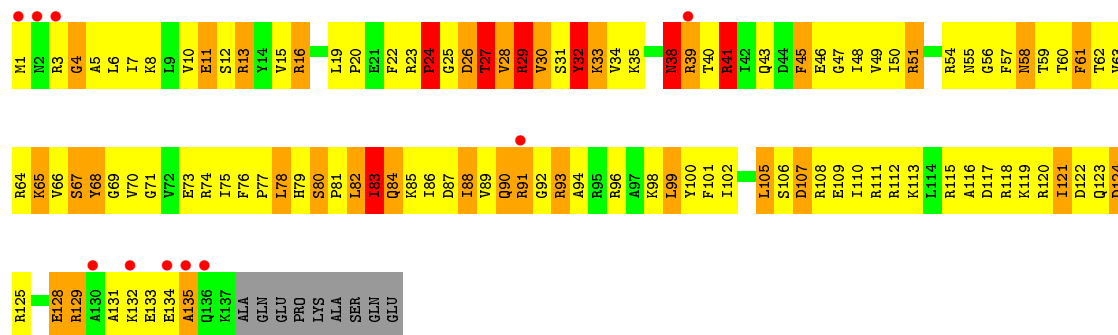
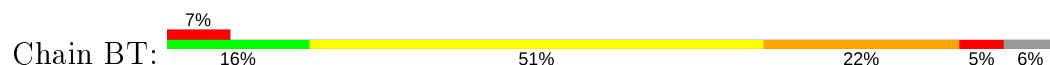
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



• Molecule 51: 50S RIBOSOMAL PROTEIN L18

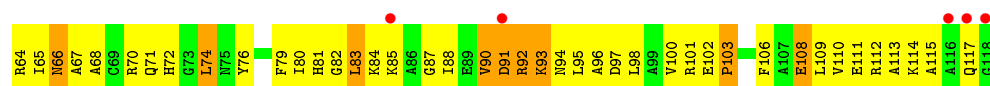


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

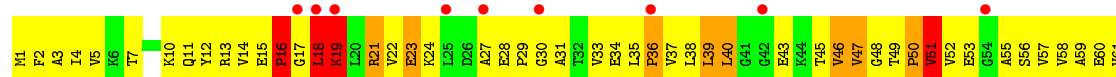


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

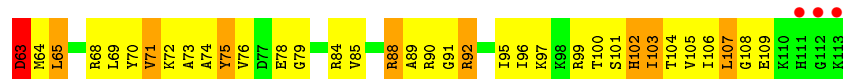




• Molecule 54: 50S RIBOSOMAL PROTEIN L21



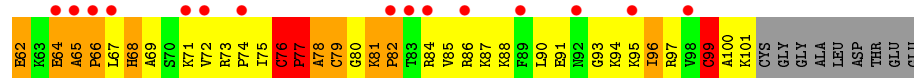
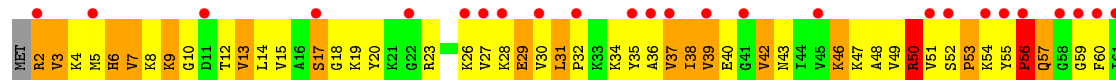
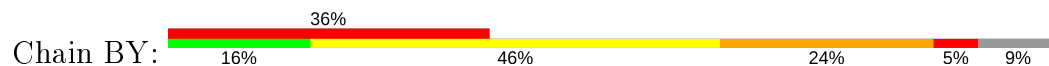
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



• Molecule 56: 50S RIBOSOMAL PROTEIN L23

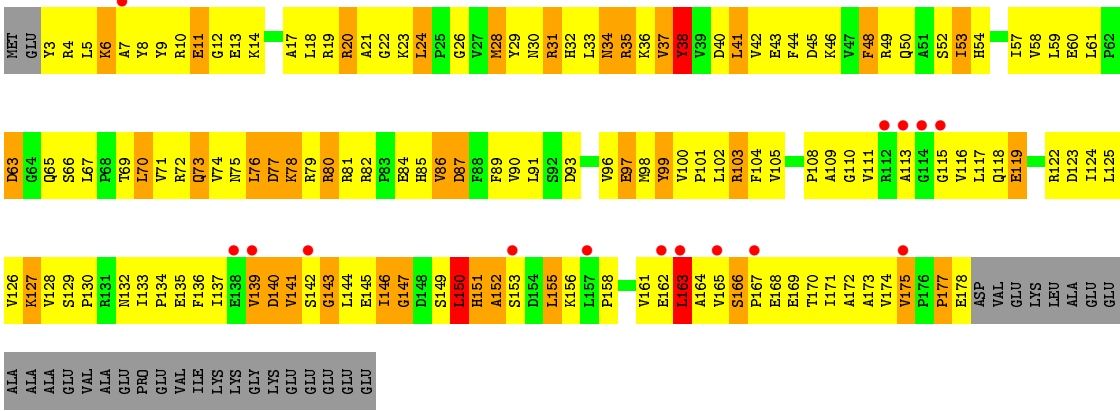


• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 197.60Å 274.93Å 282.46Å 90.00° 91.81° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.10 48.00 – 3.01 | Depositor EDS |
| % Data completeness (in resolution range) | 98.8 (50.00-3.10) 95.9 (48.00-3.01) | Depositor EDS |
| R_{merge} | 0.02 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.38 (at 3.01Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.231 , 0.268 0.232 , 0.268 | Depositor DCC |
| R_{free} test set | 28503 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 64.7 | Xtriage |
| Anisotropy | 0.187 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 85.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | 0.018 for -h,l,k 0.019 for -h,-l,-k 0.027 for h,-k,-l | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 153628 | wwPDB-VP |
| Average B, all atoms (Å ²) | 84.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, PAR, 4SU, GCP, MIA, MG, H2U, ZN, 7MG, PSU

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 | 0.58 | 3/36190 (0.0%) | 0.77 | 49/56486 (0.1%) |
| 2 | AB | 0.44 | 0/1935 | 0.72 | 1/2609 (0.0%) |
| 3 | AC | 0.50 | 1/1636 (0.1%) | 0.75 | 0/2205 |
| 4 | AD | 0.44 | 0/1733 | 0.71 | 1/2318 (0.0%) |
| 5 | AE | 0.54 | 0/1162 | 0.75 | 0/1564 |
| 6 | AF | 0.45 | 0/856 | 0.69 | 1/1154 (0.1%) |
| 7 | AG | 0.43 | 0/1276 | 0.66 | 0/1709 |
| 8 | AH | 0.45 | 0/1136 | 0.73 | 0/1527 |
| 9 | AI | 0.45 | 0/1029 | 0.71 | 0/1378 |
| 10 | AJ | 0.49 | 0/807 | 0.78 | 0/1085 |
| 11 | AK | 0.45 | 0/900 | 0.72 | 0/1213 |
| 12 | AL | 0.58 | 0/986 | 0.88 | 2/1320 (0.2%) |
| 13 | AM | 0.42 | 0/998 | 0.79 | 2/1336 (0.1%) |
| 14 | AN | 0.54 | 0/501 | 0.79 | 0/664 |
| 15 | AO | 0.42 | 0/745 | 0.66 | 0/992 |
| 16 | AP | 0.44 | 0/716 | 0.74 | 0/963 |
| 17 | AQ | 0.44 | 0/836 | 0.70 | 0/1117 |
| 18 | AR | 0.47 | 0/579 | 0.76 | 0/768 |
| 19 | AS | 0.44 | 0/642 | 0.72 | 0/865 |
| 20 | AT | 0.39 | 0/765 | 0.72 | 1/1007 (0.1%) |
| 21 | AU | 0.45 | 0/212 | 0.69 | 0/277 |
| 22 | AV | 0.49 | 0/1809 | 0.75 | 0/2819 |
| 22 | AW | 0.45 | 0/1809 | 0.73 | 0/2819 |
| 23 | AX | 0.65 | 0/334 | 0.81 | 0/519 |
| 24 | AY | 0.49 | 1/1618 (0.1%) | 0.78 | 3/2514 (0.1%) |
| 25 | AZ | 0.41 | 0/3203 | 0.68 | 1/4346 (0.0%) |
| 26 | B0 | 0.39 | 0/671 | 0.73 | 0/892 |
| 27 | B1 | 0.44 | 0/738 | 0.74 | 0/981 |
| 28 | B2 | 0.35 | 0/600 | 0.63 | 0/793 |
| 29 | B3 | 0.37 | 0/472 | 0.66 | 0/634 |
| 30 | B4 | 0.41 | 0/349 | 0.60 | 0/474 |
| 31 | B5 | 0.38 | 0/473 | 0.72 | 0/639 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | B6 | 0.66 | 0/440 | 0.98 | 2/586 (0.3%) |
| 33 | B7 | 0.43 | 0/426 | 0.71 | 0/561 |
| 34 | B8 | 0.55 | 0/515 | 0.83 | 1/679 (0.1%) |
| 35 | B9 | 0.45 | 0/310 | 0.65 | 0/407 |
| 36 | BA | 0.51 | 2/69976 (0.0%) | 0.74 | 57/109244 (0.1%) |
| 37 | BB | 0.40 | 0/2853 | 0.72 | 0/4451 |
| 38 | BC | 0.42 | 2/1774 (0.1%) | 0.67 | 0/2391 |
| 39 | BD | 0.57 | 0/2195 | 0.91 | 3/2955 (0.1%) |
| 40 | BE | 0.41 | 0/1596 | 0.71 | 0/2153 |
| 41 | BF | 0.37 | 0/1658 | 0.68 | 0/2244 |
| 42 | BG | 0.37 | 0/1499 | 0.68 | 1/2016 (0.0%) |
| 43 | BH | 0.36 | 0/1245 | 0.70 | 0/1682 |
| 46 | BN | 0.36 | 0/1131 | 0.69 | 0/1525 |
| 47 | BO | 0.50 | 0/943 | 0.76 | 0/1269 |
| 48 | BP | 0.48 | 0/1131 | 0.98 | 4/1504 (0.3%) |
| 49 | BQ | 0.45 | 0/1143 | 0.69 | 0/1527 |
| 50 | BR | 0.35 | 0/974 | 0.74 | 1/1302 (0.1%) |
| 51 | BS | 0.42 | 0/778 | 0.77 | 0/1036 |
| 52 | BT | 0.44 | 0/1155 | 0.80 | 2/1542 (0.1%) |
| 53 | BU | 0.39 | 0/975 | 0.65 | 0/1297 |
| 54 | BV | 0.36 | 0/790 | 0.70 | 0/1057 |
| 55 | BW | 0.37 | 0/907 | 0.68 | 0/1216 |
| 56 | BX | 0.43 | 0/739 | 0.66 | 1/993 (0.1%) |
| 57 | BY | 0.38 | 0/788 | 0.73 | 0/1051 |
| 58 | BZ | 0.39 | 0/1435 | 0.67 | 0/1949 |
| All | All | 0.50 | 9/165092 (0.0%) | 0.74 | 133/246624 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 3 | 51 |
| 23 | AX | 0 | 1 |
| 24 | AY | 2 | 1 |
| 36 | BA | 4 | 70 |
| 37 | BB | 0 | 2 |
| All | All | 9 | 125 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | BA | 761 | A | C5-C6 | -8.40 | 1.33 | 1.41 |
| 24 | AY | 1 | A | OP3-P | -6.72 | 1.53 | 1.61 |
| 38 | BC | 120 | MET | CG-SD | 6.37 | 1.97 | 1.81 |
| 1 | AA | 1267 | C | C5'-C4' | 6.34 | 1.58 | 1.51 |
| 36 | BA | 2506 | U | N1-C2 | 5.99 | 1.44 | 1.38 |
| 3 | AC | 2 | GLY | N-CA | 5.54 | 1.54 | 1.46 |
| 38 | BC | 218 | MET | CG-SD | 5.38 | 1.95 | 1.81 |
| 1 | AA | 858 | G | N1-C2 | 5.19 | 1.42 | 1.37 |
| 1 | AA | 299 | G | C6-O6 | 5.03 | 1.28 | 1.24 |

All (133) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1 | AA | 1498 | U | C2'-C3'-O3' | 10.24 | 132.03 | 109.50 |
| 1 | AA | 508 | C | C2'-C3'-O3' | 10.16 | 131.85 | 109.50 |
| 36 | BA | 654(I) | C | N1-C1'-C2' | 10.03 | 127.04 | 114.00 |
| 24 | AY | 75 | C | C2'-C3'-O3' | 9.40 | 130.19 | 109.50 |
| 36 | BA | 1799 | G | C2'-C3'-O3' | 9.36 | 130.09 | 109.50 |
| 1 | AA | 1504 | G | C2'-C3'-O3' | 9.11 | 129.55 | 109.50 |
| 36 | BA | 1786 | A | N9-C1'-C2' | 9.11 | 125.85 | 114.00 |
| 48 | BP | 52 | GLU | N-CA-C | 9.09 | 135.53 | 111.00 |
| 1 | AA | 687 | A | C2'-C3'-O3' | 8.91 | 129.10 | 109.50 |
| 36 | BA | 1378 | A | C2'-C3'-O3' | 8.89 | 129.05 | 109.50 |
| 24 | AY | 36 | A | C2'-C3'-O3' | 8.80 | 128.85 | 109.50 |
| 1 | AA | 1399 | C | C2'-C3'-O3' | 8.68 | 128.59 | 109.50 |
| 1 | AA | 1050 | G | N9-C1'-C2' | -8.46 | 102.69 | 112.00 |
| 1 | AA | 243 | A | C2'-C3'-O3' | 8.38 | 127.95 | 109.50 |
| 1 | AA | 109 | A | C2'-C3'-O3' | 8.35 | 127.88 | 109.50 |
| 36 | BA | 1300 | U | C2'-C3'-O3' | 8.34 | 127.86 | 109.50 |
| 1 | AA | 1239 | A | C2'-C3'-O3' | 8.25 | 127.66 | 109.50 |
| 1 | AA | 1049 | U | C2'-C3'-O3' | 8.21 | 127.57 | 109.50 |
| 36 | BA | 1819 | A | C2'-C3'-O3' | 8.10 | 127.33 | 109.50 |
| 36 | BA | 387 | U | C2'-C3'-O3' | 8.10 | 127.32 | 109.50 |
| 36 | BA | 2360 | A | N9-C1'-C2' | -8.05 | 103.15 | 112.00 |
| 1 | AA | 347 | G | N9-C1'-C2' | -8.04 | 103.16 | 112.00 |
| 1 | AA | 920 | U | C5'-C4'-C3' | -7.93 | 103.31 | 116.00 |
| 1 | AA | 369 | C | N1-C1'-C2' | -7.90 | 103.31 | 112.00 |
| 1 | AA | 30 | U | C2'-C3'-O3' | 7.77 | 126.60 | 109.50 |
| 1 | AA | 1267 | C | C5'-C4'-O4' | 7.70 | 118.34 | 109.10 |
| 1 | AA | 1267 | C | C5'-C4'-C3' | 7.70 | 128.31 | 116.00 |
| 48 | BP | 53 | GLY | N-CA-C | -7.67 | 93.92 | 113.10 |
| 1 | AA | 1101 | A | C2'-C3'-O3' | 7.65 | 126.34 | 109.50 |
| 36 | BA | 1970 | A | C5'-C4'-O4' | 7.50 | 118.10 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36 | BA | 2286 | A | N9-C1'-C2' | 7.41 | 123.64 | 114.00 |
| 36 | BA | 1992 | G | C2'-C3'-O3' | 7.41 | 125.80 | 109.50 |
| 1 | AA | 1181 | G | N9-C1'-C2' | 7.20 | 123.36 | 114.00 |
| 39 | BD | 244 | ARG | C-N-CD | -7.13 | 104.92 | 120.60 |
| 36 | BA | 1427 | A | C2'-C3'-O3' | 7.05 | 125.01 | 109.50 |
| 1 | AA | 60 | A | C2'-C3'-O3' | 7.03 | 124.96 | 109.50 |
| 36 | BA | 654(K) | C | C1'-O4'-C4' | -6.76 | 104.49 | 109.90 |
| 36 | BA | 2610 | C | C2'-C3'-O3' | 6.75 | 124.50 | 113.70 |
| 1 | AA | 1502 | A | N9-C1'-C2' | 6.75 | 122.77 | 114.00 |
| 36 | BA | 654(K) | C | N1-C1'-C2' | 6.60 | 122.58 | 114.00 |
| 1 | AA | 1186 | G | C5'-C4'-C3' | -6.49 | 105.62 | 116.00 |
| 1 | AA | 428 | G | C2'-C3'-O3' | 6.46 | 124.03 | 113.70 |
| 1 | AA | 792 | A | C2'-C3'-O3' | 6.37 | 123.89 | 113.70 |
| 36 | BA | 1653 | G | C2'-C3'-O3' | 6.37 | 123.89 | 113.70 |
| 42 | BG | 89 | GLY | N-CA-C | -6.36 | 97.21 | 113.10 |
| 4 | AD | 12 | CYS | CA-CB-SG | 6.20 | 125.16 | 114.00 |
| 1 | AA | 968 | A | C2'-C3'-O3' | 6.20 | 123.61 | 113.70 |
| 25 | AZ | 86 | ALA | N-CA-C | -6.19 | 94.30 | 111.00 |
| 52 | BT | 29 | ARG | N-CA-C | 6.18 | 127.69 | 111.00 |
| 1 | AA | 1504 | G | OP2-P-O3' | 6.18 | 118.79 | 105.20 |
| 1 | AA | 1397 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 1 | AA | 1397 | C | C5'-C4'-O4' | 6.09 | 116.41 | 109.10 |
| 1 | AA | 1283 | G | N9-C1'-C2' | -6.08 | 105.32 | 112.00 |
| 36 | BA | 783 | A | N9-C1'-C2' | -6.04 | 105.36 | 112.00 |
| 32 | B6 | 10 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 56 | BX | 57 | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 36 | BA | 975 | C | N1-C1'-C2' | 6.01 | 121.82 | 114.00 |
| 36 | BA | 2756 | U | C2'-C3'-O3' | 5.96 | 123.24 | 113.70 |
| 1 | AA | 968 | A | N9-C1'-C2' | 5.96 | 121.75 | 114.00 |
| 36 | BA | 2464 | C | N1-C1'-C2' | -5.95 | 105.45 | 112.00 |
| 48 | BP | 66 | GLY | N-CA-C | -5.95 | 98.24 | 113.10 |
| 36 | BA | 265 | A | N9-C1'-C2' | 5.93 | 121.71 | 114.00 |
| 36 | BA | 527 | C | N1-C1'-C2' | 5.93 | 121.71 | 114.00 |
| 1 | AA | 1054 | C | C5'-C4'-C3' | -5.90 | 106.56 | 116.00 |
| 13 | AM | 90 | LEU | N-CA-C | -5.88 | 95.13 | 111.00 |
| 1 | AA | 1331 | G | N9-C1'-C2' | 5.87 | 121.63 | 114.00 |
| 36 | BA | 1970 | A | C1'-O4'-C4' | -5.87 | 105.21 | 109.90 |
| 36 | BA | 2089 | U | C5'-C4'-C3' | -5.85 | 106.63 | 116.00 |
| 36 | BA | 1495 | A | N9-C1'-C2' | 5.81 | 121.56 | 114.00 |
| 50 | BR | 5 | LYS | N-CA-C | -5.77 | 95.42 | 111.00 |
| 39 | BD | 259 | THR | N-CA-C | 5.74 | 126.50 | 111.00 |
| 52 | BT | 30 | VAL | N-CA-C | 5.73 | 126.47 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | BA | 472 | A | C5'-C4'-O4' | -5.69 | 102.27 | 109.10 |
| 1 | AA | 1305 | G | N9-C1'-C2' | 5.67 | 121.37 | 114.00 |
| 32 | B6 | 9 | LEU | CA-CB-CG | 5.67 | 128.33 | 115.30 |
| 36 | BA | 1948 | G | C5'-C4'-O4' | -5.58 | 102.40 | 109.10 |
| 36 | BA | 1698 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 1 | AA | 1335 | C | N1-C1'-C2' | 5.53 | 121.18 | 114.00 |
| 1 | AA | 960 | U | N1-C1'-C2' | 5.49 | 121.14 | 114.00 |
| 1 | AA | 966 | G | N9-C1'-C2' | -5.49 | 105.97 | 112.00 |
| 36 | BA | 527 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 36 | BA | 1459 | G | N9-C1'-C2' | 5.45 | 121.08 | 114.00 |
| 1 | AA | 266 | G | C2'-C3'-O3' | 5.43 | 122.39 | 113.70 |
| 36 | BA | 1698 | A | N9-C1'-C2' | 5.42 | 121.05 | 114.00 |
| 36 | BA | 1997 | G | N9-C1'-C2' | -5.41 | 106.05 | 112.00 |
| 48 | BP | 27 | HIS | N-CA-C | 5.40 | 125.58 | 111.00 |
| 36 | BA | 2557 | G | C5'-C4'-C3' | -5.40 | 107.36 | 116.00 |
| 39 | BD | 56 | GLY | N-CA-C | -5.40 | 99.61 | 113.10 |
| 36 | BA | 629 | G | C5'-C4'-O4' | -5.38 | 102.65 | 109.10 |
| 36 | BA | 1558 | A | C2'-C3'-O3' | 5.37 | 122.30 | 113.70 |
| 36 | BA | 1493 | C | N1-C1'-C2' | 5.37 | 120.98 | 114.00 |
| 36 | BA | 945 | A | N9-C1'-C2' | 5.34 | 120.94 | 114.00 |
| 1 | AA | 547 | A | N9-C1'-C2' | 5.33 | 120.94 | 114.00 |
| 34 | B8 | 34 | TRP | N-CA-C | -5.33 | 96.62 | 111.00 |
| 2 | AB | 23 | ARG | N-CA-C | -5.32 | 96.62 | 111.00 |
| 36 | BA | 915 | C | C5'-C4'-C3' | 5.31 | 124.50 | 116.00 |
| 1 | AA | 995 | C | N1-C1'-C2' | -5.31 | 106.16 | 112.00 |
| 36 | BA | 2346 | A | N9-C1'-C2' | 5.31 | 120.90 | 114.00 |
| 36 | BA | 1819 | A | C4'-C3'-O3' | 5.31 | 123.61 | 113.00 |
| 20 | AT | 24 | LEU | CA-CB-CG | 5.29 | 127.48 | 115.30 |
| 13 | AM | 12 | ASN | N-CA-C | 5.29 | 125.28 | 111.00 |
| 1 | AA | 1157 | A | C2'-C3'-O3' | 5.28 | 122.15 | 113.70 |
| 36 | BA | 669 | G | N9-C1'-C2' | 5.26 | 120.84 | 114.00 |
| 1 | AA | 839 | U | N1-C1'-C2' | 5.25 | 120.83 | 114.00 |
| 36 | BA | 1378 | A | C4'-C3'-O3' | 5.23 | 123.46 | 113.00 |
| 6 | AF | 66 | GLU | N-CA-C | -5.22 | 96.89 | 111.00 |
| 1 | AA | 586 | C | N1-C1'-C2' | -5.22 | 106.26 | 112.00 |
| 1 | AA | 1239 | A | C4'-C3'-C2' | 5.21 | 107.81 | 102.60 |
| 1 | AA | 353 | A | C5'-C4'-O4' | -5.20 | 102.86 | 109.10 |
| 36 | BA | 857 | C | C5'-C4'-C3' | -5.19 | 107.69 | 116.00 |
| 24 | AY | 75 | C | C4'-C3'-C2' | 5.19 | 107.79 | 102.60 |
| 36 | BA | 331 | A | C2'-C3'-O3' | 5.15 | 121.94 | 113.70 |
| 36 | BA | 856 | C | C2'-C3'-O3' | 5.14 | 121.93 | 113.70 |
| 12 | AL | 88 | GLY | N-CA-C | -5.14 | 100.25 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 36 | BA | 1300 | U | C4'-C3'-O3' | 5.14 | 123.28 | 113.00 |
| 1 | AA | 1442(B) | A | N9-C1'-C2' | 5.13 | 120.66 | 114.00 |
| 36 | BA | 654(K) | C | C5'-C4'-O4' | 5.13 | 115.25 | 109.10 |
| 36 | BA | 2310 | A | N9-C1'-C2' | 5.13 | 120.66 | 114.00 |
| 1 | AA | 197 | A | N9-C1'-C2' | 5.12 | 120.65 | 114.00 |
| 36 | BA | 2714 | G | C5'-C4'-C3' | -5.11 | 107.82 | 116.00 |
| 36 | BA | 1666 | G | C5'-C4'-O4' | -5.11 | 102.97 | 109.10 |
| 36 | BA | 1781 | C | N1-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 36 | BA | 654(I) | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 12 | AL | 119 | LYS | N-CA-C | -5.09 | 97.27 | 111.00 |
| 36 | BA | 1701 | A | C5'-C4'-C3' | -5.08 | 107.88 | 116.00 |
| 36 | BA | 1022 | G | N9-C1'-C2' | 5.08 | 120.60 | 114.00 |
| 36 | BA | 2033 | A | N9-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 1 | AA | 1269 | A | C1'-O4'-C4' | -5.04 | 105.87 | 109.90 |
| 1 | AA | 266 | G | O4'-C1'-N9 | -5.03 | 104.17 | 108.20 |
| 36 | BA | 2405 | G | N9-C1'-C2' | 5.03 | 120.54 | 114.00 |
| 1 | AA | 961 | U | C5'-C4'-C3' | -5.02 | 107.96 | 116.00 |
| 1 | AA | 1504 | G | C4'-C3'-O3' | 5.02 | 123.03 | 113.00 |
| 36 | BA | 791 | C | N1-C1'-C2' | 5.01 | 120.52 | 114.00 |

All (9) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | AA | 508 | C | C3' |
| 1 | AA | 1498 | U | C3' |
| 1 | AA | 1504 | G | C3' |
| 24 | AY | 36 | A | C3' |
| 24 | AY | 75 | C | C3' |
| 36 | BA | 1300 | U | C3' |
| 36 | BA | 1378 | A | C3' |
| 36 | BA | 1799 | G | C3' |
| 36 | BA | 1819 | A | C3' |

All (125) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | AA | 1049 | U | Sidechain |
| 1 | AA | 1050 | G | Sidechain |
| 1 | AA | 1073 | U | Sidechain |
| 1 | AA | 1079 | G | Sidechain |
| 1 | AA | 1096 | C | Sidechain |
| 1 | AA | 1131 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | AA | 1145 | C | Sidechain |
| 1 | AA | 1153 | C | Sidechain |
| 1 | AA | 1181 | G | Sidechain |
| 1 | AA | 1194 | U | Sidechain |
| 1 | AA | 1281 | U | Sidechain |
| 1 | AA | 1283 | G | Sidechain |
| 1 | AA | 1305 | G | Sidechain |
| 1 | AA | 1322 | C | Sidechain |
| 1 | AA | 1331 | G | Sidechain |
| 1 | AA | 1335 | C | Sidechain |
| 1 | AA | 1338 | G | Sidechain |
| 1 | AA | 1358 | U | Sidechain |
| 1 | AA | 1370 | G | Sidechain |
| 1 | AA | 1372 | U | Sidechain |
| 1 | AA | 1503 | A | Sidechain |
| 1 | AA | 1510 | U | Sidechain |
| 1 | AA | 1522 | U | Sidechain |
| 1 | AA | 1531 | A | Sidechain |
| 1 | AA | 198 | G | Sidechain |
| 1 | AA | 250 | A | Sidechain |
| 1 | AA | 251 | G | Sidechain |
| 1 | AA | 279 | A | Sidechain |
| 1 | AA | 347 | G | Sidechain |
| 1 | AA | 380 | G | Sidechain |
| 1 | AA | 453 | A | Sidechain |
| 1 | AA | 484 | G | Sidechain |
| 1 | AA | 498 | U | Sidechain |
| 1 | AA | 50 | A | Sidechain |
| 1 | AA | 529 | G | Sidechain |
| 1 | AA | 561 | U | Sidechain |
| 1 | AA | 573 | A | Sidechain |
| 1 | AA | 603 | U | Sidechain |
| 1 | AA | 609 | A | Sidechain |
| 1 | AA | 62 | U | Sidechain |
| 1 | AA | 7 | G | Sidechain |
| 1 | AA | 727 | G | Sidechain |
| 1 | AA | 733 | A | Sidechain |
| 1 | AA | 749 | C | Sidechain |
| 1 | AA | 793 | U | Sidechain |
| 1 | AA | 941 | G | Sidechain |
| 1 | AA | 959 | A | Sidechain |
| 1 | AA | 961 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|---------|------|-----------|
| 1 | AA | 968 | A | Sidechain |
| 1 | AA | 982 | U | Sidechain |
| 1 | AA | 995 | C | Sidechain |
| 23 | AX | 16 | A | Sidechain |
| 24 | AY | 33 | U | Sidechain |
| 36 | BA | 1156 | A | Sidechain |
| 36 | BA | 1215 | G | Sidechain |
| 36 | BA | 1238 | G | Sidechain |
| 36 | BA | 1253 | A | Sidechain |
| 36 | BA | 1364 | G | Sidechain |
| 36 | BA | 1379 | A | Sidechain |
| 36 | BA | 1416 | G | Sidechain |
| 36 | BA | 1452 | A | Sidechain |
| 36 | BA | 1528(A) | A | Sidechain |
| 36 | BA | 1673 | U | Sidechain |
| 36 | BA | 1692 | U | Sidechain |
| 36 | BA | 1772 | G | Sidechain |
| 36 | BA | 1773 | A | Sidechain |
| 36 | BA | 1779 | U | Sidechain |
| 36 | BA | 1798 | U | Sidechain |
| 36 | BA | 1807 | G | Sidechain |
| 36 | BA | 1931 | U | Sidechain |
| 36 | BA | 1940 | U | Sidechain |
| 36 | BA | 1943 | U | Sidechain |
| 36 | BA | 1964 | G | Sidechain |
| 36 | BA | 1993 | U | Sidechain |
| 36 | BA | 1995 | U | Sidechain |
| 36 | BA | 1999 | C | Sidechain |
| 36 | BA | 2031 | A | Sidechain |
| 36 | BA | 2033 | A | Sidechain |
| 36 | BA | 2195 | C | Sidechain |
| 36 | BA | 2222 | G | Sidechain |
| 36 | BA | 2286 | A | Sidechain |
| 36 | BA | 2319 | G | Sidechain |
| 36 | BA | 2320 | A | Sidechain |
| 36 | BA | 2360 | A | Sidechain |
| 36 | BA | 2414 | G | Sidechain |
| 36 | BA | 2417 | C | Sidechain |
| 36 | BA | 242 | G | Sidechain |
| 36 | BA | 2452 | C | Sidechain |
| 36 | BA | 2464 | C | Sidechain |
| 36 | BA | 249 | C | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|--------|------|-----------|
| 36 | BA | 250 | G | Sidechain |
| 36 | BA | 2523 | G | Sidechain |
| 36 | BA | 2529 | G | Sidechain |
| 36 | BA | 2542 | A | Sidechain |
| 36 | BA | 2564 | A | Sidechain |
| 36 | BA | 2581 | G | Sidechain |
| 36 | BA | 2582 | G | Sidechain |
| 36 | BA | 2592 | G | Sidechain |
| 36 | BA | 2597 | G | Sidechain |
| 36 | BA | 2603 | G | Sidechain |
| 36 | BA | 2608 | G | Sidechain |
| 36 | BA | 2687 | U | Sidechain |
| 36 | BA | 271(Q) | G | Sidechain |
| 36 | BA | 2720 | U | Sidechain |
| 36 | BA | 2779 | U | Sidechain |
| 36 | BA | 463 | G | Sidechain |
| 36 | BA | 515 | A | Sidechain |
| 36 | BA | 527 | C | Sidechain |
| 36 | BA | 567 | A | Sidechain |
| 36 | BA | 59 | U | Sidechain |
| 36 | BA | 630 | G | Sidechain |
| 36 | BA | 632 | A | Sidechain |
| 36 | BA | 688 | U | Sidechain |
| 36 | BA | 690 | G | Sidechain |
| 36 | BA | 700 | G | Sidechain |
| 36 | BA | 740 | U | Sidechain |
| 36 | BA | 746 | A | Sidechain |
| 36 | BA | 764 | A | Sidechain |
| 36 | BA | 769 | G | Sidechain |
| 36 | BA | 869 | G | Sidechain |
| 36 | BA | 870 | A | Sidechain |
| 36 | BA | 956 | G | Sidechain |
| 36 | BA | 987 | G | Sidechain |
| 37 | BB | 40 | U | Sidechain |
| 37 | BB | 42 | C | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32329 | 0 | 16318 | 1085 | 2 |
| 2 | AB | 1900 | 0 | 1951 | 250 | 0 |
| 3 | AC | 1612 | 0 | 1677 | 139 | 0 |
| 4 | AD | 1703 | 0 | 1764 | 151 | 0 |
| 5 | AE | 1146 | 0 | 1207 | 100 | 0 |
| 6 | AF | 843 | 0 | 857 | 52 | 0 |
| 7 | AG | 1257 | 0 | 1296 | 120 | 0 |
| 8 | AH | 1116 | 0 | 1177 | 91 | 0 |
| 9 | AI | 1011 | 0 | 1043 | 128 | 0 |
| 10 | AJ | 794 | 0 | 840 | 135 | 0 |
| 11 | AK | 885 | 0 | 904 | 76 | 0 |
| 12 | AL | 970 | 0 | 1057 | 110 | 0 |
| 13 | AM | 987 | 0 | 1059 | 131 | 0 |
| 14 | AN | 492 | 0 | 529 | 66 | 0 |
| 15 | AO | 734 | 0 | 771 | 61 | 0 |
| 16 | AP | 700 | 0 | 720 | 65 | 0 |
| 17 | AQ | 823 | 0 | 891 | 82 | 0 |
| 18 | AR | 574 | 0 | 644 | 37 | 0 |
| 19 | AS | 629 | 0 | 652 | 125 | 0 |
| 20 | AT | 763 | 0 | 861 | 107 | 0 |
| 21 | AU | 208 | 0 | 221 | 29 | 0 |
| 22 | AV | 1619 | 0 | 822 | 61 | 0 |
| 22 | AW | 1619 | 0 | 822 | 85 | 0 |
| 23 | AX | 298 | 0 | 152 | 26 | 0 |
| 24 | AY | 1644 | 0 | 853 | 68 | 0 |
| 25 | AZ | 3142 | 0 | 3152 | 385 | 0 |
| 26 | B0 | 662 | 0 | 688 | 107 | 0 |
| 27 | B1 | 731 | 0 | 808 | 83 | 0 |
| 28 | B2 | 598 | 0 | 653 | 77 | 0 |
| 29 | B3 | 467 | 0 | 523 | 59 | 0 |
| 30 | B4 | 340 | 0 | 337 | 57 | 0 |
| 31 | B5 | 459 | 0 | 480 | 79 | 0 |
| 32 | B6 | 433 | 0 | 461 | 135 | 0 |
| 33 | B7 | 418 | 0 | 467 | 31 | 0 |
| 34 | B8 | 507 | 0 | 576 | 104 | 0 |
| 35 | B9 | 307 | 0 | 335 | 48 | 0 |
| 36 | BA | 62477 | 0 | 31497 | 2447 | 2 |
| 37 | BB | 2551 | 0 | 1295 | 115 | 0 |
| 38 | BC | 1742 | 0 | 1800 | 349 | 0 |
| 39 | BD | 2145 | 0 | 2234 | 324 | 0 |
| 40 | BE | 1563 | 0 | 1629 | 273 | 0 |
| 41 | BF | 1623 | 0 | 1677 | 250 | 0 |
| 42 | BG | 1474 | 0 | 1535 | 224 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 43 | BH | 1222 | 0 | 1282 | 170 | 0 |
| 44 | BJ | 651 | 0 | 152 | 15 | 0 |
| 45 | BK | 700 | 0 | 166 | 13 | 0 |
| 46 | BN | 1104 | 0 | 1180 | 181 | 0 |
| 47 | BO | 933 | 0 | 996 | 92 | 0 |
| 48 | BP | 1114 | 0 | 1187 | 297 | 0 |
| 49 | BQ | 1122 | 0 | 1179 | 149 | 0 |
| 50 | BR | 960 | 0 | 1021 | 148 | 0 |
| 51 | BS | 770 | 0 | 832 | 169 | 0 |
| 52 | BT | 1141 | 0 | 1202 | 250 | 0 |
| 53 | BU | 958 | 0 | 1015 | 159 | 0 |
| 54 | BV | 779 | 0 | 852 | 127 | 0 |
| 55 | BW | 896 | 0 | 953 | 104 | 0 |
| 56 | BX | 725 | 0 | 778 | 97 | 0 |
| 57 | BY | 775 | 0 | 870 | 197 | 0 |
| 58 | BZ | 1403 | 0 | 1432 | 241 | 0 |
| 59 | AA | 42 | 0 | 45 | 2 | 0 |
| 60 | AD | 1 | 0 | 0 | 1 | 0 |
| 60 | AN | 1 | 0 | 0 | 0 | 0 |
| 60 | B4 | 1 | 0 | 0 | 0 | 0 |
| 60 | B9 | 1 | 0 | 0 | 0 | 0 |
| 61 | AZ | 32 | 0 | 14 | 5 | 0 |
| 62 | AZ | 1 | 0 | 0 | 0 | 0 |
| 63 | AZ | 1 | 0 | 0 | 0 | 0 |
| All | All | 153628 | 0 | 104391 | 9953 | 2 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (9953) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:1899:G:N2 | 36:BA:1902:C:H41 | 1.36 | 1.21 |
| 36:BA:2833:G:H3' | 36:BA:2834:G:H5'' | 1.24 | 1.20 |
| 24:AY:1:A:H5' | 25:AZ:90:LYS:HZ2 | 1.06 | 1.17 |
| 2:AB:84:GLU:HB3 | 2:AB:219:VAL:HG21 | 1.22 | 1.17 |
| 55:BW:14:PRO:HG2 | 55:BW:78:GLU:HG3 | 1.22 | 1.17 |
| 42:BG:60:LEU:HD22 | 42:BG:63:ILE:HD11 | 1.27 | 1.17 |
| 36:BA:1516:C:H2' | 36:BA:1517:G:H5'' | 1.26 | 1.16 |
| 36:BA:2781:A:H5' | 36:BA:2782:G:H5' | 1.28 | 1.16 |
| 36:BA:654(L):G:H2' | 36:BA:654(M):C:H4' | 1.20 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:BU:112:ARG:HH12 | 54:BV:46:VAL:HG11 | 1.08 | 1.15 |
| 55:BW:8:ARG:HA | 55:BW:102:HIS:HB3 | 1.19 | 1.15 |
| 53:BU:24:TYR:HB2 | 53:BU:29:SER:HB3 | 1.23 | 1.15 |
| 41:BF:24:LEU:HB3 | 41:BF:25:PRO:HD2 | 1.23 | 1.15 |
| 48:BP:62:LEU:HD23 | 48:BP:62:LEU:H | 1.08 | 1.14 |
| 12:AL:47:LYS:HB3 | 12:AL:48:PRO:HD3 | 1.20 | 1.13 |
| 1:AA:1386:G:H2' | 1:AA:1387:G:H5'' | 1.31 | 1.13 |
| 32:B6:18:ARG:HG2 | 32:B6:18:ARG:HH11 | 1.08 | 1.12 |
| 28:B2:35:LEU:HD11 | 28:B2:50:ILE:HG13 | 1.21 | 1.12 |
| 57:BY:7:VAL:HB | 57:BY:8:LYS:HD2 | 1.32 | 1.12 |
| 25:AZ:68:VAL:HG23 | 25:AZ:79:HIS:HB3 | 1.30 | 1.11 |
| 36:BA:1884:A:H2' | 36:BA:1885:A:H5'' | 1.24 | 1.11 |
| 26:B0:14:ARG:HB2 | 26:B0:14:ARG:HH11 | 1.16 | 1.11 |
| 1:AA:1053:G:H4' | 1:AA:1054:C:H5' | 1.19 | 1.11 |
| 36:BA:1484:G:H2' | 36:BA:1485:G:H5'' | 1.30 | 1.10 |
| 38:BC:10:LEU:HD12 | 38:BC:32:LEU:HA | 1.29 | 1.10 |
| 2:AB:209:ARG:HH11 | 2:AB:239:VAL:HG11 | 1.11 | 1.10 |
| 42:BG:115:ARG:HH22 | 42:BG:136:ARG:HB2 | 1.13 | 1.10 |
| 36:BA:2140:C:H2' | 36:BA:2141:G:H8 | 1.17 | 1.09 |
| 36:BA:925:C:H2' | 36:BA:926:A:H5'' | 1.31 | 1.09 |
| 38:BC:180:PHE:HB3 | 38:BC:184:LYS:HB3 | 1.11 | 1.09 |
| 32:B6:30:THR:HG22 | 32:B6:31:PRO:HD2 | 1.11 | 1.09 |
| 1:AA:8:A:H62 | 4:AD:208:SER:HB2 | 0.96 | 1.09 |
| 56:BX:24:GLY:O | 56:BX:82:GLN:HA | 1.52 | 1.08 |
| 48:BP:47:ASP:HB2 | 48:BP:51:PHE:HB2 | 1.33 | 1.08 |
| 10:AJ:50:ILE:HD13 | 10:AJ:50:ILE:H | 1.14 | 1.08 |
| 36:BA:1024:G:H3' | 36:BA:1025:G:H5'' | 1.33 | 1.08 |
| 36:BA:1058:G:H2' | 36:BA:1059:G:H5'' | 1.31 | 1.08 |
| 15:AO:87:ILE:HG22 | 15:AO:88:ARG:H | 1.13 | 1.08 |
| 24:AY:1:A:H5' | 25:AZ:90:LYS:NZ | 1.68 | 1.08 |
| 22:AV:46:G:H3' | 22:AV:47:U:H5'' | 1.15 | 1.08 |
| 36:BA:1665:A:H2' | 36:BA:1666:G:H5'' | 1.30 | 1.08 |
| 57:BY:8:LYS:H | 57:BY:8:LYS:HD2 | 1.14 | 1.08 |
| 19:AS:6:LYS:HD2 | 19:AS:6:LYS:N | 1.69 | 1.07 |
| 40:BE:34:VAL:HG11 | 40:BE:78:LEU:HD22 | 1.35 | 1.07 |
| 55:BW:14:PRO:HG3 | 55:BW:101:SER:HB3 | 1.36 | 1.07 |
| 40:BE:57:LYS:HA | 40:BE:57:LYS:HE3 | 1.32 | 1.07 |
| 36:BA:2491:U:H5' | 36:BA:2570:G:H5'' | 1.31 | 1.07 |
| 51:BS:13:ARG:HG3 | 51:BS:14:VAL:H | 1.21 | 1.06 |
| 25:AZ:11:HIS:NE2 | 25:AZ:78:SER:HB2 | 1.71 | 1.06 |
| 24:AY:4:G:H2' | 24:AY:5:G:H5'' | 1.38 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 57:BY:96:ILE:HG13 | 57:BY:99:CYS:HB3 | 1.36 | 1.06 |
| 36:BA:2523:G:H2' | 36:BA:2524:G:H5'' | 1.38 | 1.06 |
| 52:BT:60:THR:HG22 | 52:BT:77:PRO:HA | 1.36 | 1.06 |
| 46:BN:73:THR:HG23 | 46:BN:82:LEU:HD11 | 1.36 | 1.05 |
| 22:AV:68:C:H2' | 22:AV:69:G:H5'' | 1.36 | 1.05 |
| 58:BZ:20:ARG:HH11 | 58:BZ:20:ARG:HB2 | 1.15 | 1.05 |
| 48:BP:9:ASN:H | 48:BP:10:PRO:HD2 | 1.19 | 1.05 |
| 2:AB:18:GLY:H | 2:AB:42:ILE:HG22 | 1.21 | 1.05 |
| 31:B5:4:HIS:HB3 | 31:B5:5:PRO:HD3 | 1.37 | 1.05 |
| 54:BV:47:VAL:HG12 | 54:BV:52:VAL:HB | 1.38 | 1.05 |
| 1:AA:9:G:H5' | 5:AE:122:GLU:OE1 | 1.55 | 1.04 |
| 22:AW:56:C:H4' | 38:BC:128:GLY:O | 1.57 | 1.04 |
| 43:BH:85:LYS:HZ3 | 43:BH:133:VAL:N | 1.54 | 1.04 |
| 52:BT:55:ASN:H | 52:BT:59:THR:HG22 | 1.21 | 1.04 |
| 43:BH:153:LYS:HD3 | 43:BH:153:LYS:H | 1.14 | 1.04 |
| 29:B3:22:ALA:HB1 | 29:B3:46:ASN:HD21 | 1.16 | 1.04 |
| 36:BA:1516:C:C2' | 36:BA:1517:G:H5'' | 1.86 | 1.04 |
| 51:BS:58:LEU:HG | 51:BS:59:LYS:H | 1.19 | 1.04 |
| 40:BE:77:ILE:HG22 | 40:BE:78:LEU:H | 1.21 | 1.04 |
| 36:BA:2893:G:H5' | 36:BA:2894:G:H5' | 1.33 | 1.04 |
| 39:BD:239:ARG:HH21 | 39:BD:239:ARG:HG2 | 1.17 | 1.04 |
| 2:AB:200:ILE:HD12 | 2:AB:200:ILE:H | 1.22 | 1.03 |
| 12:AL:47:LYS:HB3 | 12:AL:48:PRO:CD | 1.88 | 1.03 |
| 25:AZ:368:VAL:HG12 | 25:AZ:369:THR:H | 1.23 | 1.03 |
| 43:BH:167:GLU:HG2 | 43:BH:168:PRO:HD2 | 1.40 | 1.03 |
| 36:BA:1243:G:H2' | 36:BA:1244:G:H5'' | 1.37 | 1.03 |
| 52:BT:85:LYS:HZ3 | 52:BT:85:LYS:HB3 | 1.22 | 1.03 |
| 36:BA:2833:G:H3' | 36:BA:2834:G:C5' | 1.89 | 1.03 |
| 1:AA:980:C:H5' | 1:AA:980:C:H6 | 1.19 | 1.03 |
| 36:BA:629:G:H5' | 36:BA:629:G:H8 | 1.24 | 1.03 |
| 52:BT:65:LYS:HE3 | 52:BT:66:VAL:H | 1.22 | 1.03 |
| 30:B4:6:HIS:HB3 | 42:BG:67:LYS:HE3 | 1.40 | 1.03 |
| 41:BF:188:ARG:HA | 48:BP:7:ARG:HD3 | 1.40 | 1.03 |
| 36:BA:330:A:H2 | 36:BA:1210:A:H2' | 1.20 | 1.02 |
| 38:BC:164:ARG:HG2 | 38:BC:165:ASN:H | 1.19 | 1.02 |
| 58:BZ:126:VAL:HG12 | 58:BZ:163:LEU:HB2 | 1.36 | 1.02 |
| 12:AL:46:LYS:HG2 | 12:AL:47:LYS:H | 1.17 | 1.02 |
| 36:BA:2312:U:H2' | 36:BA:2313:C:H5'' | 1.37 | 1.02 |
| 57:BY:75:ILE:HD12 | 57:BY:79:CYS:HA | 1.40 | 1.02 |
| 22:AW:62:C:H2' | 22:AW:63:G:H8 | 1.22 | 1.02 |
| 37:BB:7:G:H3' | 37:BB:8:U:H5'' | 1.42 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 39:BD:85:ASP:HB2 | 39:BD:92:ILE:HD13 | 1.40 | 1.02 |
| 29:B3:35:ARG:HB2 | 29:B3:35:ARG:HH11 | 1.21 | 1.02 |
| 50:BR:45:ARG:HG3 | 50:BR:46:GLY:H | 1.23 | 1.01 |
| 26:B0:27:GLU:HB3 | 26:B0:68:GLU:HA | 1.39 | 1.01 |
| 32:B6:33:LYS:HE2 | 32:B6:33:LYS:HA | 1.41 | 1.01 |
| 34:B8:62:LEU:HD13 | 36:BA:242:G:H5'' | 1.38 | 1.01 |
| 36:BA:2756:U:H1' | 36:BA:2757:A:H5'' | 1.42 | 1.01 |
| 2:AB:68:ILE:H | 2:AB:90:MET:HE1 | 1.22 | 1.01 |
| 51:BS:97:ARG:HH21 | 51:BS:98:VAL:HA | 1.24 | 1.01 |
| 36:BA:1222:C:H2' | 36:BA:1223:G:H5'' | 1.37 | 1.01 |
| 36:BA:272(H):C:H2' | 36:BA:272(I):U:H5'' | 1.42 | 1.01 |
| 38:BC:86:ALA:HB3 | 38:BC:94:VAL:HG11 | 1.40 | 1.01 |
| 57:BY:43:ASN:HB3 | 57:BY:64:GLU:HA | 1.43 | 1.01 |
| 51:BS:78:LEU:HD11 | 51:BS:103:GLU:HB2 | 1.42 | 1.01 |
| 29:B3:8:LEU:HD22 | 29:B3:31:LEU:HA | 1.39 | 1.00 |
| 31:B5:44:THR:HG21 | 50:BR:101:ALA:HB2 | 1.43 | 1.00 |
| 46:BN:55:VAL:HG22 | 46:BN:125:GLY:HA3 | 1.43 | 1.00 |
| 57:BY:17:SER:HB2 | 57:BY:71:LYS:HE2 | 1.41 | 1.00 |
| 23:AX:26:A:H3' | 23:AX:27:A:H5'' | 1.42 | 1.00 |
| 36:BA:2101:G:H2' | 36:BA:2102:U:H5'' | 1.42 | 1.00 |
| 38:BC:42:GLU:HB3 | 38:BC:215:THR:HG23 | 1.42 | 1.00 |
| 1:AA:1320:C:H5'' | 19:AS:70:LYS:HG3 | 1.41 | 0.99 |
| 40:BE:50:GLY:HA2 | 40:BE:78:LEU:HB3 | 1.44 | 0.99 |
| 5:AE:148:VAL:HG21 | 8:AH:107:LEU:HD13 | 1.43 | 0.99 |
| 55:BW:6:ILE:HG12 | 55:BW:104:THR:HB | 1.44 | 0.99 |
| 36:BA:2761:G:H2' | 36:BA:2762:G:H5'' | 1.42 | 0.99 |
| 35:B9:30:PRO:HB2 | 36:BA:2527:C:H5' | 1.41 | 0.99 |
| 1:AA:1116:C:H2' | 1:AA:1117:G:H5'' | 1.43 | 0.99 |
| 36:BA:2110:G:H1 | 36:BA:2178:C:H41 | 1.10 | 0.99 |
| 36:BA:1747(A):G:C2' | 36:BA:1748:G:H5'' | 1.93 | 0.99 |
| 38:BC:127:LEU:HD23 | 38:BC:130:ILE:HD12 | 1.44 | 0.99 |
| 41:BF:6:VAL:HG12 | 41:BF:7:TYR:H | 1.24 | 0.99 |
| 33:B7:8:ASN:HD22 | 33:B7:8:ASN:C | 1.61 | 0.99 |
| 35:B9:17:ILE:HG21 | 35:B9:19:ARG:HH21 | 1.28 | 0.99 |
| 51:BS:97:ARG:NH2 | 51:BS:98:VAL:HA | 1.78 | 0.99 |
| 55:BW:29:LEU:HG | 55:BW:33:ARG:HD2 | 1.44 | 0.98 |
| 58:BZ:33:LEU:HD12 | 58:BZ:34:ASN:H | 1.22 | 0.98 |
| 36:BA:1884:A:C2' | 36:BA:1885:A:H5'' | 1.93 | 0.98 |
| 19:AS:46:GLY:H | 19:AS:62:ILE:HG23 | 1.24 | 0.98 |
| 36:BA:1301:A:O2' | 36:BA:1302:A:H2' | 1.61 | 0.98 |
| 57:BY:46:LYS:HG2 | 57:BY:47:LYS:H | 1.28 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:BA:1747(A):G:H2' | 36:BA:1748:G:H5'' | 1.44 | 0.98 |
| 22:AV:68:C:C2' | 22:AV:69:G:H5'' | 1.93 | 0.98 |
| 5:AE:50:GLU:HG3 | 5:AE:52:PRO:HD2 | 1.46 | 0.98 |
| 28:B2:41:ILE:HG13 | 28:B2:42:GLY:H | 1.26 | 0.98 |
| 43:BH:52:VAL:HB | 43:BH:69:ARG:HD3 | 1.43 | 0.97 |
| 32:B6:26:ASN:HD22 | 32:B6:32:ASN:HD21 | 1.03 | 0.97 |
| 36:BA:1665:A:C2' | 36:BA:1666:G:H5'' | 1.93 | 0.97 |
| 40:BE:60:ASN:OD1 | 40:BE:62:PRO:HD2 | 1.64 | 0.97 |
| 31:B5:40:LYS:NZ | 31:B5:46:CYS:H | 1.61 | 0.97 |
| 32:B6:26:ASN:HD22 | 32:B6:32:ASN:ND2 | 1.60 | 0.97 |
| 36:BA:2801(A):A:H4' | 36:BA:2802:G:H5' | 1.46 | 0.97 |
| 38:BC:163:PHE:HB3 | 38:BC:173:ALA:HB2 | 1.46 | 0.97 |
| 48:BP:62:LEU:CD2 | 48:BP:62:LEU:H | 1.78 | 0.97 |
| 32:B6:19:ARG:HG3 | 32:B6:20:ASN:H | 1.25 | 0.97 |
| 36:BA:884:C:H2' | 36:BA:885:C:H5' | 1.47 | 0.97 |
| 38:BC:70:LYS:HD2 | 38:BC:177:LYS:HZ3 | 1.24 | 0.97 |
| 19:AS:11:VAL:HA | 19:AS:38:SER:HB2 | 1.45 | 0.97 |
| 41:BF:9:ILE:HG12 | 41:BF:14:PRO:HA | 1.45 | 0.97 |
| 36:BA:1899:G:N2 | 36:BA:1902:C:N4 | 2.12 | 0.97 |
| 56:BX:12:VAL:HB | 56:BX:17:ALA:HB1 | 1.47 | 0.97 |
| 1:AA:1003:G:H2' | 1:AA:1004:A:H4' | 1.44 | 0.96 |
| 36:BA:271(L):U:H5'' | 36:BA:271(M):G:H5' | 1.44 | 0.96 |
| 24:AY:9:A:H2 | 24:AY:44:G:HO2' | 1.04 | 0.96 |
| 6:AF:67:MET:HB2 | 6:AF:68:PRO:HD2 | 1.47 | 0.96 |
| 56:BX:80:ILE:HG13 | 56:BX:80:ILE:O | 1.66 | 0.96 |
| 12:AL:20:LYS:HD3 | 12:AL:20:LYS:H | 1.31 | 0.96 |
| 32:B6:45:LYS:HD3 | 32:B6:45:LYS:H | 1.30 | 0.96 |
| 36:BA:1095:A:H2' | 36:BA:1096:A:H8 | 1.29 | 0.96 |
| 36:BA:2476:A:H2' | 36:BA:2477:C:H5'' | 1.42 | 0.96 |
| 40:BE:47:VAL:HG21 | 40:BE:86:PRO:HD2 | 1.46 | 0.96 |
| 58:BZ:69:THR:HG22 | 58:BZ:90:VAL:HA | 1.46 | 0.96 |
| 12:AL:89:ARG:HH11 | 12:AL:91:LYS:HA | 1.28 | 0.96 |
| 22:AW:55:U:H5'' | 38:BC:164:ARG:HH12 | 1.29 | 0.96 |
| 33:B7:34:ARG:HD2 | 33:B7:39:ARG:HG3 | 1.48 | 0.96 |
| 16:AP:43:LYS:HG2 | 16:AP:48:TRP:CE3 | 2.00 | 0.96 |
| 1:AA:1125:U:H3 | 10:AJ:5:ARG:HH21 | 1.14 | 0.95 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:H1 | 1.03 | 0.95 |
| 36:BA:1403:C:H5'' | 36:BA:1471:A:H1' | 1.48 | 0.95 |
| 38:BC:61:THR:HG22 | 38:BC:162:GLU:HG2 | 1.46 | 0.95 |
| 1:AA:92:C:H2' | 1:AA:93:G:H8 | 1.29 | 0.95 |
| 12:AL:46:LYS:HG2 | 12:AL:47:LYS:N | 1.79 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:32:THR:HG21 | 25:AZ:45:LYS:H | 1.26 | 0.95 |
| 30:B4:22:ILE:HD12 | 30:B4:22:ILE:H | 1.32 | 0.95 |
| 43:BH:70:THR:HG22 | 43:BH:74:ASN:HD21 | 1.31 | 0.95 |
| 15:AO:87:ILE:HG22 | 15:AO:88:ARG:N | 1.82 | 0.95 |
| 36:BA:2641:G:H5' | 36:BA:2641:G:H8 | 1.31 | 0.95 |
| 52:BT:80:SER:HB3 | 52:BT:81:PRO:HD3 | 1.49 | 0.95 |
| 1:AA:1321:C:H5'' | 1:AA:1322:C:H5'' | 1.48 | 0.95 |
| 1:AA:664:G:H22 | 1:AA:741:G:H1 | 1.00 | 0.95 |
| 36:BA:472:A:H8 | 36:BA:472:A:H5' | 1.30 | 0.95 |
| 36:BA:969:U:H2' | 36:BA:970:C:C6 | 2.02 | 0.95 |
| 49:BQ:76:LYS:HB3 | 49:BQ:91:GLU:HG3 | 1.48 | 0.95 |
| 48:BP:16:ARG:HD3 | 48:BP:18:ARG:H | 1.28 | 0.95 |
| 1:AA:8:A:N6 | 4:AD:208:SER:HB2 | 1.80 | 0.95 |
| 26:B0:49:LYS:H | 26:B0:80:HIS:HD1 | 1.14 | 0.95 |
| 42:BG:64:THR:HG23 | 42:BG:66:GLN:H | 1.32 | 0.95 |
| 27:B1:45:ASN:HD21 | 36:BA:2090:G:H21 | 1.08 | 0.94 |
| 39:BD:30:GLU:HG3 | 39:BD:63:ARG:NE | 1.81 | 0.94 |
| 5:AE:101:ILE:O | 5:AE:120:THR:HG22 | 1.67 | 0.94 |
| 25:AZ:143:ASP:HB3 | 25:AZ:146:LEU:HB3 | 1.46 | 0.94 |
| 38:BC:74:VAL:H | 38:BC:157:LYS:HE2 | 1.30 | 0.94 |
| 52:BT:85:LYS:NZ | 52:BT:85:LYS:HB3 | 1.79 | 0.94 |
| 36:BA:2375:G:H1' | 36:BA:2379:G:H22 | 1.30 | 0.94 |
| 36:BA:2726:U:H5' | 36:BA:2726:U:O2 | 1.66 | 0.94 |
| 24:AY:75:C:H6 | 25:AZ:231:ILE:HA | 1.28 | 0.94 |
| 34:B8:49:VAL:HG12 | 34:B8:53:PRO:HD3 | 1.49 | 0.94 |
| 48:BP:62:LEU:HD23 | 48:BP:62:LEU:N | 1.81 | 0.94 |
| 50:BR:2:ARG:HG3 | 50:BR:2:ARG:HH11 | 1.32 | 0.94 |
| 36:BA:2159:G:H2' | 36:BA:2160:G:H5'' | 1.50 | 0.94 |
| 39:BD:24:ILE:HD13 | 39:BD:25:THR:N | 1.82 | 0.94 |
| 10:AJ:30:SER:C | 10:AJ:80:LYS:HD3 | 1.88 | 0.94 |
| 36:BA:1902:C:O2' | 39:BD:244:ARG:HB2 | 1.66 | 0.94 |
| 41:BF:132:VAL:HG22 | 41:BF:133:ASN:H | 1.28 | 0.94 |
| 28:B2:17:SER:HB2 | 28:B2:18:PRO:HD2 | 1.49 | 0.93 |
| 36:BA:1053:C:H42 | 36:BA:1108:U:H3 | 0.99 | 0.93 |
| 39:BD:26:LYS:H | 39:BD:26:LYS:HE2 | 1.31 | 0.93 |
| 43:BH:18:GLU:HG3 | 43:BH:25:LYS:HB2 | 1.46 | 0.93 |
| 48:BP:146:VAL:HG22 | 48:BP:147:LEU:H | 1.31 | 0.93 |
| 22:AW:55:U:H5' | 38:BC:164:ARG:HH22 | 1.31 | 0.93 |
| 32:B6:6:ARG:NH1 | 32:B6:6:ARG:HB3 | 1.81 | 0.93 |
| 39:BD:35:LYS:N | 39:BD:36:PRO:HD2 | 1.82 | 0.93 |
| 38:BC:68:LEU:HD23 | 38:BC:176:GLY:HA2 | 1.46 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:10:PRO:HB2 | 13:AM:18:ALA:HB1 | 1.49 | 0.93 |
| 52:BT:83:ILE:HG13 | 52:BT:84:GLN:N | 1.84 | 0.93 |
| 1:AA:1305:G:N2 | 1:AA:1331:G:H2' | 1.81 | 0.93 |
| 36:BA:1222:C:C2' | 36:BA:1223:G:H5'' | 1.98 | 0.93 |
| 36:BA:61:G:H1 | 36:BA:94:C:H42 | 1.17 | 0.93 |
| 8:AH:114:THR:HG22 | 8:AH:130:GLY:O | 1.69 | 0.93 |
| 51:BS:49:VAL:HG12 | 51:BS:50:SER:H | 1.34 | 0.93 |
| 37:BB:40:U:H3' | 37:BB:41:U:H5'' | 1.50 | 0.93 |
| 41:BF:181:LEU:HD11 | 41:BF:186:ILE:HD11 | 1.51 | 0.93 |
| 56:BX:54:VAL:HG22 | 56:BX:81:VAL:HA | 1.50 | 0.93 |
| 47:BO:88:ASN:HD21 | 47:BO:92:GLU:HB3 | 1.31 | 0.93 |
| 52:BT:39:ARG:HD2 | 52:BT:39:ARG:H | 1.33 | 0.93 |
| 2:AB:204:ASN:HD22 | 2:AB:204:ASN:C | 1.71 | 0.92 |
| 17:AQ:24:GLU:HG2 | 17:AQ:39:SER:HB3 | 1.49 | 0.92 |
| 48:BP:16:ARG:HB2 | 48:BP:16:ARG:NH1 | 1.83 | 0.92 |
| 48:BP:23:PRO:HD2 | 48:BP:33:ARG:HE | 1.35 | 0.92 |
| 50:BR:38:VAL:HB | 50:BR:39:PRO:HD3 | 1.48 | 0.92 |
| 54:BV:72:VAL:HG23 | 54:BV:85:LYS:HB2 | 1.50 | 0.92 |
| 22:AV:46:G:H3' | 22:AV:47:U:C5' | 1.98 | 0.92 |
| 3:AC:5:ILE:HD13 | 3:AC:5:ILE:H | 1.34 | 0.92 |
| 12:AL:18:VAL:HG23 | 12:AL:19:ARG:H | 1.30 | 0.92 |
| 13:AM:97:PRO:HA | 13:AM:110:ARG:HD3 | 1.48 | 0.92 |
| 36:BA:1170:G:H22 | 36:BA:1179:C:H42 | 1.16 | 0.92 |
| 20:AT:36:LEU:HD12 | 20:AT:59:ALA:HB2 | 1.50 | 0.92 |
| 36:BA:655:A:H4' | 36:BA:656:G:H5' | 1.51 | 0.92 |
| 28:B2:65:ASN:HD22 | 28:B2:69:ARG:HH21 | 1.03 | 0.92 |
| 48:BP:6:LEU:H | 48:BP:6:LEU:HD23 | 1.35 | 0.92 |
| 50:BR:2:ARG:O | 50:BR:2:ARG:HD2 | 1.70 | 0.92 |
| 36:BA:613:G:H5' | 36:BA:613:G:H8 | 1.33 | 0.92 |
| 52:BT:55:ASN:N | 52:BT:59:THR:HG22 | 1.84 | 0.92 |
| 32:B6:30:THR:CG2 | 32:B6:31:PRO:HD2 | 1.98 | 0.92 |
| 48:BP:75:ILE:H | 48:BP:75:ILE:HD12 | 1.35 | 0.92 |
| 39:BD:28:GLU:H | 39:BD:29:PRO:HD2 | 1.34 | 0.92 |
| 52:BT:13:ARG:CZ | 52:BT:13:ARG:HA | 1.99 | 0.92 |
| 25:AZ:315:LYS:HG2 | 25:AZ:373:GLU:HG3 | 1.50 | 0.92 |
| 39:BD:261:LYS:HZ1 | 39:BD:263:ARG:NH2 | 1.65 | 0.92 |
| 26:B0:4:LYS:HD3 | 36:BA:2252:G:O6 | 1.69 | 0.92 |
| 36:BA:2287:A:N6 | 36:BA:2344:U:H3 | 1.68 | 0.92 |
| 39:BD:176:ARG:HG2 | 39:BD:176:ARG:HH11 | 1.32 | 0.91 |
| 31:B5:2:ALA:HA | 36:BA:2015:A:H1' | 1.51 | 0.91 |
| 36:BA:914:C:H2' | 36:BA:915:C:H5' | 1.50 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BT:13:ARG:NH1 | 52:BT:13:ARG:HA | 1.85 | 0.91 |
| 1:AA:405:U:H3' | 1:AA:406:G:H5' | 1.52 | 0.91 |
| 41:BF:101:LEU:HD12 | 41:BF:102:PRO:HD2 | 1.50 | 0.91 |
| 3:AC:20:SER:HB2 | 3:AC:40:ARG:HH22 | 1.36 | 0.91 |
| 36:BA:229:A:H3' | 36:BA:230:U:H5' | 1.52 | 0.91 |
| 41:BF:160:ASN:HD21 | 41:BF:162:LEU:HD13 | 1.35 | 0.91 |
| 49:BQ:141:GLN:HE22 | 58:BZ:72:ARG:HD3 | 1.36 | 0.91 |
| 19:AS:31:ILE:HG23 | 19:AS:49:ILE:HA | 1.53 | 0.91 |
| 1:AA:1281:U:H5' | 1:AA:1282:C:H5 | 1.35 | 0.91 |
| 1:AA:939:G:H5'' | 7:AG:102:ARG:NH2 | 1.85 | 0.91 |
| 36:BA:675:A:OP1 | 41:BF:63:LYS:HE2 | 1.71 | 0.91 |
| 38:BC:100:ILE:HG23 | 38:BC:127:LEU:HG | 1.53 | 0.91 |
| 1:AA:1277:C:HO2' | 1:AA:1279:A:H8 | 0.99 | 0.91 |
| 36:BA:1462:C:H4' | 36:BA:2703:C:H5' | 1.52 | 0.91 |
| 38:BC:65:PRO:HD2 | 38:BC:188:ASN:HA | 1.52 | 0.91 |
| 43:BH:12:PRO:HA | 43:BH:48:GLY:HA2 | 1.53 | 0.91 |
| 49:BQ:141:GLN:N | 58:BZ:53:ILE:HD12 | 1.85 | 0.91 |
| 1:AA:1386:G:C2' | 1:AA:1387:G:H5'' | 1.99 | 0.91 |
| 15:AO:87:ILE:CG2 | 15:AO:88:ARG:H | 1.83 | 0.91 |
| 35:B9:1:MET:HA | 35:B9:4:ARG:NH2 | 1.85 | 0.91 |
| 36:BA:1511:C:H2' | 36:BA:1512:U:H6 | 1.36 | 0.90 |
| 48:BP:58:THR:O | 48:BP:61:ARG:NE | 2.04 | 0.90 |
| 36:BA:1947:C:H2' | 36:BA:1948:G:H5'' | 1.53 | 0.90 |
| 2:AB:209:ARG:NH1 | 2:AB:239:VAL:HG11 | 1.86 | 0.90 |
| 4:AD:3:ARG:HE | 4:AD:5:ILE:HG13 | 1.35 | 0.90 |
| 7:AG:75:VAL:HG12 | 7:AG:88:PRO:HB3 | 1.51 | 0.90 |
| 24:AY:4:G:C2' | 24:AY:5:G:H5'' | 2.01 | 0.90 |
| 51:BS:15:ARG:HH11 | 51:BS:15:ARG:HB2 | 1.36 | 0.90 |
| 55:BW:72:LYS:HE3 | 55:BW:108:GLY:HA3 | 1.51 | 0.90 |
| 28:B2:41:ILE:HG13 | 28:B2:42:GLY:N | 1.85 | 0.90 |
| 38:BC:127:LEU:CD2 | 38:BC:130:ILE:HD12 | 2.01 | 0.90 |
| 54:BV:39:LEU:HD12 | 54:BV:47:VAL:HG11 | 1.53 | 0.90 |
| 53:BU:112:ARG:NH1 | 54:BV:46:VAL:HG11 | 1.85 | 0.90 |
| 22:AV:59:U:HO2' | 22:AV:60:U:H6 | 0.92 | 0.90 |
| 19:AS:49:ILE:HD12 | 19:AS:49:ILE:H | 1.37 | 0.90 |
| 25:AZ:324:LYS:HG2 | 25:AZ:364:PRO:HB3 | 1.53 | 0.90 |
| 36:BA:1378:A:O2' | 36:BA:1379:A:H5' | 1.71 | 0.90 |
| 26:B0:14:ARG:CB | 26:B0:14:ARG:HH11 | 1.84 | 0.90 |
| 36:BA:2140:C:H2' | 36:BA:2141:G:C8 | 2.06 | 0.90 |
| 9:AI:105:ASP:OD1 | 9:AI:107:ARG:HD3 | 1.71 | 0.90 |
| 32:B6:36:LEU:HD12 | 32:B6:50:ARG:NH1 | 1.86 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BA:1053:C:N4 | 36:BA:1108:U:H3 | 1.69 | 0.90 |
| 48:BP:23:PRO:HB2 | 48:BP:33:ARG:HG3 | 1.54 | 0.90 |
| 26:B0:7:LEU:HD22 | 49:BQ:85:LYS:HB2 | 1.53 | 0.90 |
| 1:AA:858:G:C6 | 1:AA:869:G:N7 | 2.40 | 0.90 |
| 1:AA:963:G:H21 | 10:AJ:55:LYS:HD3 | 1.33 | 0.90 |
| 1:AA:1305:G:H22 | 1:AA:1331:G:H2' | 1.31 | 0.89 |
| 2:AB:204:ASN:HD21 | 2:AB:206:ASP:H | 1.20 | 0.89 |
| 32:B6:15:GLU:CD | 32:B6:18:ARG:CZ | 2.40 | 0.89 |
| 36:BA:2476:A:C2' | 36:BA:2477:C:H5'' | 2.01 | 0.89 |
| 2:AB:68:ILE:H | 2:AB:90:MET:CE | 1.85 | 0.89 |
| 22:AV:4:C:H2' | 22:AV:5:G:H5'' | 1.54 | 0.89 |
| 36:BA:2151:G:H2' | 36:BA:2152:G:H8 | 1.35 | 0.89 |
| 37:BB:114:C:H4' | 51:BS:46:VAL:HG13 | 1.52 | 0.89 |
| 52:BT:65:LYS:HA | 52:BT:65:LYS:NZ | 1.86 | 0.89 |
| 32:B6:14:THR:HG22 | 32:B6:50:ARG:HB2 | 1.53 | 0.89 |
| 48:BP:71:VAL:H | 48:BP:72:PRO:CD | 1.85 | 0.89 |
| 36:BA:1947:C:C2' | 36:BA:1948:G:H5'' | 2.02 | 0.89 |
| 25:AZ:303:VAL:HG12 | 25:AZ:304:LEU:H | 1.35 | 0.89 |
| 25:AZ:355:LEU:HD23 | 25:AZ:356:PRO:HD2 | 1.53 | 0.89 |
| 36:BA:1771:C:HO2' | 36:BA:1786:A:H8 | 1.19 | 0.89 |
| 36:BA:1899:G:H21 | 36:BA:1902:C:H41 | 0.93 | 0.89 |
| 54:BV:52:VAL:HG13 | 54:BV:55:ALA:HB3 | 1.51 | 0.89 |
| 1:AA:1363(A):A:H4' | 1:AA:1364:U:H5'' | 1.51 | 0.89 |
| 1:AA:173:U:H5' | 1:AA:197:A:O4' | 1.73 | 0.89 |
| 11:AK:48:ILE:HG22 | 11:AK:49:GLY:H | 1.34 | 0.89 |
| 20:AT:73:HIS:HB3 | 20:AT:74:LYS:HD3 | 1.54 | 0.89 |
| 25:AZ:20:VAL:HG12 | 25:AZ:85:HIS:H | 1.36 | 0.89 |
| 27:B1:73:LEU:HD22 | 27:B1:94:LEU:HB3 | 1.52 | 0.89 |
| 10:AJ:96:ILE:HD13 | 10:AJ:96:ILE:H | 1.37 | 0.89 |
| 14:AN:32:SER:HB3 | 14:AN:41:ARG:HG2 | 1.55 | 0.89 |
| 49:BQ:141:GLN:NE2 | 58:BZ:72:ARG:HD3 | 1.87 | 0.89 |
| 36:BA:747:U:H5' | 55:BW:90:ARG:HH12 | 1.36 | 0.89 |
| 36:BA:83:G:N2 | 36:BA:102:G:H2' | 1.87 | 0.89 |
| 36:BA:2523:G:C2' | 36:BA:2524:G:H5'' | 2.02 | 0.89 |
| 36:BA:2729:G:H1' | 40:BE:187:ALA:HB2 | 1.54 | 0.89 |
| 48:BP:56:SER:O | 48:BP:57:THR:HG23 | 1.72 | 0.89 |
| 36:BA:84:A:H5' | 57:BY:9:LYS:HB3 | 1.55 | 0.89 |
| 36:BA:925:C:C2' | 36:BA:926:A:H5'' | 2.03 | 0.89 |
| 43:BH:12:PRO:HD2 | 43:BH:15:VAL:HG21 | 1.52 | 0.89 |
| 55:BW:69:LEU:HA | 55:BW:108:GLY:O | 1.73 | 0.89 |
| 36:BA:2189:U:H2' | 36:BA:2190:G:C4' | 2.03 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:B6:19:ARG:HD3 | 36:BA:2400:G:H4' | 1.55 | 0.88 |
| 36:BA:2693:A:H2' | 36:BA:2694:G:H8 | 1.39 | 0.88 |
| 52:BT:55:ASN:HD22 | 52:BT:58:ASN:HD21 | 1.21 | 0.88 |
| 57:BY:31:LEU:HB2 | 57:BY:32:PRO:HA | 1.55 | 0.88 |
| 17:AQ:67:LYS:HA | 17:AQ:70:ARG:HH12 | 1.38 | 0.88 |
| 10:AJ:75:ILE:HG13 | 10:AJ:76:ASN:H | 1.38 | 0.88 |
| 22:AW:62:C:H2' | 22:AW:63:G:C8 | 2.07 | 0.88 |
| 2:AB:87:ARG:HH11 | 2:AB:223:ILE:HD11 | 1.38 | 0.88 |
| 4:AD:129:ASN:HD21 | 4:AD:145:GLU:H | 1.22 | 0.88 |
| 36:BA:1598:C:H5' | 56:BX:36:LYS:HG2 | 1.55 | 0.88 |
| 25:AZ:19:HIS:CD2 | 25:AZ:20:VAL:H | 1.90 | 0.88 |
| 36:BA:2169:A:H2' | 36:BA:2170:A:C8 | 2.09 | 0.88 |
| 36:BA:2208:A:H1' | 36:BA:2219:G:C5 | 2.07 | 0.88 |
| 46:BN:5:VAL:HG12 | 46:BN:7:LYS:HG3 | 1.54 | 0.88 |
| 20:AT:26:ASN:HB2 | 20:AT:71:THR:HG23 | 1.53 | 0.88 |
| 36:BA:2640:G:H2' | 36:BA:2641:G:H5'' | 1.53 | 0.88 |
| 48:BP:59:LEU:HA | 48:BP:61:ARG:NE | 1.89 | 0.88 |
| 40:BE:117:MET:O | 40:BE:121:ASN:HA | 1.74 | 0.88 |
| 41:BF:178:PRO:HB2 | 41:BF:201:VAL:HG11 | 1.54 | 0.88 |
| 57:BY:95:LYS:HG3 | 57:BY:100:ALA:HA | 1.53 | 0.88 |
| 25:AZ:198:LYS:N | 25:AZ:198:LYS:HE2 | 1.89 | 0.88 |
| 36:BA:2464:C:HO2' | 36:BA:2465:C:H6 | 1.15 | 0.88 |
| 58:BZ:10:ARG:HH21 | 58:BZ:36:LYS:HB2 | 1.39 | 0.88 |
| 24:AY:61:C:C2' | 24:AY:62:U:H5'' | 2.04 | 0.88 |
| 36:BA:1038:C:H2' | 36:BA:1039:G:H5'' | 1.56 | 0.88 |
| 50:BR:99:LYS:HD2 | 50:BR:99:LYS:H | 1.36 | 0.88 |
| 52:BT:16:ARG:HB3 | 52:BT:16:ARG:HH11 | 1.36 | 0.88 |
| 52:BT:3:ARG:HB3 | 52:BT:6:LEU:HB2 | 1.55 | 0.88 |
| 43:BH:66:GLY:HA2 | 43:BH:69:ARG:HB3 | 1.54 | 0.87 |
| 36:BA:2189:U:H2' | 36:BA:2190:G:H4' | 1.55 | 0.87 |
| 36:BA:543:C:H42 | 36:BA:549:G:H1 | 1.22 | 0.87 |
| 42:BG:52:ILE:HG12 | 42:BG:53:LEU:H | 1.39 | 0.87 |
| 1:AA:102:G:H2' | 1:AA:103:C:H6 | 1.40 | 0.87 |
| 1:AA:975:A:H4' | 1:AA:976:G:H5'' | 1.55 | 0.87 |
| 3:AC:34:LEU:HG | 14:AN:25:VAL:HG11 | 1.55 | 0.87 |
| 36:BA:1543:C:H3' | 36:BA:1544:A:H5'' | 1.54 | 0.87 |
| 38:BC:164:ARG:O | 38:BC:171:ILE:HA | 1.74 | 0.87 |
| 38:BC:30:LYS:HZ2 | 38:BC:30:LYS:HA | 1.38 | 0.87 |
| 36:BA:1067:A:H3' | 36:BA:1068:G:H5'' | 1.55 | 0.87 |
| 2:AB:204:ASN:ND2 | 2:AB:206:ASP:H | 1.73 | 0.87 |
| 4:AD:194:LEU:HB3 | 4:AD:196:LEU:HD13 | 1.56 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:AB:18:GLY:H | 2:AB:42:ILE:CG2 | 1.87 | 0.87 |
| 58:BZ:20:ARG:NH1 | 58:BZ:20:ARG:HB2 | 1.89 | 0.87 |
| 36:BA:259:G:H21 | 36:BA:621:A:H8 | 1.23 | 0.87 |
| 13:AM:12:ASN:HD22 | 13:AM:12:ASN:H | 1.18 | 0.87 |
| 22:AW:57:G:H2' | 22:AW:58:A:H5' | 1.57 | 0.87 |
| 52:BT:55:ASN:HD22 | 52:BT:58:ASN:ND2 | 1.72 | 0.87 |
| 24:AY:1:A:H61 | 24:AY:72:U:H3 | 1.18 | 0.86 |
| 31:B5:57:VAL:HG12 | 31:B5:58:LEU:HD12 | 1.54 | 0.86 |
| 36:BA:654(L):G:H2' | 36:BA:654(M):C:C4' | 2.05 | 0.86 |
| 32:B6:30:THR:HG22 | 32:B6:31:PRO:CD | 2.01 | 0.86 |
| 36:BA:2801(A):A:H5' | 36:BA:2802:G:H8 | 1.37 | 0.86 |
| 38:BC:161:ILE:HD13 | 38:BC:173:ALA:HB1 | 1.57 | 0.86 |
| 33:B7:8:ASN:HD22 | 33:B7:9:ARG:N | 1.74 | 0.86 |
| 27:B1:89:GLU:HA | 27:B1:92:LYS:HE3 | 1.57 | 0.86 |
| 31:B5:29:THR:HG21 | 36:BA:2814:C:O2' | 1.74 | 0.86 |
| 36:BA:404:C:H4' | 36:BA:405:U:H5' | 1.55 | 0.86 |
| 58:BZ:108:PRO:HA | 58:BZ:141:VAL:CG1 | 2.05 | 0.86 |
| 32:B6:53:LYS:HD3 | 32:B6:54:ILE:H | 1.40 | 0.86 |
| 34:B8:25:MET:HG3 | 48:BP:64:LYS:HB2 | 1.56 | 0.86 |
| 36:BA:774:A:H2 | 36:BA:787:U:HO2' | 0.90 | 0.86 |
| 37:BB:80:U:H2' | 37:BB:81:G:H21 | 1.41 | 0.86 |
| 36:BA:2287:A:H62 | 36:BA:2344:U:H3 | 1.23 | 0.86 |
| 36:BA:2807:G:H3' | 36:BA:2808:U:H5'' | 1.57 | 0.86 |
| 58:BZ:151:HIS:CB | 58:BZ:170:THR:HA | 2.04 | 0.86 |
| 58:BZ:53:ILE:HG22 | 58:BZ:71:VAL:HB | 1.56 | 0.86 |
| 1:AA:194:C:H2' | 1:AA:195:A:H5'' | 1.57 | 0.86 |
| 4:AD:129:ASN:ND2 | 4:AD:145:GLU:H | 1.72 | 0.86 |
| 36:BA:2656:U:H3 | 36:BA:2665:A:H2 | 1.23 | 0.86 |
| 25:AZ:234:ARG:HA | 25:AZ:234:ARG:HE | 1.40 | 0.86 |
| 25:AZ:355:LEU:HD22 | 25:AZ:359:VAL:HB | 1.57 | 0.86 |
| 36:BA:1409:C:H2' | 36:BA:1410:G:H8 | 1.41 | 0.86 |
| 28:B2:50:ILE:HG21 | 36:BA:61:G:H5' | 1.55 | 0.86 |
| 37:BB:20:C:H2' | 37:BB:21:G:H5'' | 1.54 | 0.86 |
| 39:BD:34:VAL:C | 39:BD:36:PRO:HD2 | 1.96 | 0.86 |
| 39:BD:35:LYS:HD2 | 39:BD:36:PRO:N | 1.90 | 0.86 |
| 41:BF:24:LEU:HB3 | 41:BF:25:PRO:CD | 2.05 | 0.86 |
| 1:AA:509:A:H5' | 4:AD:54:TYR:HD2 | 1.40 | 0.86 |
| 58:BZ:152:ALA:HB1 | 58:BZ:167:PRO:HB2 | 1.58 | 0.86 |
| 58:BZ:166:SER:HB2 | 58:BZ:168:GLU:N | 1.91 | 0.85 |
| 19:AS:29:ARG:HB2 | 19:AS:48:THR:HB | 1.56 | 0.85 |
| 41:BF:135:LYS:HB3 | 41:BF:138:GLU:HG3 | 1.55 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BN:60:ILE:HD13 | 46:BN:99:LEU:HD23 | 1.55 | 0.85 |
| 53:BU:101:ARG:O | 53:BU:103:PRO:HD3 | 1.76 | 0.85 |
| 1:AA:1003:G:C2' | 1:AA:1004:A:H4' | 2.07 | 0.85 |
| 1:AA:1116:C:C2' | 1:AA:1117:G:H5'' | 2.07 | 0.85 |
| 2:AB:172:ILE:HD12 | 2:AB:172:ILE:H | 1.41 | 0.85 |
| 9:AI:114:TYR:HE1 | 10:AJ:60:ARG:H | 1.22 | 0.85 |
| 36:BA:1058:G:C2' | 36:BA:1059:G:H5'' | 2.06 | 0.85 |
| 36:BA:2476:A:H2 | 36:BA:2477:C:C5 | 1.93 | 0.85 |
| 36:BA:414:C:H1' | 36:BA:1864:U:O2' | 1.75 | 0.85 |
| 46:BN:86:PRO:HG2 | 46:BN:89:LYS:HG2 | 1.57 | 0.85 |
| 48:BP:64:LYS:O | 48:BP:66:GLY:N | 2.10 | 0.85 |
| 5:AE:126:ARG:HA | 5:AE:131:ILE:HD11 | 1.59 | 0.85 |
| 32:B6:18:ARG:HG3 | 32:B6:19:ARG:H | 1.42 | 0.85 |
| 36:BA:676:A:H8 | 36:BA:2069:G:H21 | 1.22 | 0.85 |
| 57:BY:8:LYS:N | 57:BY:8:LYS:HD2 | 1.90 | 0.85 |
| 2:AB:18:GLY:N | 2:AB:42:ILE:HG22 | 1.90 | 0.85 |
| 12:AL:41:ARG:HG2 | 12:AL:42:THR:H | 1.39 | 0.85 |
| 20:AT:89:ARG:HB2 | 20:AT:104:LEU:HD11 | 1.58 | 0.85 |
| 28:B2:51:ARG:HD3 | 28:B2:55:ARG:HH22 | 1.39 | 0.85 |
| 36:BA:612:C:C2' | 36:BA:613:G:H5'' | 2.06 | 0.85 |
| 39:BD:263:ARG:HB2 | 39:BD:263:ARG:HH11 | 1.42 | 0.85 |
| 40:BE:14:ILE:HD11 | 40:BE:173:VAL:HG11 | 1.58 | 0.85 |
| 40:BE:1:MET:HB3 | 40:BE:200:GLU:OE1 | 1.75 | 0.85 |
| 5:AE:51:VAL:HB | 5:AE:52:PRO:HD3 | 1.58 | 0.85 |
| 36:BA:2036:C:H5' | 36:BA:2036:C:H6 | 1.40 | 0.85 |
| 47:BO:87:ILE:HG21 | 47:BO:91:LEU:HA | 1.59 | 0.85 |
| 49:BQ:17:LEU:HD21 | 49:BQ:96:VAL:HG13 | 1.57 | 0.85 |
| 1:AA:1266:G:N2 | 1:AA:1268:A:OP2 | 2.10 | 0.85 |
| 11:AK:82:VAL:HG12 | 11:AK:108:ILE:HA | 1.58 | 0.85 |
| 27:B1:44:PRO:HG2 | 27:B1:46:LEU:HD23 | 1.59 | 0.85 |
| 52:BT:96:ARG:NH1 | 52:BT:96:ARG:HB2 | 1.92 | 0.85 |
| 57:BY:49:VAL:O | 57:BY:50:ARG:HB2 | 1.74 | 0.85 |
| 25:AZ:318:ALA:HA | 25:AZ:401:THR:HG22 | 1.56 | 0.85 |
| 48:BP:31:ALA:C | 48:BP:33:ARG:H | 1.79 | 0.85 |
| 13:AM:88:ARG:HG3 | 13:AM:98:VAL:HG11 | 1.57 | 0.85 |
| 1:AA:1305:G:H5' | 21:AU:4:GLY:HA3 | 1.59 | 0.85 |
| 36:BA:673:C:H6 | 36:BA:673:C:H5' | 1.42 | 0.85 |
| 52:BT:28:VAL:HG22 | 52:BT:47:GLY:N | 1.92 | 0.85 |
| 13:AM:93:ARG:HG3 | 36:BA:888:C:OP1 | 1.77 | 0.84 |
| 19:AS:6:LYS:O | 19:AS:7:LYS:HD3 | 1.77 | 0.84 |
| 22:AV:21:A:C2' | 22:AV:22:G:H5'' | 2.07 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:BT:28:VAL:CG1 | 52:BT:46:GLU:HA | 2.07 | 0.84 |
| 8:AH:98:LYS:HG3 | 8:AH:99:GLU:HG3 | 1.57 | 0.84 |
| 14:AN:13:THR:N | 14:AN:14:PRO:HD2 | 1.91 | 0.84 |
| 14:AN:29:ARG:HG2 | 14:AN:29:ARG:HH11 | 1.41 | 0.84 |
| 19:AS:10:PHE:CE1 | 19:AS:70:LYS:HD2 | 2.11 | 0.84 |
| 33:B7:38:GLY:O | 36:BA:458:G:H5'' | 1.78 | 0.84 |
| 36:BA:898:C:H2' | 36:BA:899:A:H5' | 1.57 | 0.84 |
| 24:AY:75:C:H5 | 25:AZ:232:THR:H | 1.22 | 0.84 |
| 36:BA:1697:G:H3' | 36:BA:1698:A:H5'' | 1.57 | 0.84 |
| 36:BA:1678:G:H22 | 36:BA:1989:G:H22 | 1.23 | 0.84 |
| 38:BC:53:ARG:HH11 | 38:BC:53:ARG:HB3 | 1.40 | 0.84 |
| 52:BT:11:GLU:CD | 52:BT:11:GLU:H | 1.80 | 0.84 |
| 2:AB:114:ARG:HD2 | 2:AB:141:GLU:OE2 | 1.76 | 0.84 |
| 36:BA:2245:U:H5' | 36:BA:2246:G:H5' | 1.57 | 0.84 |
| 36:BA:654(M):C:H2' | 36:BA:654(N):G:C8 | 2.13 | 0.84 |
| 7:AG:84:ASN:OD1 | 22:AW:33:U:H5' | 1.77 | 0.84 |
| 9:AI:53:VAL:HG13 | 9:AI:95:LYS:HE3 | 1.58 | 0.84 |
| 22:AW:57:G:C2' | 22:AW:58:A:H5' | 2.06 | 0.84 |
| 36:BA:271(L):U:H4' | 36:BA:271(M):G:C8 | 2.11 | 0.84 |
| 1:AA:266:G:H5'' | 1:AA:267:C:H5 | 1.43 | 0.84 |
| 36:BA:2287:A:H2 | 36:BA:2346:A:N1 | 1.76 | 0.84 |
| 36:BA:621:A:H2' | 36:BA:622:G:H5' | 1.58 | 0.84 |
| 50:BR:2:ARG:HG3 | 50:BR:2:ARG:NH1 | 1.90 | 0.84 |
| 58:BZ:155:LEU:HD23 | 58:BZ:155:LEU:H | 1.42 | 0.84 |
| 1:AA:1218:C:H2' | 1:AA:1219:U:C6 | 2.12 | 0.84 |
| 43:BH:143:GLN:HE21 | 43:BH:143:GLN:HA | 1.43 | 0.84 |
| 56:BX:30:VAL:HG22 | 56:BX:77:LYS:O | 1.78 | 0.84 |
| 12:AL:89:ARG:NH1 | 12:AL:91:LYS:HA | 1.93 | 0.84 |
| 36:BA:304:G:H1 | 36:BA:313:C:H42 | 1.23 | 0.84 |
| 42:BG:6:ALA:O | 42:BG:10:LYS:HB2 | 1.78 | 0.84 |
| 22:AW:56:C:O4' | 38:BC:132:GLY:HA3 | 1.76 | 0.84 |
| 36:BA:2593:U:H2' | 36:BA:2594:C:H6 | 1.42 | 0.84 |
| 38:BC:45:ALA:HA | 38:BC:211:SER:O | 1.78 | 0.84 |
| 30:B4:6:HIS:HA | 42:BG:67:LYS:HD2 | 1.60 | 0.84 |
| 43:BH:23:ARG:HD3 | 43:BH:36:PRO:HB3 | 1.60 | 0.84 |
| 48:BP:112:LEU:H | 48:BP:128:HIS:HD2 | 1.23 | 0.84 |
| 1:AA:522:C:H41 | 12:AL:53:ARG:HH22 | 1.25 | 0.83 |
| 36:BA:1762:A:O5' | 36:BA:1762:A:H8 | 1.59 | 0.83 |
| 36:BA:2645:G:H3' | 36:BA:2646:C:H5' | 1.60 | 0.83 |
| 42:BG:67:LYS:HD3 | 42:BG:67:LYS:N | 1.93 | 0.83 |
| 48:BP:47:ASP:HB3 | 48:BP:48:PRO:CA | 2.06 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:BR:18:LEU:HD11 | 50:BR:22:ARG:CZ | 2.08 | 0.83 |
| 52:BT:28:VAL:HG13 | 52:BT:46:GLU:HA | 1.60 | 0.83 |
| 32:B6:11:LEU:HD13 | 32:B6:12:GLU:H | 1.43 | 0.83 |
| 36:BA:2781:A:C5' | 36:BA:2782:G:H5' | 2.07 | 0.83 |
| 51:BS:48:LEU:HD23 | 51:BS:82:ILE:HG13 | 1.60 | 0.83 |
| 2:AB:80:ILE:HD12 | 2:AB:80:ILE:H | 1.41 | 0.83 |
| 36:BA:1899:G:H21 | 36:BA:1902:C:N4 | 1.75 | 0.83 |
| 38:BC:164:ARG:HG2 | 38:BC:165:ASN:N | 1.93 | 0.83 |
| 42:BG:140:ILE:HD12 | 42:BG:141:PHE:N | 1.94 | 0.83 |
| 55:BW:6:ILE:HG23 | 55:BW:104:THR:HG22 | 1.59 | 0.83 |
| 1:AA:963:G:N2 | 10:AJ:55:LYS:HD3 | 1.93 | 0.83 |
| 18:AR:73:ALA:HB3 | 18:AR:79:LEU:HD12 | 1.61 | 0.83 |
| 39:BD:270:ILE:H | 39:BD:270:ILE:HD12 | 1.43 | 0.83 |
| 46:BN:134:ARG:HH21 | 46:BN:136:GLU:HB2 | 1.43 | 0.83 |
| 14:AN:6:LEU:HB3 | 14:AN:23:ARG:NH2 | 1.94 | 0.83 |
| 25:AZ:321:TYR:HA | 25:AZ:367:ASN:HB3 | 1.60 | 0.83 |
| 32:B6:13:CYS:HB2 | 32:B6:22:ALA:HB3 | 1.60 | 0.83 |
| 34:B8:28:GLY:O | 34:B8:32:LEU:HG | 1.78 | 0.83 |
| 36:BA:1335:U:H2' | 36:BA:1336:A:C8 | 2.14 | 0.83 |
| 30:B4:9:LEU:HG | 42:BG:98:ARG:HH12 | 1.44 | 0.83 |
| 48:BP:59:LEU:HA | 48:BP:61:ARG:HE | 1.41 | 0.83 |
| 36:BA:654(L):G:C2' | 36:BA:654(M):C:H4' | 2.07 | 0.83 |
| 43:BH:70:THR:HG22 | 43:BH:74:ASN:ND2 | 1.94 | 0.83 |
| 46:BN:2:LYS:NZ | 53:BU:95:LEU:HD21 | 1.92 | 0.83 |
| 2:AB:61:LEU:HA | 2:AB:64:ARG:NE | 1.94 | 0.83 |
| 10:AJ:24:VAL:HG21 | 10:AJ:37:PRO:HG3 | 1.60 | 0.83 |
| 34:B8:8:LYS:O | 34:B8:12:LYS:HG3 | 1.78 | 0.83 |
| 36:BA:2128:C:HO2' | 36:BA:2129:C:H6 | 1.26 | 0.83 |
| 50:BR:18:LEU:HD11 | 50:BR:22:ARG:NE | 1.92 | 0.83 |
| 36:BA:1484:G:C2' | 36:BA:1485:G:H5'' | 2.08 | 0.83 |
| 38:BC:58:VAL:HG22 | 38:BC:201:PRO:HG2 | 1.58 | 0.83 |
| 1:AA:1218:C:H2' | 1:AA:1219:U:H6 | 1.41 | 0.83 |
| 20:AT:51:GLU:HA | 20:AT:54:LYS:HE3 | 1.59 | 0.83 |
| 25:AZ:195:TRP:HA | 25:AZ:198:LYS:HD2 | 1.60 | 0.83 |
| 36:BA:1286:A:H2' | 36:BA:1288:U:OP2 | 1.76 | 0.83 |
| 43:BH:97:ARG:HG2 | 43:BH:98:LEU:H | 1.42 | 0.83 |
| 50:BR:55:ALA:HA | 50:BR:80:PHE:CE1 | 2.12 | 0.83 |
| 1:AA:351:G:H4' | 1:AA:352:C:OP1 | 1.79 | 0.82 |
| 1:AA:979:C:C3' | 1:AA:980:C:H5'' | 2.09 | 0.82 |
| 24:AY:61:C:H2' | 24:AY:62:U:H5'' | 1.60 | 0.82 |
| 26:B0:36:ILE:HG22 | 26:B0:60:PHE:HB3 | 1.61 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BC:30:LYS:NZ | 38:BC:178:ALA:HB1 | 1.94 | 0.82 |
| 39:BD:80:ALA:HB3 | 39:BD:94:LEU:O | 1.79 | 0.82 |
| 40:BE:6:GLY:HA2 | 40:BE:51:PHE:CZ | 2.14 | 0.82 |
| 50:BR:7:GLY:O | 50:BR:8:ARG:HB2 | 1.78 | 0.82 |
| 52:BT:68:TYR:O | 52:BT:70:VAL:N | 2.11 | 0.82 |
| 1:AA:160:A:H1' | 1:AA:344:A:C5 | 2.15 | 0.82 |
| 34:B8:52:LYS:N | 34:B8:53:PRO:HD2 | 1.93 | 0.82 |
| 36:BA:27:G:N2 | 36:BA:512:G:H2' | 1.94 | 0.82 |
| 36:BA:796:C:H2' | 36:BA:797:C:C6 | 2.14 | 0.82 |
| 46:BN:57:ALA:HB3 | 46:BN:124:ALA:HA | 1.61 | 0.82 |
| 50:BR:47:PHE:O | 50:BR:51:LEU:HD13 | 1.79 | 0.82 |
| 9:AI:9:ARG:HG2 | 9:AI:14:VAL:HG22 | 1.61 | 0.82 |
| 36:BA:672:C:C2' | 36:BA:673:C:H5'' | 2.09 | 0.82 |
| 55:BW:6:ILE:HG12 | 55:BW:104:THR:CB | 2.09 | 0.82 |
| 36:BA:1169:G:H1 | 36:BA:1180:C:H42 | 1.28 | 0.82 |
| 48:BP:16:ARG:CZ | 48:BP:18:ARG:HB2 | 2.09 | 0.82 |
| 52:BT:50:ILE:HD11 | 52:BT:64:ARG:CB | 2.10 | 0.82 |
| 1:AA:547:A:H4' | 1:AA:548:G:O5' | 1.79 | 0.82 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.23 | 0.82 |
| 10:AJ:55:LYS:HE3 | 10:AJ:55:LYS:N | 1.95 | 0.82 |
| 12:AL:41:ARG:HH22 | 12:AL:57:LYS:NZ | 1.78 | 0.82 |
| 36:BA:1779:U:H5 | 36:BA:1784:A:N7 | 1.77 | 0.82 |
| 36:BA:2175:C:H4' | 38:BC:221:SER:HB3 | 1.60 | 0.82 |
| 36:BA:272(J):C:H2' | 36:BA:274:G:H5'' | 1.60 | 0.82 |
| 36:BA:2124:G:H1' | 38:BC:42:GLU:HG3 | 1.60 | 0.82 |
| 43:BH:98:LEU:HB2 | 43:BH:125:VAL:HG21 | 1.61 | 0.82 |
| 51:BS:85:VAL:HG23 | 51:BS:106:ARG:HG3 | 1.59 | 0.82 |
| 54:BV:21:ARG:HB3 | 54:BV:91:TYR:HB2 | 1.60 | 0.82 |
| 9:AI:4:TYR:CD2 | 9:AI:88:TYR:HB2 | 2.14 | 0.82 |
| 36:BA:2807:G:H1 | 36:BA:2893:G:H1 | 1.24 | 0.82 |
| 36:BA:629:G:H5' | 36:BA:629:G:C8 | 2.14 | 0.82 |
| 39:BD:263:ARG:HH11 | 39:BD:263:ARG:CB | 1.93 | 0.82 |
| 39:BD:263:ARG:NH1 | 39:BD:263:ARG:HB2 | 1.93 | 0.82 |
| 36:BA:708:C:H42 | 36:BA:723:G:H1 | 1.26 | 0.82 |
| 39:BD:261:LYS:NZ | 39:BD:263:ARG:NH2 | 2.27 | 0.82 |
| 39:BD:30:GLU:HG3 | 39:BD:63:ARG:HE | 1.43 | 0.82 |
| 41:BF:6:VAL:HG12 | 41:BF:7:TYR:N | 1.94 | 0.82 |
| 42:BG:124:SER:HB2 | 42:BG:131:TYR:CE1 | 2.14 | 0.82 |
| 46:BN:22:THR:HG22 | 46:BN:61:ARG:HB3 | 1.60 | 0.82 |
| 2:AB:200:ILE:N | 2:AB:200:ILE:HD12 | 1.95 | 0.82 |
| 18:AR:45:SER:H | 18:AR:51:LEU:HG | 1.44 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:B0:48:GLY:H | 26:B0:51:VAL:HB | 1.42 | 0.82 |
| 36:BA:1243:G:C2' | 36:BA:1244:G:H5'' | 2.09 | 0.82 |
| 38:BC:180:PHE:HB3 | 38:BC:184:LYS:CB | 2.04 | 0.82 |
| 39:BD:35:LYS:HB3 | 39:BD:35:LYS:HZ2 | 1.45 | 0.82 |
| 50:BR:99:LYS:HA | 50:BR:112:ALA:HA | 1.61 | 0.82 |
| 53:BU:112:ARG:HH12 | 54:BV:46:VAL:CG1 | 1.91 | 0.82 |
| 19:AS:29:ARG:HB3 | 19:AS:48:THR:H | 1.45 | 0.82 |
| 36:BA:1291:C:H2' | 36:BA:1292:U:H5' | 1.62 | 0.82 |
| 38:BC:86:ALA:HB3 | 38:BC:94:VAL:CG1 | 2.10 | 0.82 |
| 50:BR:73:VAL:O | 50:BR:76:VAL:HG12 | 1.79 | 0.82 |
| 32:B6:18:ARG:HG2 | 32:B6:18:ARG:NH1 | 1.82 | 0.82 |
| 36:BA:1543:C:H3' | 36:BA:1544:A:C5' | 2.09 | 0.82 |
| 36:BA:1689:A:H62 | 36:BA:1698:A:H2 | 1.28 | 0.82 |
| 48:BP:83:VAL:HG12 | 48:BP:112:LEU:HD21 | 1.62 | 0.82 |
| 54:BV:36:PRO:HA | 54:BV:56:SER:HB3 | 1.61 | 0.82 |
| 13:AM:97:PRO:CA | 13:AM:110:ARG:HD3 | 2.09 | 0.81 |
| 26:B0:43:THR:O | 26:B0:43:THR:HG23 | 1.78 | 0.81 |
| 29:B3:15:TYR:O | 29:B3:20:LYS:HE3 | 1.80 | 0.81 |
| 41:BF:132:VAL:HG23 | 41:BF:162:LEU:HD23 | 1.62 | 0.81 |
| 41:BF:167:ALA:HB1 | 41:BF:173:VAL:HG11 | 1.60 | 0.81 |
| 42:BG:18:GLU:O | 42:BG:22:ARG:HB2 | 1.80 | 0.81 |
| 1:AA:198:G:HO2' | 1:AA:199:G:H8 | 0.84 | 0.81 |
| 19:AS:32:LYS:HA | 19:AS:50:ALA:HB3 | 1.61 | 0.81 |
| 32:B6:15:GLU:OE2 | 32:B6:41:PRO:CB | 2.28 | 0.81 |
| 42:BG:43:LEU:HD11 | 42:BG:153:ARG:HG3 | 1.61 | 0.81 |
| 48:BP:24:GLY:HA3 | 48:BP:33:ARG:NH1 | 1.95 | 0.81 |
| 1:AA:198:G:O2' | 1:AA:199:G:H8 | 1.62 | 0.81 |
| 2:AB:204:ASN:HD22 | 2:AB:205:ASP:N | 1.78 | 0.81 |
| 34:B8:25:MET:CG | 48:BP:64:LYS:HB2 | 2.09 | 0.81 |
| 49:BQ:141:GLN:O | 58:BZ:53:ILE:HB | 1.79 | 0.81 |
| 53:BU:8:VAL:HG23 | 53:BU:11:ARG:HH21 | 1.45 | 0.81 |
| 57:BY:75:ILE:CD1 | 57:BY:79:CYS:HA | 2.11 | 0.81 |
| 1:AA:192:U:H2' | 1:AA:193:C:H6 | 1.45 | 0.81 |
| 21:AU:12:LYS:HG2 | 21:AU:22:ARG:HB3 | 1.62 | 0.81 |
| 25:AZ:101:GLY:HA3 | 25:AZ:210:ILE:HD11 | 1.60 | 0.81 |
| 41:BF:84:VAL:HG12 | 41:BF:85:GLY:N | 1.94 | 0.81 |
| 50:BR:74:LYS:HD2 | 50:BR:77:ARG:HH21 | 1.45 | 0.81 |
| 36:BA:2312:U:C2' | 36:BA:2313:C:H5'' | 2.10 | 0.81 |
| 38:BC:128:GLY:HA2 | 38:BC:137:LEU:CD2 | 2.11 | 0.81 |
| 1:AA:1314:C:OP2 | 19:AS:6:LYS:HG3 | 1.79 | 0.81 |
| 2:AB:97:TRP:CH2 | 2:AB:173:ALA:HA | 2.15 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 31:B5:4:HIS:HB3 | 31:B5:5:PRO:CD | 2.08 | 0.81 |
| 36:BA:472:A:H5' | 36:BA:472:A:C8 | 2.15 | 0.81 |
| 43:BH:12:PRO:CA | 43:BH:48:GLY:HA2 | 2.10 | 0.81 |
| 46:BN:3:THR:HG22 | 46:BN:4:TYR:H | 1.46 | 0.81 |
| 36:BA:83:G:H22 | 36:BA:102:G:H2' | 1.44 | 0.81 |
| 36:BA:2801(A):A:C4' | 36:BA:2802:G:H5' | 2.10 | 0.81 |
| 40:BE:116:VAL:O | 40:BE:117:MET:HB2 | 1.77 | 0.81 |
| 41:BF:25:PRO:HB3 | 41:BF:119:ARG:HB2 | 1.63 | 0.81 |
| 1:AA:1432:G:OP1 | 52:BT:107:ASP:HB2 | 1.79 | 0.81 |
| 22:AV:72:C:H2' | 22:AV:73:A:H5'' | 1.62 | 0.81 |
| 36:BA:2126:A:H4' | 36:BA:2127:G:O5' | 1.81 | 0.81 |
| 38:BC:180:PHE:CB | 38:BC:184:LYS:HB3 | 2.03 | 0.81 |
| 40:BE:11:MET:HB2 | 40:BE:23:VAL:O | 1.81 | 0.81 |
| 48:BP:124:LYS:HD3 | 48:BP:143:GLY:HA3 | 1.60 | 0.81 |
| 49:BQ:134:ARG:NH2 | 58:BZ:122:ARG:HE | 1.78 | 0.81 |
| 53:BU:70:ARG:HA | 53:BU:74:LEU:O | 1.79 | 0.81 |
| 55:BW:13:SER:HB3 | 55:BW:16:LYS:HD2 | 1.62 | 0.81 |
| 57:BY:28:LYS:HB3 | 57:BY:37:VAL:HB | 1.63 | 0.81 |
| 1:AA:979:C:H2' | 1:AA:980:C:H5'' | 1.63 | 0.81 |
| 3:AC:130:VAL:O | 3:AC:134:ILE:HG13 | 1.81 | 0.81 |
| 36:BA:330:A:C2 | 36:BA:1210:A:H2' | 2.10 | 0.81 |
| 36:BA:1409:C:H2' | 36:BA:1410:G:C8 | 2.16 | 0.81 |
| 36:BA:2185:C:H2' | 36:BA:2186:G:H5' | 1.63 | 0.81 |
| 52:BT:33:LYS:HG3 | 52:BT:43:GLN:HB2 | 1.62 | 0.81 |
| 1:AA:573:A:H5' | 1:AA:573:A:H8 | 1.46 | 0.81 |
| 13:AM:91:ARG:HB3 | 13:AM:98:VAL:HG22 | 1.62 | 0.81 |
| 36:BA:1314:C:H5' | 36:BA:1314:C:H6 | 1.44 | 0.81 |
| 39:BD:30:GLU:HG3 | 39:BD:63:ARG:CZ | 2.10 | 0.81 |
| 51:BS:83:LYS:HG2 | 51:BS:105:ALA:HB3 | 1.63 | 0.81 |
| 1:AA:1320:C:H5' | 1:AA:1320:C:H6 | 1.45 | 0.81 |
| 13:AM:90:LEU:HA | 13:AM:93:ARG:HB2 | 1.63 | 0.81 |
| 22:AW:54:U:H2' | 22:AW:55:U:O4' | 1.81 | 0.81 |
| 25:AZ:330:ARG:O | 25:AZ:364:PRO:HG3 | 1.79 | 0.81 |
| 36:BA:1198:U:H2' | 36:BA:1199:U:C6 | 2.16 | 0.81 |
| 36:BA:1948:G:H8 | 36:BA:1948:G:H5' | 1.45 | 0.81 |
| 36:BA:471:A:H2' | 36:BA:472:A:H5'' | 1.63 | 0.81 |
| 41:BF:5:ALA:HB2 | 41:BF:24:LEU:HD11 | 1.62 | 0.81 |
| 1:AA:266:G:H5'' | 1:AA:267:C:C5 | 2.15 | 0.80 |
| 36:BA:1859:A:H61 | 36:BA:1883:G:H1' | 1.46 | 0.80 |
| 36:BA:2836:U:H2' | 36:BA:2837:G:C8 | 2.16 | 0.80 |
| 48:BP:84:ASN:HA | 48:BP:115:LEU:O | 1.80 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:747:U:H5' | 55:BW:90:ARG:NH1 | 1.95 | 0.80 |
| 1:AA:1281:U:H5' | 1:AA:1282:C:C5 | 2.16 | 0.80 |
| 3:AC:7:PRO:O | 3:AC:11:ARG:HG2 | 1.81 | 0.80 |
| 10:AJ:50:ILE:N | 10:AJ:50:ILE:HD13 | 1.94 | 0.80 |
| 25:AZ:301:GLY:CA | 25:AZ:347:THR:HB | 2.10 | 0.80 |
| 28:B2:17:SER:HB2 | 28:B2:18:PRO:CD | 2.11 | 0.80 |
| 32:B6:6:ARG:HH11 | 32:B6:6:ARG:HB3 | 1.45 | 0.80 |
| 36:BA:628:G:C2' | 36:BA:629:G:H5'' | 2.12 | 0.80 |
| 46:BN:2:LYS:HZ1 | 53:BU:95:LEU:HD21 | 1.44 | 0.80 |
| 55:BW:40:ASN:O | 55:BW:41:LYS:HG2 | 1.81 | 0.80 |
| 7:AG:113:GLU:CG | 7:AG:119:ARG:HG2 | 2.12 | 0.80 |
| 38:BC:29:VAL:HG23 | 38:BC:30:LYS:HD2 | 1.63 | 0.80 |
| 46:BN:73:THR:CG2 | 46:BN:82:LEU:HD11 | 2.11 | 0.80 |
| 48:BP:105:LEU:O | 48:BP:106:LEU:HB2 | 1.78 | 0.80 |
| 53:BU:15:LYS:O | 53:BU:19:LYS:HG3 | 1.82 | 0.80 |
| 19:AS:78:ARG:H | 19:AS:81:ARG:NH1 | 1.79 | 0.80 |
| 36:BA:2640:G:C2' | 36:BA:2641:G:H5'' | 2.12 | 0.80 |
| 48:BP:97:PRO:O | 48:BP:98:GLU:HB3 | 1.80 | 0.80 |
| 58:BZ:103:ARG:HD2 | 58:BZ:136:PHE:HB2 | 1.64 | 0.80 |
| 36:BA:266:G:H2' | 36:BA:267:C:H5'' | 1.64 | 0.80 |
| 37:BB:7:G:C3' | 37:BB:8:U:H5'' | 2.11 | 0.80 |
| 25:AZ:104:LEU:HD12 | 25:AZ:105:VAL:H | 1.43 | 0.80 |
| 25:AZ:311:THR:HG22 | 25:AZ:312:PRO:HD2 | 1.63 | 0.80 |
| 38:BC:49:ILE:HG22 | 38:BC:204:ALA:HB1 | 1.62 | 0.80 |
| 42:BG:56:ALA:HA | 42:BG:153:ARG:HH21 | 1.47 | 0.80 |
| 43:BH:16:SER:HB2 | 43:BH:27:LYS:HB2 | 1.64 | 0.80 |
| 1:AA:1266:G:H22 | 1:AA:1268:A:H5'' | 1.45 | 0.80 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:N1 | 1.78 | 0.80 |
| 26:B0:10:THR:HG22 | 26:B0:12:ASN:H | 1.46 | 0.80 |
| 29:B3:22:ALA:O | 29:B3:25:ALA:HB3 | 1.82 | 0.80 |
| 41:BF:160:ASN:ND2 | 41:BF:162:LEU:HD13 | 1.96 | 0.80 |
| 2:AB:77:ALA:HB2 | 2:AB:211:ILE:HD13 | 1.62 | 0.80 |
| 4:AD:107:ARG:HH21 | 4:AD:194:LEU:HD12 | 1.47 | 0.80 |
| 5:AE:6:PHE:HB3 | 5:AE:34:VAL:HG22 | 1.64 | 0.80 |
| 8:AH:10:LEU:HD22 | 8:AH:83:ILE:HD11 | 1.61 | 0.80 |
| 57:BY:87:LYS:C | 57:BY:88:LYS:HD2 | 2.01 | 0.80 |
| 2:AB:215:LEU:O | 2:AB:219:VAL:HG23 | 1.82 | 0.80 |
| 32:B6:15:GLU:OE1 | 32:B6:18:ARG:NE | 2.15 | 0.80 |
| 36:BA:2184:G:H2' | 36:BA:2185:C:C1' | 2.12 | 0.80 |
| 36:BA:2631:G:N2 | 40:BE:61:ARG:HH12 | 1.79 | 0.80 |
| 36:BA:500:G:N2 | 36:BA:502:A:H3' | 1.96 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BA:969:U:H2' | 36:BA:970:C:H6 | 1.45 | 0.80 |
| 19:AS:46:GLY:N | 19:AS:62:ILE:HG23 | 1.97 | 0.80 |
| 25:AZ:124:ARG:HB2 | 25:AZ:163:PHE:HE2 | 1.46 | 0.80 |
| 36:BA:2370:G:H2' | 36:BA:2371:G:C8 | 2.16 | 0.80 |
| 53:BU:88:ILE:O | 53:BU:88:ILE:HG13 | 1.79 | 0.80 |
| 36:BA:81:G:H21 | 57:BY:2:ARG:HH12 | 1.26 | 0.80 |
| 1:AA:961:U:HO2' | 1:AA:962:C:H6 | 1.30 | 0.79 |
| 10:AJ:30:SER:O | 10:AJ:80:LYS:HD3 | 1.81 | 0.79 |
| 28:B2:65:ASN:ND2 | 28:B2:69:ARG:HH21 | 1.78 | 0.79 |
| 42:BG:52:ILE:HD13 | 42:BG:52:ILE:H | 1.47 | 0.79 |
| 48:BP:47:ASP:HB3 | 48:BP:48:PRO:HA | 1.64 | 0.79 |
| 52:BT:66:VAL:HG12 | 52:BT:71:GLY:HA2 | 1.64 | 0.79 |
| 53:BU:92:ARG:HD2 | 54:BV:11:GLN:CG | 2.12 | 0.79 |
| 1:AA:751:U:H4' | 15:AO:24:SER:HB2 | 1.64 | 0.79 |
| 31:B5:40:LYS:HZ3 | 31:B5:46:CYS:H | 1.25 | 0.79 |
| 36:BA:1614:A:H2' | 36:BA:1615:C:H5' | 1.65 | 0.79 |
| 36:BA:2893:G:C5' | 36:BA:2894:G:H5' | 2.12 | 0.79 |
| 36:BA:2129:C:OP2 | 38:BC:6:ARG:HB3 | 1.82 | 0.79 |
| 41:BF:3:GLU:O | 41:BF:24:LEU:HG | 1.81 | 0.79 |
| 50:BR:84:ALA:HB3 | 50:BR:85:PRO:HD3 | 1.64 | 0.79 |
| 3:AC:19:GLU:HG2 | 3:AC:54:ARG:HE | 1.46 | 0.79 |
| 5:AE:12:LEU:HD22 | 5:AE:13:ILE:N | 1.98 | 0.79 |
| 22:AV:68:C:H2' | 22:AV:69:G:C5' | 2.12 | 0.79 |
| 38:BC:30:LYS:HZ1 | 38:BC:178:ALA:HB1 | 1.44 | 0.79 |
| 2:AB:96:ARG:HD3 | 2:AB:148:TYR:HE1 | 1.47 | 0.79 |
| 10:AJ:54:PHE:CE2 | 10:AJ:55:LYS:HD2 | 2.18 | 0.79 |
| 12:AL:27:LEU:HB2 | 12:AL:62:SER:HB2 | 1.64 | 0.79 |
| 25:AZ:281:ILE:O | 25:AZ:284:ASP:HB2 | 1.83 | 0.79 |
| 34:B8:30:ARG:HA | 34:B8:30:ARG:HE | 1.48 | 0.79 |
| 39:BD:35:LYS:NZ | 39:BD:35:LYS:HB3 | 1.96 | 0.79 |
| 36:BA:2428:G:O2' | 48:BP:56:SER:HB2 | 1.81 | 0.79 |
| 52:BT:13:ARG:HH12 | 52:BT:15:VAL:HG12 | 1.46 | 0.79 |
| 55:BW:29:LEU:O | 55:BW:33:ARG:HG3 | 1.81 | 0.79 |
| 14:AN:13:THR:H | 14:AN:14:PRO:HD2 | 1.44 | 0.79 |
| 19:AS:29:ARG:CB | 19:AS:48:THR:HB | 2.11 | 0.79 |
| 36:BA:1494:A:C2' | 36:BA:1495:A:H5'' | 2.13 | 0.79 |
| 36:BA:1494:A:H2' | 36:BA:1495:A:H5'' | 1.65 | 0.79 |
| 42:BG:57:ALA:HB2 | 42:BG:90:LEU:HD21 | 1.63 | 0.79 |
| 47:BO:4:PRO:O | 47:BO:5:GLN:HB2 | 1.82 | 0.79 |
| 6:AF:43:LEU:H | 6:AF:43:LEU:HD22 | 1.46 | 0.79 |
| 29:B3:28:LEU:HD23 | 29:B3:28:LEU:N | 1.96 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 34:B8:50:LEU:H | 34:B8:53:PRO:HD3 | 1.48 | 0.79 |
| 41:BF:4:VAL:HA | 41:BF:19:GLU:HG3 | 1.62 | 0.79 |
| 50:BR:45:ARG:HG3 | 50:BR:46:GLY:N | 1.98 | 0.79 |
| 36:BA:2693:A:H2' | 36:BA:2694:G:C8 | 2.17 | 0.79 |
| 36:BA:860:U:H5 | 36:BA:917:A:N7 | 1.80 | 0.79 |
| 39:BD:210:GLY:O | 39:BD:211:ARG:HB3 | 1.82 | 0.79 |
| 10:AJ:49:VAL:O | 10:AJ:60:ARG:HB3 | 1.81 | 0.79 |
| 15:AO:10:LYS:HA | 15:AO:10:LYS:HE3 | 1.63 | 0.79 |
| 36:BA:622:G:O2' | 36:BA:623:G:H5' | 1.82 | 0.79 |
| 58:BZ:126:VAL:HG12 | 58:BZ:163:LEU:CB | 2.13 | 0.79 |
| 1:AA:1139:G:H5' | 1:AA:1140:C:OP1 | 1.82 | 0.79 |
| 2:AB:77:ALA:O | 2:AB:81:VAL:HG23 | 1.82 | 0.79 |
| 17:AQ:52:LYS:HD2 | 17:AQ:52:LYS:H | 1.46 | 0.79 |
| 29:B3:22:ALA:HB1 | 29:B3:46:ASN:ND2 | 1.96 | 0.79 |
| 36:BA:1010:A:H1' | 36:BA:1153:C:H1' | 1.65 | 0.79 |
| 40:BE:77:ILE:HG22 | 40:BE:78:LEU:N | 1.96 | 0.79 |
| 41:BF:206:ILE:HG22 | 41:BF:207:GLY:H | 1.45 | 0.79 |
| 51:BS:101:LEU:O | 51:BS:101:LEU:HD12 | 1.82 | 0.79 |
| 52:BT:56:GLY:O | 52:BT:59:THR:HG23 | 1.83 | 0.79 |
| 22:AV:62:C:H5' | 22:AV:62:C:H6 | 1.46 | 0.79 |
| 22:AW:38:A:H2' | 22:AW:39:U:H5'' | 1.64 | 0.79 |
| 36:BA:1348:G:H2' | 36:BA:1349:A:H5'' | 1.62 | 0.79 |
| 36:BA:1639:U:C2' | 36:BA:1640:C:H5'' | 2.13 | 0.79 |
| 36:BA:782:A:C2 | 39:BD:226:MET:HG2 | 2.17 | 0.79 |
| 42:BG:51:ARG:HD3 | 42:BG:53:LEU:HD21 | 1.65 | 0.79 |
| 1:AA:429:U:H2' | 4:AD:25:ARG:HH12 | 1.47 | 0.78 |
| 36:BA:484:C:OP1 | 57:BY:49:VAL:HG13 | 1.83 | 0.78 |
| 51:BS:35:ILE:H | 51:BS:53:SER:HB2 | 1.48 | 0.78 |
| 1:AA:980:C:H5' | 1:AA:980:C:C6 | 2.12 | 0.78 |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:HE2 | 1.46 | 0.78 |
| 27:B1:37:ILE:HD12 | 27:B1:37:ILE:O | 1.82 | 0.78 |
| 38:BC:94:VAL:HG12 | 38:BC:95:GLY:N | 1.97 | 0.78 |
| 55:BW:70:TYR:CE2 | 55:BW:72:LYS:HG2 | 2.18 | 0.78 |
| 57:BY:96:ILE:CG1 | 57:BY:99:CYS:HB3 | 2.14 | 0.78 |
| 3:AC:131:ARG:HD3 | 3:AC:166:GLU:OE1 | 1.84 | 0.78 |
| 12:AL:32:PHE:HB3 | 12:AL:84:LEU:HD22 | 1.66 | 0.78 |
| 22:AV:61:C:H2' | 22:AV:62:C:H5'' | 1.65 | 0.78 |
| 24:AY:75:C:C6 | 25:AZ:231:ILE:HA | 2.17 | 0.78 |
| 27:B1:80:LEU:HD23 | 27:B1:81:LYS:H | 1.48 | 0.78 |
| 36:BA:271(M):G:H2' | 36:BA:271(N):U:H5'' | 1.63 | 0.78 |
| 40:BE:9:VAL:HG12 | 40:BE:25:VAL:O | 1.83 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 47:BO:71:ARG:HH11 | 47:BO:71:ARG:HG3 | 1.48 | 0.78 |
| 48:BP:83:VAL:HG23 | 48:BP:105:LEU:HD22 | 1.64 | 0.78 |
| 49:BQ:133:ARG:HH11 | 49:BQ:133:ARG:HB2 | 1.48 | 0.78 |
| 58:BZ:33:LEU:CD1 | 58:BZ:34:ASN:H | 1.96 | 0.78 |
| 1:AA:950:U:H2' | 1:AA:951:G:H8 | 1.48 | 0.78 |
| 3:AC:180:ALA:O | 3:AC:181:ASN:HB3 | 1.80 | 0.78 |
| 8:AH:89:PRO:HA | 8:AH:92:ARG:NH1 | 1.98 | 0.78 |
| 25:AZ:21:ASP:H | 61:AZ:501:GCP:C3B | 1.97 | 0.78 |
| 36:BA:733:G:N7 | 36:BA:761:A:C6 | 2.51 | 0.78 |
| 32:B6:45:LYS:HD3 | 32:B6:45:LYS:N | 1.97 | 0.78 |
| 36:BA:2760:C:H2' | 36:BA:2761:G:H5'' | 1.65 | 0.78 |
| 36:BA:2789:C:H1' | 36:BA:2892:A:N1 | 1.98 | 0.78 |
| 31:B5:3:LYS:HD3 | 36:BA:747:U:OP2 | 1.83 | 0.78 |
| 43:BH:153:LYS:CD | 43:BH:153:LYS:H | 1.94 | 0.78 |
| 58:BZ:130:PRO:HA | 58:BZ:133:ILE:HD11 | 1.65 | 0.78 |
| 4:AD:7:PRO:HB2 | 4:AD:10:ARG:HD2 | 1.65 | 0.78 |
| 12:AL:24:VAL:O | 12:AL:24:VAL:HG12 | 1.84 | 0.78 |
| 15:AO:29:VAL:HG11 | 15:AO:67:LEU:HD21 | 1.65 | 0.78 |
| 30:B4:10:VAL:HG23 | 30:B4:11:PRO:HD2 | 1.66 | 0.78 |
| 36:BA:654(N):G:H2' | 36:BA:654(O):G:O4' | 1.83 | 0.78 |
| 40:BE:24:THR:HG21 | 40:BE:188:VAL:HG11 | 1.65 | 0.78 |
| 41:BF:51:THR:HG23 | 41:BF:92:PRO:HD2 | 1.65 | 0.78 |
| 50:BR:27:SER:O | 50:BR:34:ILE:HD11 | 1.83 | 0.78 |
| 1:AA:1127:G:H1 | 1:AA:1145:C:N4 | 1.82 | 0.78 |
| 2:AB:200:ILE:CD1 | 2:AB:200:ILE:H | 1.95 | 0.78 |
| 34:B8:61:LEU:HD13 | 34:B8:62:LEU:H | 1.47 | 0.78 |
| 36:BA:1528(A):A:H62 | 36:BA:1541:G:N2 | 1.82 | 0.78 |
| 38:BC:191:ALA:HA | 38:BC:194:ARG:HD2 | 1.64 | 0.78 |
| 38:BC:66:HIS:CD2 | 38:BC:184:LYS:HD3 | 2.19 | 0.78 |
| 46:BN:28:THR:HG23 | 46:BN:29:LYS:HG3 | 1.65 | 0.78 |
| 1:AA:1503:A:N7 | 23:AX:15:A:C6 | 2.52 | 0.78 |
| 2:AB:33:TYR:HB3 | 2:AB:41:ILE:HG22 | 1.66 | 0.78 |
| 28:B2:64:LEU:HD23 | 28:B2:64:LEU:O | 1.83 | 0.78 |
| 36:BA:612:C:H2' | 36:BA:613:G:C5' | 2.13 | 0.78 |
| 48:BP:16:ARG:NE | 48:BP:18:ARG:HB2 | 1.99 | 0.78 |
| 9:AI:4:TYR:HB2 | 9:AI:19:LEU:HB2 | 1.66 | 0.78 |
| 25:AZ:66:ALA:HB3 | 25:AZ:81:ASP:HB3 | 1.66 | 0.78 |
| 26:B0:27:GLU:HG3 | 26:B0:69:PHE:HD1 | 1.46 | 0.78 |
| 36:BA:392:C:H2' | 36:BA:393:C:H6 | 1.48 | 0.78 |
| 36:BA:672:C:H2' | 36:BA:673:C:C5' | 2.14 | 0.78 |
| 2:AB:36:ARG:NE | 2:AB:36:ARG:HA | 1.99 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:AJ:65:LEU:HD13 | 14:AN:56:VAL:H | 1.48 | 0.78 |
| 25:AZ:148:ASP:HA | 25:AZ:172:ARG:HH22 | 1.49 | 0.78 |
| 30:B4:5:ILE:O | 30:B4:5:ILE:HG12 | 1.84 | 0.78 |
| 38:BC:59:ARG:CZ | 38:BC:142:ALA:HB2 | 2.13 | 0.78 |
| 46:BN:133:GLN:HG2 | 46:BN:135:PRO:HD3 | 1.66 | 0.78 |
| 52:BT:89:VAL:HG12 | 52:BT:91:ARG:HG3 | 1.63 | 0.78 |
| 1:AA:265:G:H2' | 1:AA:266:G:H5'' | 1.65 | 0.77 |
| 22:AV:21:A:H2' | 22:AV:22:G:H5'' | 1.62 | 0.77 |
| 26:B0:7:LEU:HB3 | 49:BQ:85:LYS:HG3 | 1.66 | 0.77 |
| 32:B6:15:GLU:HB2 | 32:B6:20:ASN:HB3 | 1.66 | 0.77 |
| 55:BW:107:LEU:H | 55:BW:107:LEU:HD12 | 1.47 | 0.77 |
| 58:BZ:40:ASP:HB3 | 58:BZ:43:GLU:HG2 | 1.66 | 0.77 |
| 2:AB:61:LEU:HD12 | 2:AB:64:ARG:HD2 | 1.66 | 0.77 |
| 20:AT:14:LYS:O | 20:AT:18:GLN:HB2 | 1.83 | 0.77 |
| 29:B3:35:ARG:CB | 29:B3:35:ARG:HH11 | 1.98 | 0.77 |
| 31:B5:16:ARG:HD2 | 31:B5:20:ARG:NH2 | 1.98 | 0.77 |
| 37:BB:13:A:O2' | 37:BB:14:U:H3' | 1.83 | 0.77 |
| 52:BT:10:VAL:O | 52:BT:13:ARG:HG2 | 1.83 | 0.77 |
| 10:AJ:89:ASP:HB3 | 10:AJ:91:PRO:HD3 | 1.64 | 0.77 |
| 25:AZ:34:VAL:HG21 | 25:AZ:199:ILE:HG21 | 1.65 | 0.77 |
| 36:BA:1434:A:H61 | 36:BA:1558:A:N6 | 1.81 | 0.77 |
| 37:BB:60:C:H2' | 37:BB:61:G:H8 | 1.49 | 0.77 |
| 48:BP:34:GLY:O | 48:BP:35:HIS:HB2 | 1.85 | 0.77 |
| 13:AM:22:ILE:HG21 | 13:AM:66:LEU:HD23 | 1.64 | 0.77 |
| 17:AQ:66:SER:OG | 17:AQ:69:LYS:HB2 | 1.84 | 0.77 |
| 25:AZ:230:THR:OG1 | 25:AZ:295:ARG:HD2 | 1.84 | 0.77 |
| 32:B6:15:GLU:OE2 | 32:B6:41:PRO:HB3 | 1.83 | 0.77 |
| 36:BA:614(A):U:H4' | 36:BA:614(B):G:H5'' | 1.67 | 0.77 |
| 42:BG:44:GLY:O | 42:BG:47:LYS:HE2 | 1.84 | 0.77 |
| 51:BS:85:VAL:C | 51:BS:106:ARG:HG2 | 2.04 | 0.77 |
| 4:AD:19:LEU:HD23 | 4:AD:21:LEU:HD21 | 1.67 | 0.77 |
| 11:AK:57:THR:CG2 | 11:AK:60:ALA:H | 1.98 | 0.77 |
| 19:AS:11:VAL:HA | 19:AS:38:SER:CB | 2.14 | 0.77 |
| 20:AT:63:ILE:HG22 | 20:AT:64:ASP:N | 1.99 | 0.77 |
| 34:B8:32:LEU:HD12 | 34:B8:36:LYS:NZ | 1.99 | 0.77 |
| 38:BC:41:VAL:HG12 | 38:BC:43:VAL:HG23 | 1.64 | 0.77 |
| 43:BH:20:ALA:HB1 | 43:BH:21:PRO:CD | 2.15 | 0.77 |
| 36:BA:1227:G:OP1 | 53:BU:13:LYS:HD2 | 1.83 | 0.77 |
| 1:AA:967:C:H4' | 9:AI:125:TYR:HE2 | 1.49 | 0.77 |
| 12:AL:91:LYS:O | 12:AL:92:ASP:HB2 | 1.83 | 0.77 |
| 25:AZ:303:VAL:HG12 | 25:AZ:304:LEU:N | 2.00 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:1678:G:N2 | 36:BA:1989:G:H22 | 1.81 | 0.77 |
| 56:BX:18:TYR:HA | 56:BX:21:PHE:CE1 | 2.19 | 0.77 |
| 58:BZ:19:ARG:HH12 | 58:BZ:84:GLU:HA | 1.48 | 0.77 |
| 9:AI:53:VAL:HG13 | 9:AI:95:LYS:CE | 2.15 | 0.77 |
| 40:BE:47:VAL:O | 40:BE:49:LEU:HD22 | 1.84 | 0.77 |
| 53:BU:92:ARG:HD3 | 53:BU:94:ASN:HB3 | 1.65 | 0.77 |
| 54:BV:36:PRO:HA | 54:BV:56:SER:CB | 2.15 | 0.77 |
| 8:AH:7:ALA:HB2 | 8:AH:85:ARG:HD3 | 1.67 | 0.77 |
| 24:AY:72:U:H2' | 24:AY:73:G:H5'' | 1.65 | 0.77 |
| 31:B5:3:LYS:HA | 31:B5:3:LYS:HE3 | 1.67 | 0.77 |
| 51:BS:67:ARG:NH2 | 51:BS:100:ALA:HB3 | 1.99 | 0.77 |
| 51:BS:24:LEU:HB3 | 51:BS:85:VAL:HG12 | 1.67 | 0.77 |
| 25:AZ:202:LEU:O | 25:AZ:206:ILE:HG13 | 1.84 | 0.77 |
| 25:AZ:277:LEU:HD12 | 25:AZ:279:GLU:H | 1.47 | 0.77 |
| 36:BA:654(J):A:H8 | 36:BA:654(L):G:H1' | 1.48 | 0.77 |
| 38:BC:186:ALA:HB1 | 38:BC:190:ARG:NH2 | 1.99 | 0.77 |
| 40:BE:47:VAL:HG21 | 40:BE:86:PRO:CD | 2.14 | 0.77 |
| 10:AJ:40:LEU:HD23 | 10:AJ:40:LEU:H | 1.48 | 0.77 |
| 1:AA:265:G:H5' | 17:AQ:64:PRO:O | 1.85 | 0.77 |
| 36:BA:1484:G:H2' | 36:BA:1485:G:C5' | 2.13 | 0.77 |
| 36:BA:1722:A:O2' | 36:BA:1739:U:H5'' | 1.84 | 0.77 |
| 36:BA:672:C:H2' | 36:BA:673:C:H5'' | 1.67 | 0.77 |
| 42:BG:115:ARG:NH2 | 42:BG:136:ARG:HB2 | 1.95 | 0.77 |
| 36:BA:2593:U:H2' | 36:BA:2594:C:C6 | 2.20 | 0.76 |
| 36:BA:271(E):U:H2' | 36:BA:271(F):C:C6 | 2.20 | 0.76 |
| 36:BA:615:G:OP2 | 41:BF:40:GLN:HG3 | 1.86 | 0.76 |
| 40:BE:51:PHE:O | 40:BE:74:PRO:HB3 | 1.84 | 0.76 |
| 35:B9:7:VAL:HG13 | 35:B9:34:GLN:HG2 | 1.67 | 0.76 |
| 36:BA:296:C:O2' | 36:BA:297:C:H5' | 1.84 | 0.76 |
| 40:BE:199:ARG:HG2 | 40:BE:200:GLU:H | 1.51 | 0.76 |
| 52:BT:64:ARG:HD2 | 52:BT:73:GLU:OE1 | 1.86 | 0.76 |
| 30:B4:14:ILE:HG13 | 30:B4:31:ILE:HG21 | 1.67 | 0.76 |
| 36:BA:1095:A:H2' | 36:BA:1096:A:C8 | 2.19 | 0.76 |
| 42:BG:96:ARG:O | 42:BG:97:ASP:HB2 | 1.85 | 0.76 |
| 47:BO:87:ILE:CG2 | 47:BO:91:LEU:HA | 2.15 | 0.76 |
| 54:BV:69:LYS:HB2 | 54:BV:88:ARG:HD3 | 1.66 | 0.76 |
| 1:AA:176:C:H2' | 1:AA:177:C:C6 | 2.21 | 0.76 |
| 21:AU:6:ARG:HD3 | 21:AU:15:ARG:NH1 | 2.00 | 0.76 |
| 27:B1:80:LEU:HD23 | 27:B1:81:LYS:N | 2.01 | 0.76 |
| 35:B9:35:ARG:O | 35:B9:35:ARG:HG2 | 1.86 | 0.76 |
| 36:BA:1899:G:O2' | 36:BA:1900:A:H5'' | 1.84 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BC:131:LEU:HD22 | 38:BC:136:LEU:HD12 | 1.66 | 0.76 |
| 5:AE:80:ILE:HD11 | 5:AE:138:ALA:HA | 1.68 | 0.76 |
| 13:AM:90:LEU:O | 13:AM:91:ARG:HB2 | 1.84 | 0.76 |
| 28:B2:43:GLN:HG2 | 28:B2:44:LEU:H | 1.50 | 0.76 |
| 36:BA:1847:A:H4' | 36:BA:1848:A:OP2 | 1.84 | 0.76 |
| 38:BC:70:LYS:CD | 38:BC:177:LYS:HZ3 | 1.98 | 0.76 |
| 47:BO:88:ASN:ND2 | 47:BO:92:GLU:HB3 | 1.99 | 0.76 |
| 31:B5:3:LYS:HD3 | 36:BA:747:U:P | 2.26 | 0.76 |
| 36:BA:2151:G:H2' | 36:BA:2152:G:C8 | 2.19 | 0.76 |
| 36:BA:581:C:H2' | 36:BA:582:G:H8 | 1.51 | 0.76 |
| 10:AJ:33:GLN:O | 10:AJ:75:ILE:HG12 | 1.84 | 0.76 |
| 19:AS:6:LYS:HG2 | 19:AS:7:LYS:HE3 | 1.67 | 0.76 |
| 36:BA:1231:G:H2' | 36:BA:1232:G:H8 | 1.50 | 0.76 |
| 36:BA:1290:C:H2' | 36:BA:1291:C:H6 | 1.50 | 0.76 |
| 36:BA:143(A):C:H4' | 56:BX:38:GLU:OE1 | 1.85 | 0.76 |
| 36:BA:2022:U:O2' | 36:BA:2617:C:H5' | 1.85 | 0.76 |
| 50:BR:92:GLY:H | 50:BR:94:TYR:HE2 | 1.34 | 0.76 |
| 34:B8:21:LYS:HZ3 | 34:B8:48:PHE:HZ | 1.34 | 0.76 |
| 38:BC:164:ARG:O | 38:BC:171:ILE:HD12 | 1.85 | 0.76 |
| 36:BA:1353:A:H4' | 39:BD:38:LYS:HE3 | 1.68 | 0.76 |
| 1:AA:1452:C:H5'' | 1:AA:1456:G:OP1 | 1.85 | 0.76 |
| 10:AJ:23:ILE:HG23 | 10:AJ:85:LEU:HD22 | 1.67 | 0.76 |
| 25:AZ:224:PRO:HG3 | 25:AZ:345:ARG:HD3 | 1.64 | 0.76 |
| 36:BA:1019:U:HO2' | 36:BA:1021:A:H2 | 1.34 | 0.76 |
| 36:BA:1798:U:H5' | 39:BD:259:THR:HG22 | 1.66 | 0.76 |
| 51:BS:15:ARG:HH12 | 51:BS:18:ILE:HD11 | 1.51 | 0.76 |
| 52:BT:80:SER:CB | 52:BT:81:PRO:HD3 | 2.16 | 0.76 |
| 57:BY:79:CYS:SG | 57:BY:80:GLY:N | 2.58 | 0.76 |
| 11:AK:57:THR:HG22 | 11:AK:60:ALA:H | 1.50 | 0.76 |
| 1:AA:1305:G:C5' | 21:AU:4:GLY:HA3 | 2.16 | 0.76 |
| 24:AY:75:C:H1' | 25:AZ:231:ILE:CD1 | 2.16 | 0.76 |
| 31:B5:4:HIS:CB | 31:B5:5:PRO:HD3 | 2.15 | 0.76 |
| 36:BA:1947:C:H2' | 36:BA:1948:G:C5' | 2.16 | 0.76 |
| 36:BA:2836:U:H2' | 36:BA:2837:G:H8 | 1.49 | 0.76 |
| 38:BC:107:TRP:CZ3 | 38:BC:131:LEU:HD21 | 2.20 | 0.76 |
| 50:BR:7:GLY:O | 50:BR:8:ARG:NE | 2.18 | 0.76 |
| 1:AA:490:G:H2' | 1:AA:491:G:H8 | 1.51 | 0.75 |
| 9:AI:49:PRO:HB3 | 9:AI:101:PHE:HD2 | 1.50 | 0.75 |
| 10:AJ:62:HIS:HB2 | 14:AN:59:ALA:HB3 | 1.67 | 0.75 |
| 31:B5:50:GLY:HA3 | 31:B5:56:LYS:HD3 | 1.67 | 0.75 |
| 38:BC:75:LEU:HG | 38:BC:112:ALA:O | 1.85 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:BT:32:TYR:HD2 | 52:BT:32:TYR:N | 1.84 | 0.75 |
| 1:AA:1023:G:H2' | 1:AA:1024:G:H5' | 1.67 | 0.75 |
| 1:AA:1052:U:O4 | 1:AA:1200:C:H2' | 1.86 | 0.75 |
| 2:AB:155:LEU:HD21 | 2:AB:159:PRO:HG3 | 1.66 | 0.75 |
| 4:AD:61:LYS:CE | 4:AD:62:GLN:HE21 | 2.00 | 0.75 |
| 36:BA:548:A:H2' | 36:BA:549:G:H5' | 1.68 | 0.75 |
| 42:BG:66:GLN:OE1 | 42:BG:94:LEU:HD23 | 1.85 | 0.75 |
| 49:BQ:60:ARG:HB3 | 49:BQ:60:ARG:HH11 | 1.50 | 0.75 |
| 55:BW:65:LEU:HD23 | 55:BW:68:ARG:NE | 2.02 | 0.75 |
| 36:BA:2317:C:H2' | 36:BA:2318:G:H5' | 1.66 | 0.75 |
| 43:BH:153:LYS:HD3 | 43:BH:153:LYS:N | 1.96 | 0.75 |
| 51:BS:66:ALA:HB1 | 51:BS:99:LYS:HD3 | 1.68 | 0.75 |
| 25:AZ:35:THR:CG2 | 25:AZ:203:LEU:HD11 | 2.17 | 0.75 |
| 35:B9:10:ILE:O | 35:B9:11:CYS:HB3 | 1.86 | 0.75 |
| 36:BA:2315:G:H2' | 36:BA:2316:C:H6 | 1.51 | 0.75 |
| 39:BD:60:ARG:HG3 | 39:BD:86:PRO:HB2 | 1.67 | 0.75 |
| 43:BH:18:GLU:CG | 43:BH:25:LYS:HB2 | 2.15 | 0.75 |
| 1:AA:979:C:C2' | 1:AA:980:C:H5'' | 2.15 | 0.75 |
| 2:AB:84:GLU:HB3 | 2:AB:219:VAL:CG2 | 2.12 | 0.75 |
| 15:AO:17:ARG:HD3 | 15:AO:26:GLU:HG3 | 1.67 | 0.75 |
| 36:BA:1590:U:H2' | 36:BA:1591:G:H5'' | 1.68 | 0.75 |
| 38:BC:175:VAL:HG21 | 38:BC:189:ILE:HG12 | 1.69 | 0.75 |
| 46:BN:28:THR:HG23 | 46:BN:29:LYS:N | 2.01 | 0.75 |
| 1:AA:280:C:O2 | 17:AQ:38:ARG:HG3 | 1.87 | 0.75 |
| 36:BA:2113:U:H2' | 36:BA:2114:A:H8 | 1.50 | 0.75 |
| 38:BC:100:ILE:O | 38:BC:104:LEU:HD23 | 1.87 | 0.75 |
| 36:BA:2170:A:H5' | 38:BC:133:PRO:HG2 | 1.69 | 0.75 |
| 43:BH:41:MET:HG3 | 43:BH:42:ARG:O | 1.85 | 0.75 |
| 48:BP:50:ARG:HG3 | 48:BP:51:PHE:N | 2.01 | 0.75 |
| 57:BY:42:VAL:HG21 | 57:BY:67:LEU:HD12 | 1.68 | 0.75 |
| 58:BZ:100:VAL:HG23 | 58:BZ:126:VAL:HG21 | 1.67 | 0.75 |
| 58:BZ:20:ARG:HH11 | 58:BZ:20:ARG:CB | 1.97 | 0.75 |
| 1:AA:963:G:H21 | 10:AJ:55:LYS:CD | 2.00 | 0.75 |
| 11:AK:84:VAL:HG11 | 11:AK:95:ILE:HD11 | 1.67 | 0.75 |
| 36:BA:2028:U:H2' | 36:BA:2029:G:C8 | 2.22 | 0.75 |
| 36:BA:2375:G:H1' | 36:BA:2379:G:N2 | 2.02 | 0.75 |
| 37:BB:87:G:H3' | 37:BB:88:C:H5'' | 1.68 | 0.75 |
| 51:BS:85:VAL:O | 51:BS:106:ARG:HG2 | 1.86 | 0.75 |
| 51:BS:13:ARG:HG3 | 51:BS:14:VAL:N | 2.01 | 0.75 |
| 56:BX:89:ILE:HG22 | 56:BX:92:LEU:H | 1.52 | 0.75 |
| 49:BQ:62:GLY:HA2 | 58:BZ:116:VAL:HG21 | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:33:LEU:HD12 | 58:BZ:34:ASN:N | 2.00 | 0.75 |
| 8:AH:83:ILE:HD12 | 8:AH:137:VAL:HG22 | 1.66 | 0.75 |
| 22:AV:61:C:C2' | 22:AV:62:C:H5'' | 2.17 | 0.75 |
| 25:AZ:213:PRO:HG2 | 25:AZ:215:ARG:HH21 | 1.52 | 0.75 |
| 28:B2:19:VAL:HG12 | 28:B2:23:LYS:HE3 | 1.68 | 0.75 |
| 36:BA:1503:U:H2' | 36:BA:1504:C:C6 | 2.22 | 0.75 |
| 37:BB:40:U:H3' | 37:BB:41:U:C5' | 2.17 | 0.75 |
| 49:BQ:133:ARG:CB | 49:BQ:133:ARG:HH11 | 1.99 | 0.75 |
| 52:BT:80:SER:HB3 | 52:BT:81:PRO:CD | 2.16 | 0.75 |
| 11:AK:62:GLN:HG2 | 11:AK:63:LEU:HD23 | 1.66 | 0.75 |
| 22:AV:72:C:C2' | 22:AV:73:A:H5'' | 2.17 | 0.75 |
| 25:AZ:256:VAL:HG12 | 25:AZ:379:ALA:HB2 | 1.69 | 0.75 |
| 25:AZ:330:ARG:HG3 | 25:AZ:395:VAL:HB | 1.69 | 0.75 |
| 33:B7:8:ASN:C | 33:B7:8:ASN:ND2 | 2.35 | 0.75 |
| 36:BA:2184:G:H2' | 36:BA:2185:C:H1' | 1.67 | 0.75 |
| 52:BT:82:LEU:HD12 | 52:BT:82:LEU:H | 1.52 | 0.75 |
| 54:BV:18:LEU:HD23 | 54:BV:19:LYS:N | 2.01 | 0.75 |
| 55:BW:68:ARG:O | 55:BW:109:GLU:HA | 1.85 | 0.75 |
| 35:B9:35:ARG:HD3 | 36:BA:2742:C:OP1 | 1.87 | 0.74 |
| 36:BA:2813:A:H61 | 36:BA:2887:U:H3 | 1.30 | 0.74 |
| 36:BA:833:U:H5'' | 48:BP:48:PRO:CB | 2.17 | 0.74 |
| 39:BD:176:ARG:NH1 | 39:BD:176:ARG:HG2 | 2.01 | 0.74 |
| 39:BD:26:LYS:HE2 | 39:BD:26:LYS:N | 2.02 | 0.74 |
| 40:BE:87:GLU:O | 40:BE:89:ASP:N | 2.20 | 0.74 |
| 41:BF:155:LEU:HD11 | 41:BF:176:LEU:HD13 | 1.68 | 0.74 |
| 36:BA:598:G:H5' | 48:BP:15:ARG:HB2 | 1.68 | 0.74 |
| 52:BT:50:ILE:HD11 | 52:BT:64:ARG:HB3 | 1.65 | 0.74 |
| 55:BW:29:LEU:CG | 55:BW:33:ARG:HD2 | 2.17 | 0.74 |
| 2:AB:98:LEU:O | 2:AB:101:MET:HG3 | 1.87 | 0.74 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CG | 2.22 | 0.74 |
| 13:AM:3:ARG:HB2 | 30:B4:34:GLU:HG2 | 1.68 | 0.74 |
| 36:BA:2108:C:H2' | 36:BA:2108:C:O2 | 1.86 | 0.74 |
| 36:BA:2712:U:H1' | 36:BA:2712(A):A:C8 | 2.22 | 0.74 |
| 36:BA:984:A:H5'' | 36:BA:985:C:H5 | 1.53 | 0.74 |
| 41:BF:101:LEU:HD12 | 41:BF:102:PRO:CD | 2.17 | 0.74 |
| 48:BP:106:LEU:HD11 | 48:BP:112:LEU:HD23 | 1.70 | 0.74 |
| 52:BT:106:SER:HA | 52:BT:110:ILE:HG12 | 1.69 | 0.74 |
| 1:AA:1321:C:H5'' | 1:AA:1322:C:C5' | 2.15 | 0.74 |
| 5:AE:100:VAL:HG12 | 5:AE:118:ILE:HG22 | 1.68 | 0.74 |
| 22:AV:20:U:H3' | 22:AV:21:A:H5' | 1.68 | 0.74 |
| 28:B2:53:LEU:O | 28:B2:57:ILE:HG12 | 1.88 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:1608:A:H1' | 36:BA:1610:A:OP2 | 1.85 | 0.74 |
| 36:BA:2101:G:H2' | 36:BA:2102:U:C5' | 2.15 | 0.74 |
| 36:BA:2206:G:N2 | 36:BA:2207:G:H5' | 2.02 | 0.74 |
| 36:BA:2577:A:H5'' | 36:BA:2578:G:H5' | 1.68 | 0.74 |
| 37:BB:106:G:H2' | 37:BB:107:G:H8 | 1.51 | 0.74 |
| 38:BC:128:GLY:HA2 | 38:BC:137:LEU:HD23 | 1.70 | 0.74 |
| 41:BF:154:VAL:HG22 | 41:BF:191:ARG:HB3 | 1.68 | 0.74 |
| 41:BF:192:LEU:HD21 | 41:BF:194:MET:HG3 | 1.68 | 0.74 |
| 58:BZ:144:LEU:HD11 | 58:BZ:150:LEU:HD22 | 1.68 | 0.74 |
| 4:AD:47:ARG:HD3 | 4:AD:49:ARG:HH21 | 1.52 | 0.74 |
| 36:BA:774:A:H2 | 36:BA:787:U:O2' | 1.70 | 0.74 |
| 50:BR:2:ARG:C | 50:BR:2:ARG:HD2 | 2.06 | 0.74 |
| 50:BR:34:ILE:HB | 50:BR:114:VAL:HG23 | 1.69 | 0.74 |
| 56:BX:10:ALA:HB1 | 56:BX:11:PRO:HD2 | 1.68 | 0.74 |
| 57:BY:50:ARG:HG3 | 57:BY:56:PRO:O | 1.86 | 0.74 |
| 1:AA:961:U:O2' | 1:AA:962:C:H6 | 1.70 | 0.74 |
| 3:AC:80:GLY:O | 3:AC:82:GLU:HG3 | 1.87 | 0.74 |
| 4:AD:12:CYS:O | 4:AD:33:MET:HE1 | 1.88 | 0.74 |
| 19:AS:5:LEU:C | 19:AS:6:LYS:HD2 | 2.08 | 0.74 |
| 36:BA:2159:G:H2' | 36:BA:2160:G:C5' | 2.17 | 0.74 |
| 41:BF:159:GLY:HA2 | 41:BF:164:ARG:HH21 | 1.52 | 0.74 |
| 46:BN:89:LYS:O | 46:BN:93:THR:HG22 | 1.87 | 0.74 |
| 48:BP:111:ARG:HH21 | 48:BP:111:ARG:HG2 | 1.52 | 0.74 |
| 58:BZ:10:ARG:HH21 | 58:BZ:36:LYS:CB | 2.01 | 0.74 |
| 9:AI:40:LEU:HD11 | 9:AI:70:LYS:HG2 | 1.68 | 0.74 |
| 36:BA:2176:A:H2 | 38:BC:172:HIS:CE1 | 2.06 | 0.74 |
| 36:BA:1658:C:OP1 | 40:BE:132:HIS:ND1 | 2.20 | 0.74 |
| 47:BO:115:VAL:HG13 | 47:BO:121:VAL:HG21 | 1.69 | 0.74 |
| 58:BZ:17:ALA:HA | 58:BZ:20:ARG:HG2 | 1.68 | 0.74 |
| 11:AK:52:GLY:H | 11:AK:55:LYS:CE | 2.00 | 0.74 |
| 17:AQ:57:VAL:HA | 17:AQ:77:VAL:HG23 | 1.68 | 0.74 |
| 27:B1:44:PRO:HG2 | 27:B1:46:LEU:CD2 | 2.17 | 0.74 |
| 36:BA:1264:G:H3' | 36:BA:1265:A:H5'' | 1.70 | 0.74 |
| 36:BA:2413:G:H21 | 48:BP:70:GLN:HE22 | 1.36 | 0.74 |
| 9:AI:95:LYS:HD3 | 9:AI:96:LEU:N | 2.02 | 0.74 |
| 12:AL:5:PRO:HG2 | 12:AL:10:LEU:HD21 | 1.70 | 0.74 |
| 13:AM:11:ARG:HG2 | 13:AM:12:ASN:HD22 | 1.52 | 0.74 |
| 36:BA:2189:U:C2' | 36:BA:2190:G:H4' | 2.17 | 0.74 |
| 53:BU:95:LEU:C | 53:BU:97:ASP:H | 1.90 | 0.74 |
| 4:AD:175:SER:HB3 | 4:AD:186:LEU:HD11 | 1.68 | 0.74 |
| 16:AP:20:VAL:HG23 | 16:AP:34:GLU:O | 1.88 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:B2:65:ASN:HD22 | 28:B2:69:ARG:NH2 | 1.83 | 0.74 |
| 36:BA:2307:G:H21 | 36:BA:2308:G:H5' | 1.52 | 0.74 |
| 36:BA:612:C:H2' | 36:BA:613:G:H5'' | 1.67 | 0.74 |
| 40:BE:35:GLN:HG2 | 40:BE:36:ARG:H | 1.51 | 0.74 |
| 30:B4:25:TYR:HB2 | 42:BG:101:ILE:HD13 | 1.68 | 0.74 |
| 1:AA:1226:C:H4' | 1:AA:1227:A:OP1 | 1.85 | 0.74 |
| 25:AZ:324:LYS:HD3 | 25:AZ:325:LYS:N | 2.03 | 0.74 |
| 25:AZ:388:ILE:O | 25:AZ:395:VAL:HG22 | 1.88 | 0.74 |
| 36:BA:1061:U:H4' | 36:BA:1070:A:O4' | 1.88 | 0.74 |
| 38:BC:164:ARG:CG | 38:BC:165:ASN:H | 1.99 | 0.74 |
| 38:BC:184:LYS:HE2 | 38:BC:184:LYS:N | 2.03 | 0.74 |
| 48:BP:122:PRO:HA | 48:BP:141:ALA:O | 1.87 | 0.74 |
| 48:BP:121:LYS:O | 48:BP:123:LEU:HD23 | 1.87 | 0.74 |
| 51:BS:40:ILE:HG22 | 51:BS:47:THR:HG23 | 1.70 | 0.74 |
| 51:BS:78:LEU:HD11 | 51:BS:103:GLU:CB | 2.17 | 0.74 |
| 53:BU:93:LYS:H | 53:BU:93:LYS:HD2 | 1.53 | 0.74 |
| 54:BV:28:GLU:HB3 | 54:BV:29:PRO:HD2 | 1.68 | 0.74 |
| 56:BX:64:LYS:NZ | 56:BX:73:ARG:HH21 | 1.86 | 0.74 |
| 16:AP:34:GLU:OE2 | 16:AP:55:ARG:HD3 | 1.88 | 0.73 |
| 36:BA:2416:C:H2' | 36:BA:2417:C:H6 | 1.53 | 0.73 |
| 5:AE:6:PHE:CB | 5:AE:34:VAL:HG22 | 2.17 | 0.73 |
| 25:AZ:263:ARG:HE | 25:AZ:293:VAL:HG12 | 1.52 | 0.73 |
| 25:AZ:368:VAL:HG12 | 25:AZ:369:THR:N | 2.01 | 0.73 |
| 25:AZ:54:PRO:O | 25:AZ:55:GLU:HB3 | 1.86 | 0.73 |
| 30:B4:14:ILE:HG13 | 30:B4:31:ILE:CG2 | 2.18 | 0.73 |
| 39:BD:267:SER:O | 39:BD:269:PHE:N | 2.22 | 0.73 |
| 42:BG:11:TYR:HA | 42:BG:15:VAL:HG23 | 1.69 | 0.73 |
| 42:BG:16:ARG:HH11 | 42:BG:16:ARG:HG3 | 1.51 | 0.73 |
| 46:BN:36:GLY:O | 46:BN:42:TRP:HB2 | 1.87 | 0.73 |
| 36:BA:252:G:OP2 | 48:BP:50:ARG:NH1 | 2.21 | 0.73 |
| 37:BB:91:C:OP1 | 49:BQ:16:ARG:HG2 | 1.88 | 0.73 |
| 51:BS:58:LEU:HG | 51:BS:59:LYS:N | 2.01 | 0.73 |
| 53:BU:48:ALA:O | 53:BU:52:ARG:HG3 | 1.87 | 0.73 |
| 1:AA:92:C:H2' | 1:AA:93:G:C8 | 2.19 | 0.73 |
| 10:AJ:90:LEU:H | 10:AJ:91:PRO:HD3 | 1.53 | 0.73 |
| 12:AL:59:ARG:HD3 | 12:AL:65:GLU:OE2 | 1.88 | 0.73 |
| 26:B0:27:GLU:OE2 | 36:BA:856:C:H1' | 1.88 | 0.73 |
| 36:BA:2580:U:C5' | 40:BE:131:ALA:H | 2.01 | 0.73 |
| 42:BG:76:SER:OG | 42:BG:84:LYS:HG3 | 1.88 | 0.73 |
| 43:BH:158:HIS:NE2 | 43:BH:170:ARG:HA | 2.03 | 0.73 |
| 52:BT:54:ARG:HA | 52:BT:59:THR:HB | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:151:HIS:HB2 | 58:BZ:170:THR:HA | 1.68 | 0.73 |
| 1:AA:1226:C:C5 | 13:AM:104:ARG:HB2 | 2.24 | 0.73 |
| 1:AA:66:G:H4' | 1:AA:173:U:C5 | 2.23 | 0.73 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CB | 2.18 | 0.73 |
| 36:BA:1798:U:C5' | 39:BD:259:THR:HG22 | 2.17 | 0.73 |
| 36:BA:2315:G:H2' | 36:BA:2316:C:C6 | 2.23 | 0.73 |
| 50:BR:2:ARG:HH11 | 50:BR:2:ARG:N | 1.85 | 0.73 |
| 1:AA:1148:U:H2' | 1:AA:1149:C:O4' | 1.87 | 0.73 |
| 36:BA:272(J):C:C2' | 36:BA:274:G:H5'' | 2.19 | 0.73 |
| 36:BA:94(A):G:H2' | 36:BA:95:G:O4' | 1.87 | 0.73 |
| 38:BC:215:THR:HB | 38:BC:221:SER:HA | 1.68 | 0.73 |
| 43:BH:106:THR:HG22 | 43:BH:112:PRO:HA | 1.68 | 0.73 |
| 52:BT:91:ARG:O | 52:BT:117:ASP:HB3 | 1.88 | 0.73 |
| 56:BX:35:THR:HG22 | 56:BX:37:THR:H | 1.51 | 0.73 |
| 1:AA:950:U:H2' | 1:AA:951:G:C8 | 2.23 | 0.73 |
| 5:AE:144:THR:O | 5:AE:148:VAL:HG23 | 1.87 | 0.73 |
| 9:AI:48:GLU:N | 9:AI:49:PRO:HD2 | 2.03 | 0.73 |
| 13:AM:25:ILE:HD11 | 13:AM:60:VAL:HG13 | 1.71 | 0.73 |
| 1:AA:453:A:H5'' | 16:AP:72:ARG:HD2 | 1.70 | 0.73 |
| 22:AV:69:G:H8 | 22:AV:69:G:H5' | 1.52 | 0.73 |
| 34:B8:61:LEU:CD1 | 34:B8:62:LEU:H | 2.01 | 0.73 |
| 22:AW:55:U:H5' | 38:BC:164:ARG:NH2 | 2.03 | 0.73 |
| 36:BA:1813:G:H4' | 39:BD:44:ASN:O | 1.88 | 0.73 |
| 42:BG:38:VAL:HG22 | 42:BG:93:THR:HG23 | 1.69 | 0.73 |
| 36:BA:1012:U:O4 | 46:BN:28:THR:HG21 | 1.89 | 0.73 |
| 26:B0:69:PHE:CD2 | 26:B0:79:VAL:HG22 | 2.24 | 0.73 |
| 36:BA:1786:A:H2 | 36:BA:2606:C:H1' | 1.54 | 0.73 |
| 36:BA:723:G:H2' | 36:BA:724:U:C6 | 2.24 | 0.73 |
| 41:BF:159:GLY:HA2 | 41:BF:164:ARG:NH2 | 2.04 | 0.73 |
| 42:BG:5:VAL:HG12 | 42:BG:6:ALA:H | 1.54 | 0.73 |
| 43:BH:17:VAL:HG12 | 43:BH:18:GLU:H | 1.53 | 0.73 |
| 51:BS:36:TYR:HD1 | 51:BS:36:TYR:N | 1.86 | 0.73 |
| 57:BY:14:LEU:HD12 | 57:BY:23:ARG:O | 1.89 | 0.73 |
| 1:AA:453:A:HO2' | 1:AA:454:C:H6 | 1.35 | 0.73 |
| 7:AG:121:ALA:O | 7:AG:125:MET:HG3 | 1.89 | 0.73 |
| 8:AH:20:TYR:HE2 | 8:AH:75:ARG:HD2 | 1.53 | 0.73 |
| 13:AM:11:ARG:HG2 | 13:AM:12:ASN:ND2 | 2.03 | 0.73 |
| 38:BC:59:ARG:HG3 | 38:BC:164:ARG:HG3 | 1.70 | 0.73 |
| 39:BD:94:LEU:HB2 | 39:BD:104:TYR:HE2 | 1.53 | 0.73 |
| 42:BG:67:LYS:H | 42:BG:67:LYS:HD3 | 1.53 | 0.73 |
| 57:BY:81:LYS:HD3 | 57:BY:97:ARG:O | 1.89 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1040:U:H2' | 1:AA:1041:A:H8 | 1.54 | 0.73 |
| 7:AG:46:ALA:O | 7:AG:50:ILE:HG12 | 1.88 | 0.73 |
| 12:AL:6:THR:OG1 | 12:AL:9:GLN:HG3 | 1.88 | 0.73 |
| 25:AZ:301:GLY:HA2 | 25:AZ:347:THR:HB | 1.71 | 0.73 |
| 36:BA:1230:C:H2' | 36:BA:1231:G:C8 | 2.23 | 0.73 |
| 36:BA:2308:G:O6 | 36:BA:2310:A:H2' | 1.89 | 0.73 |
| 36:BA:428:A:H3' | 36:BA:429:A:C8 | 2.23 | 0.73 |
| 48:BP:9:ASN:N | 48:BP:10:PRO:HD2 | 1.99 | 0.73 |
| 49:BQ:3:MET:HB2 | 49:BQ:4:PRO:HD2 | 1.70 | 0.73 |
| 52:BT:102:ILE:HB | 52:BT:110:ILE:CD1 | 2.19 | 0.73 |
| 54:BV:77:ALA:O | 54:BV:79:VAL:HG23 | 1.89 | 0.73 |
| 1:AA:1285:A:H4' | 1:AA:1286:A:O5' | 1.88 | 0.73 |
| 1:AA:266:G:C5' | 1:AA:267:C:C5 | 2.71 | 0.73 |
| 3:AC:58:GLU:H | 3:AC:65:ALA:HB3 | 1.53 | 0.73 |
| 23:AX:25:A:O2' | 23:AX:26:A:H5' | 1.88 | 0.73 |
| 24:AY:62:U:H5' | 24:AY:62:U:H6 | 1.53 | 0.73 |
| 27:B1:80:LEU:HD22 | 27:B1:82:LEU:HD22 | 1.71 | 0.73 |
| 29:B3:31:LEU:HD23 | 29:B3:32:GLN:N | 2.04 | 0.73 |
| 34:B8:49:VAL:CG1 | 34:B8:53:PRO:HD3 | 2.18 | 0.73 |
| 52:BT:131:ALA:C | 52:BT:133:GLU:H | 1.90 | 0.73 |
| 6:AF:19:LEU:O | 6:AF:19:LEU:HD23 | 1.88 | 0.72 |
| 17:AQ:45:HIS:O | 17:AQ:73:VAL:HG23 | 1.89 | 0.72 |
| 1:AA:192:U:H5' | 20:AT:102:GLY:O | 1.89 | 0.72 |
| 20:AT:39:LYS:O | 20:AT:43:LEU:HG | 1.89 | 0.72 |
| 36:BA:1750:G:O2' | 36:BA:1751:C:H5' | 1.89 | 0.72 |
| 46:BN:58:ASP:C | 46:BN:60:ILE:H | 1.92 | 0.72 |
| 47:BO:26:LYS:HB2 | 47:BO:30:ALA:HB2 | 1.69 | 0.72 |
| 36:BA:662:G:OP1 | 48:BP:18:ARG:HD2 | 1.89 | 0.72 |
| 51:BS:58:LEU:HD23 | 51:BS:65:VAL:HG13 | 1.71 | 0.72 |
| 58:BZ:163:LEU:HG | 58:BZ:165:VAL:HG23 | 1.69 | 0.72 |
| 9:AI:40:LEU:CD1 | 9:AI:70:LYS:HG2 | 2.19 | 0.72 |
| 11:AK:69:ALA:HB1 | 11:AK:103:LEU:HD21 | 1.69 | 0.72 |
| 35:B9:1:MET:SD | 36:BA:2478:A:OP2 | 2.46 | 0.72 |
| 36:BA:1666:G:H2' | 36:BA:1667:G:H5' | 1.69 | 0.72 |
| 43:BH:52:VAL:HG21 | 43:BH:69:ARG:HB2 | 1.71 | 0.72 |
| 50:BR:49:ASP:OD1 | 50:BR:95:THR:HG22 | 1.88 | 0.72 |
| 56:BX:12:VAL:HG23 | 56:BX:13:LEU:N | 2.04 | 0.72 |
| 57:BY:8:LYS:H | 57:BY:8:LYS:CD | 1.95 | 0.72 |
| 5:AE:20:GLN:HE22 | 5:AE:25:ARG:NH2 | 1.87 | 0.72 |
| 36:BA:1386:C:H2' | 36:BA:1387:C:H6 | 1.54 | 0.72 |
| 36:BA:2179:C:H5'' | 36:BA:2180:U:OP1 | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 38:BC:152:ILE:HA | 38:BC:155:GLU:OE2 | 1.88 | 0.72 |
| 38:BC:30:LYS:HD3 | 38:BC:185:LEU:HD11 | 1.71 | 0.72 |
| 40:BE:35:GLN:HG2 | 40:BE:36:ARG:N | 2.04 | 0.72 |
| 52:BT:50:ILE:HG23 | 52:BT:99:LEU:HD12 | 1.70 | 0.72 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.23 | 0.72 |
| 1:AA:177:C:H2' | 1:AA:178:C:C6 | 2.25 | 0.72 |
| 1:AA:454:C:H5' | 1:AA:455:C:OP2 | 1.89 | 0.72 |
| 1:AA:858:G:H8 | 1:AA:858:G:C5' | 2.01 | 0.72 |
| 22:AV:53:G:O2' | 22:AV:54:U:H5' | 1.90 | 0.72 |
| 36:BA:1590:U:C2' | 36:BA:1591:G:H5'' | 2.18 | 0.72 |
| 36:BA:272(H):C:C2' | 36:BA:272(I):U:H5'' | 2.19 | 0.72 |
| 48:BP:100:LEU:HB2 | 48:BP:106:LEU:HD22 | 1.71 | 0.72 |
| 57:BY:86:ARG:HB3 | 57:BY:88:LYS:HE3 | 1.71 | 0.72 |
| 57:BY:86:ARG:HG2 | 57:BY:87:LYS:H | 1.55 | 0.72 |
| 58:BZ:117:LEU:HA | 58:BZ:174:VAL:HG22 | 1.68 | 0.72 |
| 36:BA:2283:C:H2' | 36:BA:2284:C:H5' | 1.71 | 0.72 |
| 36:BA:237:C:O2' | 36:BA:238:C:H5' | 1.90 | 0.72 |
| 37:BB:87:G:C3' | 37:BB:88:C:H5'' | 2.18 | 0.72 |
| 22:AW:56:C:H5' | 38:BC:137:LEU:HB2 | 1.71 | 0.72 |
| 39:BD:27:THR:CG2 | 39:BD:83:GLU:HG2 | 2.19 | 0.72 |
| 46:BN:63:THR:HB | 46:BN:66:LYS:HZ3 | 1.54 | 0.72 |
| 36:BA:812:C:H5' | 48:BP:25:SER:HB2 | 1.70 | 0.72 |
| 50:BR:21:TYR:HD1 | 50:BR:21:TYR:N | 1.87 | 0.72 |
| 51:BS:54:LEU:C | 51:BS:56:LEU:H | 1.93 | 0.72 |
| 4:AD:3:ARG:HE | 4:AD:5:ILE:CG1 | 2.01 | 0.72 |
| 14:AN:22:THR:O | 14:AN:23:ARG:HB2 | 1.89 | 0.72 |
| 14:AN:23:ARG:HD2 | 14:AN:28:GLY:O | 1.89 | 0.72 |
| 16:AP:53:VAL:HG23 | 16:AP:54:GLU:H | 1.55 | 0.72 |
| 36:BA:1639:U:H2' | 36:BA:1640:C:H5'' | 1.72 | 0.72 |
| 36:BA:686:G:N2 | 36:BA:788:A:H61 | 1.87 | 0.72 |
| 42:BG:11:TYR:HA | 42:BG:15:VAL:CG2 | 2.18 | 0.72 |
| 46:BN:12:ARG:HG2 | 46:BN:50:ASP:OD2 | 1.89 | 0.72 |
| 1:AA:1452:C:H5' | 1:AA:1456:G:C2 | 2.25 | 0.72 |
| 25:AZ:32:THR:HG21 | 25:AZ:45:LYS:N | 2.02 | 0.72 |
| 36:BA:2378:A:H62 | 36:BA:2379:G:H21 | 1.35 | 0.72 |
| 36:BA:547:A:H2' | 36:BA:548:A:C8 | 2.25 | 0.72 |
| 36:BA:742:G:H2' | 36:BA:743:G:H8 | 1.55 | 0.72 |
| 38:BC:7:TYR:CE2 | 38:BC:11:LEU:HD11 | 2.24 | 0.72 |
| 39:BD:222:ARG:O | 39:BD:225:ALA:HB3 | 1.88 | 0.72 |
| 13:AM:10:PRO:CB | 13:AM:18:ALA:HB1 | 2.20 | 0.72 |
| 32:B6:26:ASN:ND2 | 32:B6:32:ASN:HD21 | 1.82 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:B8:30:ARG:NE | 34:B8:30:ARG:HA | 2.03 | 0.72 |
| 40:BE:96:PHE:HA | 40:BE:100:GLU:OE1 | 1.89 | 0.72 |
| 52:BT:102:ILE:HB | 52:BT:110:ILE:HD13 | 1.71 | 0.72 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:C8 | 2.25 | 0.72 |
| 1:AA:662:G:O2' | 1:AA:836:G:H5' | 1.88 | 0.72 |
| 4:AD:107:ARG:NH2 | 4:AD:194:LEU:HD12 | 2.03 | 0.72 |
| 38:BC:35:ALA:HB3 | 38:BC:39:GLU:OE2 | 1.90 | 0.72 |
| 39:BD:8:PRO:HB3 | 39:BD:14:ARG:HB2 | 1.72 | 0.72 |
| 42:BG:133:LEU:HD11 | 42:BG:157:ILE:HD12 | 1.72 | 0.72 |
| 46:BN:9:VAL:HG21 | 46:BN:41:ASP:OD2 | 1.90 | 0.72 |
| 56:BX:35:THR:CG2 | 56:BX:37:THR:H | 2.03 | 0.72 |
| 58:BZ:151:HIS:HA | 58:BZ:171:ILE:HG12 | 1.71 | 0.72 |
| 7:AG:15:ASP:HB2 | 7:AG:20:ASP:O | 1.90 | 0.72 |
| 8:AH:68:ARG:HH11 | 8:AH:68:ARG:HG2 | 1.52 | 0.72 |
| 13:AM:10:PRO:HG2 | 13:AM:45:VAL:HG11 | 1.72 | 0.72 |
| 36:BA:2779:U:H1' | 36:BA:2781:A:C5 | 2.25 | 0.72 |
| 33:B7:11:LYS:HE2 | 36:BA:686:G:H5'' | 1.72 | 0.72 |
| 38:BC:180:PHE:O | 38:BC:185:LEU:HG | 1.90 | 0.72 |
| 38:BC:10:LEU:CD1 | 38:BC:32:LEU:HA | 2.16 | 0.72 |
| 41:BF:33:LEU:HD21 | 41:BF:112:MET:HB3 | 1.72 | 0.72 |
| 42:BG:57:ALA:CB | 42:BG:90:LEU:HD21 | 2.18 | 0.72 |
| 2:AB:90:MET:HE3 | 2:AB:91:PRO:HD3 | 1.71 | 0.71 |
| 19:AS:10:PHE:CZ | 19:AS:70:LYS:HD2 | 2.25 | 0.71 |
| 25:AZ:21:ASP:H | 61:AZ:501:GCP:H3B1 | 1.54 | 0.71 |
| 25:AZ:92:MET:HG3 | 25:AZ:93:ILE:N | 2.05 | 0.71 |
| 26:B0:20:ARG:CG | 26:B0:20:ARG:HH11 | 2.03 | 0.71 |
| 36:BA:2113:U:H2' | 36:BA:2114:A:C8 | 2.25 | 0.71 |
| 38:BC:94:VAL:HG12 | 38:BC:95:GLY:H | 1.54 | 0.71 |
| 40:BE:49:LEU:O | 40:BE:78:LEU:HB2 | 1.90 | 0.71 |
| 46:BN:30:ILE:O | 46:BN:34:LEU:HB2 | 1.90 | 0.71 |
| 52:BT:23:ARG:HB2 | 52:BT:24:PRO:HD2 | 1.72 | 0.71 |
| 57:BY:50:ARG:HB3 | 57:BY:53:PRO:HG3 | 1.72 | 0.71 |
| 1:AA:1053:G:C4' | 1:AA:1054:C:H5' | 2.11 | 0.71 |
| 1:AA:509:A:H5' | 4:AD:54:TYR:CD2 | 2.25 | 0.71 |
| 10:AJ:6:ILE:HG13 | 10:AJ:72:VAL:HB | 1.72 | 0.71 |
| 20:AT:53:LEU:HB3 | 20:AT:57:ARG:HH12 | 1.55 | 0.71 |
| 20:AT:73:HIS:C | 20:AT:74:LYS:HD3 | 2.10 | 0.71 |
| 32:B6:15:GLU:OE1 | 32:B6:18:ARG:CZ | 2.38 | 0.71 |
| 36:BA:221:A:H4' | 36:BA:222:A:O5' | 1.90 | 0.71 |
| 36:BA:2317:C:C2' | 36:BA:2318:G:H5' | 2.20 | 0.71 |
| 36:BA:2632:A:N3 | 40:BE:61:ARG:NH1 | 2.38 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BA:81:G:H21 | 57:BY:2:ARG:NH1 | 1.86 | 0.71 |
| 36:BA:848:G:N3 | 36:BA:933:A:H1' | 2.05 | 0.71 |
| 40:BE:38:THR:HB | 40:BE:41:LYS:HG2 | 1.72 | 0.71 |
| 36:BA:2303:G:O2' | 42:BG:132:ASN:HB2 | 1.89 | 0.71 |
| 50:BR:117:VAL:HG22 | 50:BR:118:GLU:H | 1.53 | 0.71 |
| 52:BT:33:LYS:HE2 | 52:BT:43:GLN:HE21 | 1.54 | 0.71 |
| 58:BZ:128:VAL:HG22 | 58:BZ:129:SER:H | 1.52 | 0.71 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.26 | 0.71 |
| 1:AA:384:G:H2' | 1:AA:385:C:C6 | 2.25 | 0.71 |
| 2:AB:15:VAL:H | 2:AB:16:HIS:CE1 | 2.08 | 0.71 |
| 14:AN:13:THR:H | 14:AN:14:PRO:CD | 2.03 | 0.71 |
| 36:BA:2408:U:H2' | 36:BA:2409:G:C8 | 2.25 | 0.71 |
| 39:BD:28:GLU:N | 39:BD:29:PRO:HD2 | 2.03 | 0.71 |
| 40:BE:132:HIS:HA | 40:BE:135:HIS:HE1 | 1.54 | 0.71 |
| 40:BE:24:THR:HG21 | 40:BE:188:VAL:CG1 | 2.19 | 0.71 |
| 42:BG:133:LEU:CD1 | 42:BG:157:ILE:HB | 2.20 | 0.71 |
| 51:BS:62:LYS:H | 51:BS:65:VAL:HG23 | 1.54 | 0.71 |
| 52:BT:85:LYS:NZ | 52:BT:85:LYS:CB | 2.52 | 0.71 |
| 54:BV:38:LEU:HD23 | 54:BV:39:LEU:N | 2.05 | 0.71 |
| 1:AA:639:G:O2' | 1:AA:640:A:H5' | 1.89 | 0.71 |
| 2:AB:68:ILE:N | 2:AB:90:MET:HE1 | 2.01 | 0.71 |
| 7:AG:8:GLU:HG3 | 7:AG:9:VAL:H | 1.54 | 0.71 |
| 2:AB:178:ARG:HH12 | 8:AH:74:PRO:HB3 | 1.55 | 0.71 |
| 32:B6:5:VAL:N | 32:B6:9:LEU:H | 1.88 | 0.71 |
| 36:BA:203:C:H3' | 36:BA:204:A:H5'' | 1.72 | 0.71 |
| 36:BA:2243:U:H2' | 36:BA:2244:U:C6 | 2.25 | 0.71 |
| 36:BA:2464:C:O2' | 36:BA:2465:C:H6 | 1.73 | 0.71 |
| 36:BA:613:G:C8 | 36:BA:613:G:H5' | 2.22 | 0.71 |
| 48:BP:38:GLN:HG3 | 48:BP:39:LYS:H | 1.53 | 0.71 |
| 1:AA:1377:A:H2' | 7:AG:7:ALA:HB2 | 1.72 | 0.71 |
| 13:AM:90:LEU:O | 13:AM:91:ARG:CB | 2.38 | 0.71 |
| 16:AP:44:THR:O | 16:AP:45:THR:HB | 1.90 | 0.71 |
| 17:AQ:76:LEU:HD12 | 17:AQ:77:VAL:H | 1.54 | 0.71 |
| 22:AV:20:U:H3' | 22:AV:21:A:C5' | 2.21 | 0.71 |
| 36:BA:2023:G:H5' | 36:BA:2617:C:H4' | 1.72 | 0.71 |
| 36:BA:2661:G:O2' | 36:BA:2662:A:H5' | 1.90 | 0.71 |
| 36:BA:481:G:OP2 | 57:BY:47:LYS:HB2 | 1.91 | 0.71 |
| 40:BE:47:VAL:HG23 | 40:BE:84:PHE:O | 1.91 | 0.71 |
| 56:BX:12:VAL:HG12 | 56:BX:27:THR:O | 1.90 | 0.71 |
| 1:AA:627:G:H2' | 1:AA:628:G:H8 | 1.56 | 0.71 |
| 1:AA:977:A:O2' | 1:AA:978:A:C5' | 2.39 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:AS:63:THR:HG22 | 19:AS:66:MET:SD | 2.30 | 0.71 |
| 32:B6:11:LEU:HD13 | 32:B6:12:GLU:N | 2.05 | 0.71 |
| 32:B6:11:LEU:HD11 | 32:B6:51:GLU:HG3 | 1.72 | 0.71 |
| 36:BA:2170:A:H5'' | 38:BC:134:ARG:NH2 | 2.06 | 0.71 |
| 38:BC:53:ARG:NH1 | 38:BC:53:ARG:HB3 | 2.04 | 0.71 |
| 43:BH:105:LEU:HD23 | 43:BH:105:LEU:H | 1.55 | 0.71 |
| 49:BQ:141:GLN:H | 58:BZ:53:ILE:HD12 | 1.55 | 0.71 |
| 52:BT:23:ARG:O | 52:BT:25:GLY:N | 2.24 | 0.71 |
| 4:AD:43:HIS:O | 4:AD:45:GLN:N | 2.22 | 0.71 |
| 8:AH:86:ILE:HG21 | 8:AH:133:LEU:HD23 | 1.73 | 0.71 |
| 9:AI:114:TYR:CE1 | 10:AJ:60:ARG:N | 2.55 | 0.71 |
| 11:AK:52:GLY:H | 11:AK:55:LYS:HE3 | 1.53 | 0.71 |
| 13:AM:82:MET:HG2 | 13:AM:82:MET:O | 1.90 | 0.71 |
| 24:AY:76:A:O4' | 25:AZ:237:VAL:HG11 | 1.90 | 0.71 |
| 36:BA:1539:G:C2 | 36:BA:1540:U:H1' | 2.25 | 0.71 |
| 36:BA:1794:U:H2' | 36:BA:1795:C:C6 | 2.26 | 0.71 |
| 36:BA:471:A:C2' | 36:BA:472:A:H5'' | 2.20 | 0.71 |
| 36:BA:673:C:H5' | 36:BA:673:C:C6 | 2.25 | 0.71 |
| 38:BC:83:ILE:HG23 | 38:BC:95:GLY:HA3 | 1.73 | 0.71 |
| 39:BD:108:PRO:HG2 | 39:BD:111:LEU:HB2 | 1.72 | 0.71 |
| 40:BE:79:ARG:NH1 | 40:BE:195:LEU:HD21 | 2.06 | 0.71 |
| 40:BE:37:ARG:HA | 40:BE:42:ASP:OD2 | 1.90 | 0.71 |
| 36:BA:322:A:OP2 | 41:BF:169:ASN:HB2 | 1.88 | 0.71 |
| 58:BZ:102:LEU:HD22 | 58:BZ:137:ILE:HB | 1.71 | 0.71 |
| 27:B1:33:LYS:HD3 | 27:B1:33:LYS:N | 2.04 | 0.71 |
| 41:BF:33:LEU:O | 41:BF:37:VAL:HG23 | 1.91 | 0.71 |
| 26:B0:7:LEU:HD21 | 49:BQ:81:VAL:HG23 | 1.71 | 0.71 |
| 52:BT:28:VAL:O | 52:BT:29:ARG:HD3 | 1.91 | 0.71 |
| 55:BW:73:ALA:HB3 | 55:BW:106:ILE:HG13 | 1.72 | 0.71 |
| 3:AC:154:SER:HA | 3:AC:165:THR:HA | 1.72 | 0.71 |
| 18:AR:32:ARG:HA | 18:AR:69:THR:HG21 | 1.72 | 0.71 |
| 25:AZ:142:ASP:O | 25:AZ:144:PRO:HD3 | 1.90 | 0.71 |
| 26:B0:14:ARG:NH1 | 26:B0:14:ARG:HB2 | 2.00 | 0.71 |
| 36:BA:1639:U:O2' | 36:BA:1640:C:H5'' | 1.91 | 0.71 |
| 36:BA:392:C:H2' | 36:BA:393:C:C6 | 2.25 | 0.71 |
| 41:BF:6:VAL:CG1 | 41:BF:7:TYR:H | 2.01 | 0.71 |
| 50:BR:28:LEU:HD12 | 50:BR:114:VAL:HG23 | 1.71 | 0.71 |
| 51:BS:58:LEU:CG | 51:BS:59:LYS:H | 1.98 | 0.71 |
| 1:AA:148:G:H2' | 1:AA:149:A:H8 | 1.55 | 0.71 |
| 2:AB:152:PHE:O | 2:AB:153:ARG:HB3 | 1.91 | 0.71 |
| 9:AI:37:PHE:HB3 | 9:AI:43:ALA:HB2 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:1161:C:H2' | 36:BA:1162:G:H8 | 1.56 | 0.71 |
| 36:BA:1335:U:H2' | 36:BA:1336:A:H8 | 1.56 | 0.71 |
| 36:BA:1709:U:H2' | 36:BA:1710:C:C6 | 2.26 | 0.71 |
| 22:AW:20:U:H5' | 36:BA:2112:G:H1 | 1.56 | 0.71 |
| 38:BC:99:ILE:HD12 | 38:BC:102:LYS:NZ | 2.05 | 0.71 |
| 40:BE:34:VAL:O | 40:BE:35:GLN:HB2 | 1.91 | 0.71 |
| 50:BR:2:ARG:CG | 50:BR:2:ARG:HH11 | 2.03 | 0.71 |
| 51:BS:17:ARG:C | 51:BS:19:LYS:H | 1.95 | 0.71 |
| 51:BS:36:TYR:CD1 | 51:BS:36:TYR:N | 2.57 | 0.71 |
| 57:BY:42:VAL:HG12 | 57:BY:65:ALA:HB3 | 1.73 | 0.71 |
| 13:AM:66:LEU:H | 13:AM:66:LEU:HD12 | 1.54 | 0.70 |
| 35:B9:4:ARG:O | 35:B9:36:GLN:HA | 1.91 | 0.70 |
| 36:BA:1116:C:H2' | 36:BA:1117:G:H8 | 1.56 | 0.70 |
| 36:BA:1251:C:OP1 | 53:BU:10:ARG:HG3 | 1.89 | 0.70 |
| 36:BA:259:G:H1' | 36:BA:621:A:O2' | 1.91 | 0.70 |
| 36:BA:654(J):A:C8 | 36:BA:654(L):G:H1' | 2.26 | 0.70 |
| 38:BC:163:PHE:HA | 38:BC:172:HIS:O | 1.90 | 0.70 |
| 36:BA:1569:A:O2' | 39:BD:38:LYS:HG3 | 1.90 | 0.70 |
| 46:BN:17:ASP:OD2 | 46:BN:56:ASN:HB3 | 1.91 | 0.70 |
| 26:B0:7:LEU:HD21 | 49:BQ:81:VAL:CG2 | 2.21 | 0.70 |
| 57:BY:77:PRO:HB2 | 57:BY:99:CYS:SG | 2.31 | 0.70 |
| 58:BZ:119:GLU:HG2 | 58:BZ:122:ARG:NH1 | 2.05 | 0.70 |
| 5:AE:31:LEU:HD23 | 5:AE:45:PHE:HD1 | 1.56 | 0.70 |
| 17:AQ:26:GLN:O | 17:AQ:27:PHE:HB3 | 1.89 | 0.70 |
| 29:B3:26:LEU:HB2 | 29:B3:28:LEU:HD21 | 1.73 | 0.70 |
| 32:B6:5:VAL:N | 32:B6:8:LYS:HB3 | 2.06 | 0.70 |
| 36:BA:416:C:H42 | 36:BA:2407:G:H1 | 1.39 | 0.70 |
| 36:BA:2641:G:H5' | 36:BA:2641:G:C8 | 2.22 | 0.70 |
| 36:BA:915:C:H2' | 36:BA:916:G:H8 | 1.54 | 0.70 |
| 48:BP:16:ARG:HB2 | 48:BP:16:ARG:HH11 | 1.56 | 0.70 |
| 54:BV:49:THR:HB | 54:BV:50:PRO:CD | 2.21 | 0.70 |
| 1:AA:1127:G:H1 | 1:AA:1145:C:H42 | 1.38 | 0.70 |
| 2:AB:122:PHE:HA | 2:AB:139:LYS:NZ | 2.06 | 0.70 |
| 3:AC:68:VAL:HG12 | 3:AC:70:VAL:HG23 | 1.72 | 0.70 |
| 7:AG:16:LEU:CD1 | 9:AI:42:ARG:HA | 2.20 | 0.70 |
| 28:B2:2:LYS:O | 28:B2:5:GLU:HG2 | 1.91 | 0.70 |
| 36:BA:1252:G:N3 | 53:BU:33:ARG:HD2 | 2.05 | 0.70 |
| 36:BA:121:G:H4' | 36:BA:149:A:H5' | 1.74 | 0.70 |
| 36:BA:1512:U:O2 | 36:BA:1512:U:H2' | 1.90 | 0.70 |
| 36:BA:612:C:O2' | 36:BA:613:G:H5'' | 1.91 | 0.70 |
| 38:BC:30:LYS:HA | 38:BC:30:LYS:NZ | 2.05 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:AW:57:G:H2' | 22:AW:58:A:C5' | 2.21 | 0.70 |
| 22:AW:59:U:H2' | 22:AW:60:U:H5' | 1.73 | 0.70 |
| 36:BA:1053:C:H2' | 36:BA:1054:A:H8 | 1.57 | 0.70 |
| 36:BA:1981:A:H5'' | 36:BA:1982:C:OP2 | 1.91 | 0.70 |
| 36:BA:2207:G:O2' | 36:BA:2208:A:H5'' | 1.91 | 0.70 |
| 36:BA:2875:C:H4' | 52:BT:5:ALA:HB2 | 1.72 | 0.70 |
| 1:AA:1510:U:H2' | 1:AA:1511:G:C8 | 2.26 | 0.70 |
| 2:AB:42:ILE:HD11 | 2:AB:202:PRO:HB2 | 1.72 | 0.70 |
| 34:B8:33:ASN:ND2 | 36:BA:2419:U:H5'' | 2.05 | 0.70 |
| 36:BA:481:G:H1' | 36:BA:506:G:N2 | 2.05 | 0.70 |
| 39:BD:35:LYS:O | 39:BD:37:LEU:N | 2.25 | 0.70 |
| 39:BD:3:VAL:CG1 | 39:BD:17:THR:HB | 2.22 | 0.70 |
| 40:BE:48:GLN:NE2 | 40:BE:78:LEU:HD13 | 2.07 | 0.70 |
| 52:BT:32:TYR:CD2 | 52:BT:32:TYR:N | 2.57 | 0.70 |
| 52:BT:65:LYS:HA | 52:BT:65:LYS:HZ2 | 1.56 | 0.70 |
| 57:BY:7:VAL:HB | 57:BY:8:LYS:CD | 2.17 | 0.70 |
| 57:BY:86:ARG:HD3 | 57:BY:88:LYS:HG3 | 1.73 | 0.70 |
| 49:BQ:140:ALA:HB3 | 58:BZ:53:ILE:HD11 | 1.73 | 0.70 |
| 1:AA:1120:G:H2' | 1:AA:1121:U:H6 | 1.55 | 0.70 |
| 1:AA:542:G:OP1 | 4:AD:10:ARG:NH2 | 2.25 | 0.70 |
| 9:AI:26:VAL:HG22 | 9:AI:61:ALA:HB3 | 1.71 | 0.70 |
| 10:AJ:90:LEU:H | 10:AJ:91:PRO:CD | 2.05 | 0.70 |
| 15:AO:17:ARG:HH11 | 15:AO:17:ARG:HG3 | 1.56 | 0.70 |
| 34:B8:47:LYS:NZ | 34:B8:47:LYS:HB2 | 2.07 | 0.70 |
| 36:BA:1348:G:C2' | 36:BA:1349:A:H5'' | 2.20 | 0.70 |
| 38:BC:215:THR:HB | 38:BC:221:SER:CA | 2.22 | 0.70 |
| 38:BC:77:ILE:O | 38:BC:95:GLY:HA2 | 1.90 | 0.70 |
| 47:BO:47:ILE:HG23 | 47:BO:48:PRO:HD2 | 1.71 | 0.70 |
| 54:BV:49:THR:HB | 54:BV:50:PRO:HD2 | 1.73 | 0.70 |
| 1:AA:299:G:H2' | 1:AA:300:A:C8 | 2.27 | 0.70 |
| 1:AA:534:U:H6 | 1:AA:534:U:H5' | 1.56 | 0.70 |
| 20:AT:26:ASN:HB3 | 20:AT:71:THR:OG1 | 1.91 | 0.70 |
| 32:B6:36:LEU:HD12 | 32:B6:50:ARG:HH12 | 1.53 | 0.70 |
| 36:BA:191:A:O2' | 36:BA:192:C:H5' | 1.92 | 0.70 |
| 36:BA:2050:C:H1' | 40:BE:156:MET:HE2 | 1.72 | 0.70 |
| 36:BA:2761:G:C2' | 36:BA:2762:G:H5'' | 2.19 | 0.70 |
| 39:BD:27:THR:O | 39:BD:27:THR:HG23 | 1.91 | 0.70 |
| 40:BE:57:LYS:O | 40:BE:58:ARG:HG3 | 1.91 | 0.70 |
| 1:AA:250:A:H4' | 1:AA:251:G:O5' | 1.92 | 0.70 |
| 1:AA:254:G:H21 | 17:AQ:16:GLN:HE22 | 1.39 | 0.70 |
| 2:AB:22:LYS:HA | 2:AB:22:LYS:HE2 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:AB:80:ILE:CD1 | 2:AB:80:ILE:H | 2.04 | 0.70 |
| 10:AJ:16:LEU:HD11 | 10:AJ:70:ARG:HG2 | 1.74 | 0.70 |
| 24:AY:65:C:H5' | 25:AZ:341:GLN:HG2 | 1.74 | 0.70 |
| 25:AZ:99:MET:HE2 | 25:AZ:102:ALA:HB2 | 1.74 | 0.70 |
| 29:B3:40:THR:O | 29:B3:44:ARG:HB2 | 1.91 | 0.70 |
| 50:BR:117:VAL:O | 50:BR:118:GLU:HB2 | 1.90 | 0.70 |
| 52:BT:61:PHE:CE2 | 52:BT:76:PHE:HB2 | 2.27 | 0.70 |
| 25:AZ:272:MET:HE1 | 25:AZ:284:ASP:OD2 | 1.91 | 0.70 |
| 36:BA:1665:A:C3' | 36:BA:1666:G:H5'' | 2.21 | 0.70 |
| 36:BA:936:C:H2' | 36:BA:937:U:C6 | 2.27 | 0.70 |
| 38:BC:49:ILE:HG22 | 38:BC:204:ALA:CB | 2.22 | 0.70 |
| 41:BF:51:THR:CG2 | 41:BF:92:PRO:HD2 | 2.22 | 0.70 |
| 42:BG:42:GLY:O | 42:BG:89:GLY:HA2 | 1.92 | 0.70 |
| 48:BP:47:ASP:CB | 48:BP:48:PRO:HA | 2.22 | 0.70 |
| 8:AH:11:THR:HA | 8:AH:14:ARG:NH1 | 2.06 | 0.70 |
| 22:AW:72:C:O2' | 22:AW:73:A:H5' | 1.92 | 0.70 |
| 36:BA:1142(A):A:H4' | 46:BN:25:ARG:HH22 | 1.56 | 0.70 |
| 36:BA:1464:C:HO2' | 36:BA:1528:A:H8 | 1.34 | 0.70 |
| 36:BA:1771:C:H1' | 36:BA:1786:A:C8 | 2.27 | 0.70 |
| 36:BA:2131:G:H5'' | 36:BA:2132:U:O5' | 1.92 | 0.70 |
| 36:BA:2313:C:H6 | 36:BA:2313:C:H5' | 1.56 | 0.70 |
| 36:BA:991:C:H5' | 36:BA:991:C:H6 | 1.57 | 0.70 |
| 38:BC:75:LEU:HD21 | 38:BC:113:VAL:HG22 | 1.72 | 0.70 |
| 40:BE:107:THR:O | 40:BE:190:GLY:HA2 | 1.92 | 0.70 |
| 49:BQ:29:PHE:HB2 | 49:BQ:105:GLU:OE2 | 1.91 | 0.70 |
| 50:BR:100:LEU:H | 50:BR:100:LEU:HD22 | 1.57 | 0.70 |
| 51:BS:97:ARG:O | 51:BS:99:LYS:HG2 | 1.92 | 0.70 |
| 58:BZ:126:VAL:CG1 | 58:BZ:163:LEU:HB2 | 2.20 | 0.70 |
| 1:AA:977:A:O2' | 1:AA:978:A:H5'' | 1.91 | 0.69 |
| 4:AD:64:LEU:HB2 | 4:AD:198:VAL:HG21 | 1.74 | 0.69 |
| 11:AK:48:ILE:HG22 | 11:AK:49:GLY:N | 2.07 | 0.69 |
| 34:B8:49:VAL:O | 34:B8:50:LEU:HB2 | 1.92 | 0.69 |
| 36:BA:1041:G:O2' | 36:BA:1042:G:H5' | 1.91 | 0.69 |
| 36:BA:1747(A):G:H2' | 36:BA:1748:G:C5' | 2.21 | 0.69 |
| 43:BH:143:GLN:CA | 43:BH:143:GLN:HE21 | 2.05 | 0.69 |
| 46:BN:67:LEU:HD23 | 46:BN:87:LEU:HD12 | 1.74 | 0.69 |
| 51:BS:24:LEU:HD13 | 51:BS:41:ASP:HB2 | 1.74 | 0.69 |
| 4:AD:155:LEU:HB2 | 4:AD:158:ILE:HG12 | 1.74 | 0.69 |
| 22:AV:62:C:H2' | 22:AV:63:G:H8 | 1.56 | 0.69 |
| 24:AY:44:G:H4' | 24:AY:45:U:OP1 | 1.92 | 0.69 |
| 29:B3:18:ASP:OD2 | 29:B3:49:LYS:HE3 | 1.91 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:142:A:H8 | 36:BA:1408:C:H1' | 1.57 | 0.69 |
| 36:BA:952:G:P | 49:BQ:16:ARG:HH12 | 2.16 | 0.69 |
| 46:BN:58:ASP:O | 46:BN:60:ILE:N | 2.25 | 0.69 |
| 50:BR:11:ASN:O | 50:BR:12:ARG:HB2 | 1.92 | 0.69 |
| 56:BX:12:VAL:HG23 | 56:BX:13:LEU:H | 1.57 | 0.69 |
| 56:BX:27:THR:HG22 | 56:BX:80:ILE:HG22 | 1.74 | 0.69 |
| 57:BY:13:VAL:HG22 | 57:BY:73:ARG:C | 2.12 | 0.69 |
| 57:BY:27:VAL:HG12 | 57:BY:28:LYS:H | 1.56 | 0.69 |
| 57:BY:50:ARG:O | 57:BY:53:PRO:HD3 | 1.92 | 0.69 |
| 2:AB:121:LEU:O | 2:AB:121:LEU:HD23 | 1.92 | 0.69 |
| 2:AB:51:LEU:O | 2:AB:55:PHE:HD2 | 1.75 | 0.69 |
| 6:AF:33:TYR:CD2 | 6:AF:75:LEU:HA | 2.28 | 0.69 |
| 15:AO:39:LEU:HD13 | 15:AO:56:LEU:HB2 | 1.72 | 0.69 |
| 18:AR:37:VAL:CG1 | 18:AR:78:LEU:HB3 | 2.22 | 0.69 |
| 31:B5:33:CYS:HG | 31:B5:36:CYS:HG | 1.40 | 0.69 |
| 58:BZ:19:ARG:HH12 | 58:BZ:84:GLU:CA | 2.04 | 0.69 |
| 2:AB:145:LEU:HD13 | 2:AB:149:LEU:HD12 | 1.75 | 0.69 |
| 1:AA:1125:U:H5 | 10:AJ:73:ASP:OD2 | 1.75 | 0.69 |
| 13:AM:66:LEU:HD12 | 13:AM:66:LEU:N | 2.06 | 0.69 |
| 14:AN:13:THR:N | 14:AN:14:PRO:CD | 2.54 | 0.69 |
| 10:AJ:50:ILE:HD11 | 14:AN:41:ARG:HD2 | 1.73 | 0.69 |
| 25:AZ:331:HIS:O | 25:AZ:332:THR:HG23 | 1.92 | 0.69 |
| 28:B2:18:PRO:HG2 | 28:B2:19:VAL:H | 1.57 | 0.69 |
| 28:B2:35:LEU:CD1 | 28:B2:50:ILE:HG13 | 2.13 | 0.69 |
| 30:B4:7:PRO:O | 30:B4:8:LYS:HB3 | 1.91 | 0.69 |
| 32:B6:12:GLU:HA | 32:B6:23:THR:HG22 | 1.72 | 0.69 |
| 35:B9:18:ARG:HD2 | 36:BA:1034:G:H5' | 1.72 | 0.69 |
| 36:BA:1065:U:O2' | 36:BA:1066:U:H5'' | 1.92 | 0.69 |
| 36:BA:996:A:H4' | 53:BU:92:ARG:NE | 2.06 | 0.69 |
| 36:BA:674:G:H1' | 41:BF:74:ARG:HD3 | 1.74 | 0.69 |
| 1:AA:643:C:H2' | 1:AA:644:G:H8 | 1.57 | 0.69 |
| 25:AZ:324:LYS:HG2 | 25:AZ:364:PRO:CB | 2.22 | 0.69 |
| 27:B1:29:GLY:O | 27:B1:30:VAL:HG22 | 1.92 | 0.69 |
| 32:B6:18:ARG:HH11 | 32:B6:18:ARG:CG | 1.97 | 0.69 |
| 36:BA:1184:G:O2' | 36:BA:1185:C:H5' | 1.91 | 0.69 |
| 36:BA:2101:G:C2' | 36:BA:2102:U:H5'' | 2.19 | 0.69 |
| 36:BA:2648:C:H2' | 36:BA:2649:U:C6 | 2.27 | 0.69 |
| 36:BA:2712:U:O2' | 36:BA:2713:A:H5' | 1.91 | 0.69 |
| 38:BC:62:VAL:HG21 | 38:BC:192:PHE:HA | 1.73 | 0.69 |
| 36:BA:806:C:OP2 | 48:BP:39:LYS:HD2 | 1.91 | 0.69 |
| 48:BP:71:VAL:H | 48:BP:72:PRO:HD3 | 1.57 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:23:LYS:HD3 | 58:BZ:38:TYR:CE1 | 2.28 | 0.69 |
| 1:AA:353:A:H5' | 1:AA:353:A:H8 | 1.58 | 0.69 |
| 2:AB:167:PRO:HG2 | 2:AB:192:SER:OG | 1.92 | 0.69 |
| 8:AH:86:ILE:HD11 | 8:AH:136:GLU:HG2 | 1.73 | 0.69 |
| 36:BA:1434:A:H61 | 36:BA:1558:A:H62 | 1.39 | 0.69 |
| 36:BA:1495:A:N3 | 36:BA:1496:A:C2 | 2.60 | 0.69 |
| 36:BA:1414:G:H1 | 36:BA:1588:C:H42 | 1.40 | 0.69 |
| 36:BA:2249:U:H4' | 36:BA:2275:C:C5 | 2.27 | 0.69 |
| 36:BA:2308:G:H2' | 36:BA:2309:A:C8 | 2.28 | 0.69 |
| 36:BA:30:G:H2' | 36:BA:31:C:C6 | 2.26 | 0.69 |
| 42:BG:122:PRO:HD3 | 42:BG:181:ARG:HB3 | 1.72 | 0.69 |
| 1:AA:624:C:O3' | 16:AP:10:GLY:HA2 | 1.92 | 0.69 |
| 4:AD:150:GLU:CD | 4:AD:151:LYS:N | 2.46 | 0.69 |
| 9:AI:104:ARG:C | 9:AI:104:ARG:HD3 | 2.12 | 0.69 |
| 24:AY:20:H2U:H4' | 24:AY:21:A:C5' | 2.23 | 0.69 |
| 29:B3:43:ILE:O | 29:B3:47:VAL:HG23 | 1.92 | 0.69 |
| 36:BA:1786:A:C2 | 36:BA:2606:C:H1' | 2.28 | 0.69 |
| 36:BA:2245:U:H5' | 36:BA:2246:G:C5' | 2.23 | 0.69 |
| 36:BA:2350:C:H2' | 36:BA:2351:G:O4' | 1.93 | 0.69 |
| 36:BA:2807:G:C3' | 36:BA:2808:U:H5'' | 2.23 | 0.69 |
| 38:BC:114:VAL:CG2 | 38:BC:149:ILE:HD11 | 2.23 | 0.69 |
| 39:BD:131:LEU:N | 39:BD:131:LEU:HD12 | 2.07 | 0.69 |
| 39:BD:210:GLY:O | 39:BD:211:ARG:CB | 2.39 | 0.69 |
| 39:BD:25:THR:HG22 | 39:BD:26:LYS:HD2 | 1.75 | 0.69 |
| 42:BG:176:LEU:HD23 | 42:BG:176:LEU:O | 1.91 | 0.69 |
| 36:BA:2312:U:O3' | 42:BG:71:THR:HG21 | 1.92 | 0.69 |
| 36:BA:1242:A:N1 | 48:BP:8:PRO:HG3 | 2.07 | 0.69 |
| 58:BZ:151:HIS:HB3 | 58:BZ:170:THR:HA | 1.74 | 0.69 |
| 58:BZ:40:ASP:HB3 | 58:BZ:43:GLU:CD | 2.12 | 0.69 |
| 2:AB:80:ILE:N | 2:AB:80:ILE:HD12 | 2.07 | 0.69 |
| 11:AK:15:ALA:HB1 | 11:AK:78:GLN:HB2 | 1.73 | 0.69 |
| 13:AM:49:THR:HG22 | 13:AM:51:ALA:H | 1.58 | 0.69 |
| 31:B5:19:ARG:HG3 | 36:BA:2046:G:H5' | 1.74 | 0.69 |
| 32:B6:52:VAL:HG22 | 32:B6:53:LYS:H | 1.56 | 0.69 |
| 36:BA:1290:C:H2' | 36:BA:1291:C:C6 | 2.27 | 0.69 |
| 36:BA:1353:A:H2' | 36:BA:1354:A:C8 | 2.28 | 0.69 |
| 36:BA:1419:A:O2' | 36:BA:1420:U:H5'' | 1.93 | 0.69 |
| 36:BA:2124:G:N2 | 38:BC:218:MET:HG2 | 2.07 | 0.69 |
| 36:BA:2777:G:H5'' | 36:BA:2778:A:H5' | 1.75 | 0.69 |
| 36:BA:428:A:H3' | 36:BA:429:A:H8 | 1.58 | 0.69 |
| 36:BA:719:C:O2' | 36:BA:720:C:H5' | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BC:14:VAL:CG2 | 38:BC:32:LEU:HD11 | 2.22 | 0.69 |
| 47:BO:71:ARG:HB3 | 47:BO:72:PRO:HD2 | 1.72 | 0.69 |
| 50:BR:34:ILE:HB | 50:BR:114:VAL:CG2 | 2.21 | 0.69 |
| 58:BZ:40:ASP:HB3 | 58:BZ:43:GLU:CG | 2.22 | 0.69 |
| 1:AA:102:G:H2' | 1:AA:103:C:C6 | 2.25 | 0.69 |
| 1:AA:29:G:O2' | 1:AA:30:U:H5' | 1.93 | 0.69 |
| 2:AB:194:PRO:O | 2:AB:196:LEU:N | 2.26 | 0.69 |
| 2:AB:36:ARG:HA | 2:AB:36:ARG:CZ | 2.21 | 0.69 |
| 13:AM:14:ARG:H | 13:AM:44:ARG:HH11 | 1.41 | 0.69 |
| 30:B4:30:GLU:O | 30:B4:31:ILE:HD12 | 1.93 | 0.69 |
| 36:BA:2666:C:H5' | 36:BA:2667:C:OP2 | 1.93 | 0.69 |
| 36:BA:915:C:H2' | 36:BA:916:G:C8 | 2.28 | 0.69 |
| 40:BE:52:LEU:HD23 | 40:BE:75:VAL:HB | 1.74 | 0.69 |
| 47:BO:98:VAL:HG12 | 47:BO:117:LEU:HB3 | 1.73 | 0.69 |
| 55:BW:17:VAL:C | 55:BW:19:LEU:H | 1.95 | 0.69 |
| 57:BY:46:LYS:HG2 | 57:BY:47:LYS:N | 2.05 | 0.69 |
| 3:AC:3:ASN:O | 3:AC:4:LYS:HB2 | 1.93 | 0.69 |
| 25:AZ:243:GLU:HA | 25:AZ:243:GLU:OE1 | 1.93 | 0.69 |
| 26:B0:20:ARG:HG2 | 26:B0:20:ARG:HH11 | 1.57 | 0.69 |
| 36:BA:1038:C:C2' | 36:BA:1039:G:H5'' | 2.23 | 0.69 |
| 36:BA:1721:G:C6 | 36:BA:1739:U:H5' | 2.28 | 0.69 |
| 36:BA:1991:U:H2' | 36:BA:1992:G:H5'' | 1.74 | 0.69 |
| 36:BA:2283:C:C2' | 36:BA:2284:C:H5' | 2.23 | 0.69 |
| 36:BA:6:A:H2' | 36:BA:7:G:H8 | 1.57 | 0.69 |
| 36:BA:74:A:H5'' | 36:BA:75:G:O4' | 1.92 | 0.69 |
| 36:BA:784:A:H5'' | 39:BD:227:ASN:ND2 | 2.08 | 0.69 |
| 49:BQ:60:ARG:CB | 49:BQ:60:ARG:HH11 | 2.06 | 0.69 |
| 50:BR:12:ARG:HB3 | 50:BR:16:HIS:CD2 | 2.27 | 0.69 |
| 52:BT:129:ARG:NH2 | 52:BT:131:ALA:HB3 | 2.08 | 0.69 |
| 1:AA:1498:U:H4' | 1:AA:1519:A:C2 | 2.28 | 0.69 |
| 8:AH:20:TYR:CE2 | 8:AH:75:ARG:HD2 | 2.28 | 0.69 |
| 10:AJ:50:ILE:CD1 | 10:AJ:50:ILE:H | 1.83 | 0.69 |
| 21:AU:5:ASP:O | 21:AU:11:GLY:HA3 | 1.93 | 0.69 |
| 28:B2:12:GLU:O | 28:B2:16:LEU:HG | 1.92 | 0.69 |
| 28:B2:25:VAL:C | 28:B2:27:GLU:H | 1.95 | 0.69 |
| 30:B4:10:VAL:CG2 | 30:B4:11:PRO:HD2 | 2.22 | 0.69 |
| 27:B1:45:ASN:ND2 | 36:BA:2090:G:H21 | 1.87 | 0.69 |
| 36:BA:2170:A:H4' | 38:BC:133:PRO:CB | 2.22 | 0.69 |
| 39:BD:8:PRO:HB3 | 39:BD:14:ARG:CB | 2.23 | 0.69 |
| 41:BF:205:ARG:O | 41:BF:206:ILE:HD13 | 1.93 | 0.69 |
| 42:BG:76:SER:HB3 | 42:BG:83:ARG:HB3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 49:BQ:134:ARG:HA | 49:BQ:137:TYR:HD2 | 1.57 | 0.69 |
| 50:BR:52:ILE:HD13 | 50:BR:79:LEU:HD21 | 1.74 | 0.69 |
| 50:BR:57:ARG:O | 50:BR:59:ASP:N | 2.26 | 0.69 |
| 51:BS:92:TYR:CG | 51:BS:93:LYS:N | 2.61 | 0.69 |
| 1:AA:1152:A:H5'' | 10:AJ:13:HIS:CD2 | 2.29 | 0.68 |
| 6:AF:25:ILE:HD13 | 6:AF:25:ILE:O | 1.92 | 0.68 |
| 9:AI:4:TYR:CE2 | 9:AI:88:TYR:HB2 | 2.28 | 0.68 |
| 19:AS:24:ALA:O | 19:AS:25:LYS:HG3 | 1.93 | 0.68 |
| 22:AW:19:G:C5 | 36:BA:2169:A:H1' | 2.28 | 0.68 |
| 24:AY:27:C:H2' | 24:AY:28:C:C6 | 2.29 | 0.68 |
| 30:B4:5:ILE:H | 30:B4:5:ILE:HD13 | 1.58 | 0.68 |
| 36:BA:484:C:O2' | 36:BA:485:C:H5' | 1.93 | 0.68 |
| 39:BD:118:VAL:HG22 | 39:BD:119:ALA:H | 1.58 | 0.68 |
| 46:BN:56:ASN:H | 46:BN:125:GLY:HA3 | 1.58 | 0.68 |
| 50:BR:32:GLY:HA2 | 50:BR:116:LEU:HD12 | 1.75 | 0.68 |
| 3:AC:11:ARG:NH2 | 3:AC:182:ILE:HD12 | 2.07 | 0.68 |
| 7:AG:79:ARG:HH21 | 22:AW:33:U:H4' | 1.57 | 0.68 |
| 7:AG:72:ARG:HA | 7:AG:96:GLN:HE22 | 1.58 | 0.68 |
| 23:AX:26:A:H3' | 23:AX:27:A:C5' | 2.19 | 0.68 |
| 29:B3:28:LEU:H | 29:B3:28:LEU:HD23 | 1.57 | 0.68 |
| 36:BA:2131:G:OP1 | 36:BA:2132:U:H3' | 1.92 | 0.68 |
| 33:B7:37:LYS:HE2 | 36:BA:469:G:O6 | 1.94 | 0.68 |
| 38:BC:100:ILE:HG23 | 38:BC:127:LEU:CG | 2.23 | 0.68 |
| 38:BC:100:ILE:CG2 | 38:BC:127:LEU:HG | 2.22 | 0.68 |
| 38:BC:99:ILE:HD12 | 38:BC:102:LYS:HZ3 | 1.57 | 0.68 |
| 39:BD:24:ILE:O | 39:BD:25:THR:O | 2.10 | 0.68 |
| 39:BD:43:ARG:HD2 | 39:BD:44:ASN:OD1 | 1.93 | 0.68 |
| 42:BG:114:ILE:HG23 | 42:BG:117:PHE:HB2 | 1.76 | 0.68 |
| 47:BO:1:MET:HB3 | 47:BO:32:TYR:HD2 | 1.58 | 0.68 |
| 48:BP:47:ASP:HB3 | 48:BP:49:ARG:N | 2.08 | 0.68 |
| 51:BS:106:ARG:HB3 | 51:BS:106:ARG:NH1 | 2.08 | 0.68 |
| 57:BY:86:ARG:HG2 | 57:BY:87:LYS:N | 2.07 | 0.68 |
| 1:AA:1125:U:C5 | 10:AJ:73:ASP:OD2 | 2.47 | 0.68 |
| 16:AP:53:VAL:HG23 | 16:AP:54:GLU:N | 2.07 | 0.68 |
| 25:AZ:147:LEU:HG | 25:AZ:172:ARG:NH1 | 2.08 | 0.68 |
| 25:AZ:301:GLY:HA3 | 25:AZ:347:THR:HB | 1.75 | 0.68 |
| 36:BA:1064:C:H3' | 36:BA:1065:U:H5'' | 1.75 | 0.68 |
| 36:BA:1747(A):G:O2' | 36:BA:1748:G:H5'' | 1.94 | 0.68 |
| 46:BN:32:THR:HG22 | 46:BN:37:LYS:HB3 | 1.74 | 0.68 |
| 55:BW:3:ALA:CB | 55:BW:58:ALA:HB2 | 2.23 | 0.68 |
| 58:BZ:37:VAL:O | 58:BZ:38:TYR:HB3 | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1001:A:H2' | 1:AA:1001:A:N3 | 2.07 | 0.68 |
| 1:AA:878:G:H5' | 8:AH:89:PRO:HG2 | 1.75 | 0.68 |
| 1:AA:943:U:H2' | 1:AA:944:G:H5' | 1.75 | 0.68 |
| 27:B1:45:ASN:HD21 | 36:BA:2090:G:N2 | 1.89 | 0.68 |
| 36:BA:1858:G:H22 | 36:BA:1883:G:H2' | 1.58 | 0.68 |
| 36:BA:2159:G:C2' | 36:BA:2160:G:H5'' | 2.21 | 0.68 |
| 36:BA:2415:G:O3' | 48:BP:66:GLY:HA3 | 1.93 | 0.68 |
| 43:BH:42:ARG:O | 43:BH:43:VAL:HG13 | 1.92 | 0.68 |
| 52:BT:32:TYR:O | 52:BT:33:LYS:HB2 | 1.91 | 0.68 |
| 55:BW:29:LEU:HD21 | 55:BW:33:ARG:NH1 | 2.08 | 0.68 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:H6 | 1.58 | 0.68 |
| 3:AC:16:ARG:HA | 3:AC:16:ARG:HH11 | 1.58 | 0.68 |
| 6:AF:69:GLU:O | 6:AF:72:VAL:HG12 | 1.94 | 0.68 |
| 13:AM:119:GLY:O | 13:AM:120:LYS:HB2 | 1.91 | 0.68 |
| 27:B1:67:ILE:N | 27:B1:68:PRO:HD2 | 2.08 | 0.68 |
| 29:B3:4:LEU:HD11 | 29:B3:39:ASP:OD1 | 1.94 | 0.68 |
| 34:B8:50:LEU:C | 34:B8:53:PRO:HD2 | 2.14 | 0.68 |
| 36:BA:1666:G:C2' | 36:BA:1667:G:H5' | 2.22 | 0.68 |
| 36:BA:34:C:H5' | 36:BA:35:G:OP2 | 1.93 | 0.68 |
| 36:BA:621:A:H2' | 36:BA:622:G:C5' | 2.23 | 0.68 |
| 39:BD:44:ASN:HB3 | 39:BD:49:ILE:HA | 1.75 | 0.68 |
| 49:BQ:134:ARG:CZ | 58:BZ:122:ARG:HE | 2.07 | 0.68 |
| 50:BR:63:ARG:HG3 | 50:BR:80:PHE:HE2 | 1.58 | 0.68 |
| 51:BS:90:GLY:O | 51:BS:92:TYR:N | 2.27 | 0.68 |
| 1:AA:1189:C:OP1 | 10:AJ:51:ARG:NH2 | 2.26 | 0.68 |
| 1:AA:429:U:H2' | 4:AD:25:ARG:NH1 | 2.09 | 0.68 |
| 2:AB:219:VAL:O | 2:AB:222:ILE:HG12 | 1.93 | 0.68 |
| 4:AD:107:ARG:HH12 | 4:AD:114:ARG:HH21 | 1.39 | 0.68 |
| 9:AI:118:LYS:O | 9:AI:119:ALA:CB | 2.41 | 0.68 |
| 16:AP:25:ARG:HH11 | 16:AP:25:ARG:HG3 | 1.57 | 0.68 |
| 17:AQ:24:GLU:HG2 | 17:AQ:39:SER:CB | 2.21 | 0.68 |
| 22:AV:72:C:C3' | 22:AV:73:A:H5'' | 2.24 | 0.68 |
| 39:BD:96:HIS:CE1 | 39:BD:102:LYS:NZ | 2.62 | 0.68 |
| 47:BO:107:ARG:NH1 | 52:BT:35:LYS:HD2 | 2.08 | 0.68 |
| 51:BS:38:GLN:O | 51:BS:39:ILE:HG13 | 1.94 | 0.68 |
| 53:BU:68:ALA:O | 53:BU:71:GLN:HB3 | 1.93 | 0.68 |
| 1:AA:982:U:H4' | 1:AA:983:A:O5' | 1.94 | 0.68 |
| 8:AH:8:ASP:O | 8:AH:12:ARG:HG3 | 1.94 | 0.68 |
| 10:AJ:54:PHE:O | 10:AJ:56:HIS:N | 2.27 | 0.68 |
| 22:AW:18:G:H1' | 22:AW:57:G:O6 | 1.94 | 0.68 |
| 25:AZ:124:ARG:HB2 | 25:AZ:163:PHE:CE2 | 2.28 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B1:89:GLU:HA | 27:B1:92:LYS:CE | 2.23 | 0.68 |
| 36:BA:628:G:H2' | 36:BA:629:G:H5'' | 1.76 | 0.68 |
| 37:BB:50:G:OP1 | 51:BS:63:THR:HG23 | 1.94 | 0.68 |
| 39:BD:248:SER:HB2 | 39:BD:249:PRO:HD2 | 1.76 | 0.68 |
| 40:BE:167:VAL:O | 40:BE:167:VAL:HG13 | 1.92 | 0.68 |
| 42:BG:42:GLY:HA2 | 42:BG:90:LEU:H | 1.58 | 0.68 |
| 43:BH:76:VAL:C | 43:BH:78:GLY:H | 1.97 | 0.68 |
| 36:BA:2394:C:OP1 | 48:BP:63:PRO:HD2 | 1.94 | 0.68 |
| 51:BS:61:ASN:O | 51:BS:62:LYS:HB2 | 1.93 | 0.68 |
| 54:BV:81:TYR:HE2 | 54:BV:83:ARG:HE | 1.39 | 0.68 |
| 57:BY:67:LEU:HD21 | 57:BY:71:LYS:HE2 | 1.74 | 0.68 |
| 58:BZ:35:ARG:NE | 58:BZ:35:ARG:HA | 2.08 | 0.68 |
| 1:AA:1296:C:H4' | 1:AA:1302:U:C5 | 2.29 | 0.68 |
| 5:AE:145:LYS:O | 5:AE:149:GLU:HG2 | 1.93 | 0.68 |
| 9:AI:24:GLY:HA2 | 9:AI:59:PHE:O | 1.93 | 0.68 |
| 10:AJ:75:ILE:HG13 | 10:AJ:76:ASN:N | 2.08 | 0.68 |
| 18:AR:73:ALA:CB | 18:AR:79:LEU:HD12 | 2.23 | 0.68 |
| 19:AS:10:PHE:HE1 | 19:AS:70:LYS:HD2 | 1.58 | 0.68 |
| 20:AT:25:ARG:HH11 | 20:AT:25:ARG:HG3 | 1.58 | 0.68 |
| 24:AY:27:C:H2' | 24:AY:28:C:H6 | 1.59 | 0.68 |
| 32:B6:11:LEU:HD21 | 32:B6:51:GLU:CG | 2.24 | 0.68 |
| 35:B9:31:LYS:HE2 | 36:BA:2478:A:H5' | 1.76 | 0.68 |
| 36:BA:1067:A:H3' | 36:BA:1068:G:C5' | 2.23 | 0.68 |
| 36:BA:1161:C:H2' | 36:BA:1162:G:C8 | 2.27 | 0.68 |
| 36:BA:1540:U:H3' | 36:BA:1541:G:H3' | 1.75 | 0.68 |
| 36:BA:2137:C:H42 | 36:BA:2154:G:H22 | 1.41 | 0.68 |
| 36:BA:2662:A:H2' | 36:BA:2663:G:O4' | 1.92 | 0.68 |
| 39:BD:247:ALA:HA | 39:BD:254:THR:HG22 | 1.75 | 0.68 |
| 47:BO:107:ARG:HH21 | 47:BO:115:VAL:HG11 | 1.58 | 0.68 |
| 48:BP:112:LEU:H | 48:BP:128:HIS:CD2 | 2.09 | 0.68 |
| 53:BU:36:ARG:HG2 | 53:BU:40:PHE:CE1 | 2.28 | 0.68 |
| 58:BZ:71:VAL:HG11 | 58:BZ:74:VAL:HG23 | 1.75 | 0.68 |
| 1:AA:1004:A:H5'' | 1:AA:1025:U:C4 | 2.29 | 0.68 |
| 1:AA:918:A:H2' | 1:AA:919:A:C8 | 2.29 | 0.68 |
| 21:AU:12:LYS:HG2 | 21:AU:22:ARG:CB | 2.24 | 0.68 |
| 26:B0:36:ILE:HD11 | 36:BA:2355:C:C1' | 2.23 | 0.68 |
| 27:B1:53:VAL:HG22 | 27:B1:74:VAL:HG13 | 1.75 | 0.68 |
| 36:BA:2728:U:O2' | 36:BA:2729:G:H5' | 1.91 | 0.68 |
| 43:BH:157:TYR:O | 43:BH:158:HIS:HB2 | 1.93 | 0.68 |
| 48:BP:146:VAL:HG22 | 48:BP:147:LEU:N | 2.08 | 0.68 |
| 50:BR:55:ALA:HA | 50:BR:80:PHE:HE1 | 1.53 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:128:VAL:HG22 | 58:BZ:129:SER:N | 2.09 | 0.68 |
| 7:AG:129:GLU:OE1 | 7:AG:131:LYS:HE2 | 1.93 | 0.68 |
| 24:AY:75:C:N4 | 25:AZ:232:THR:HG1 | 1.91 | 0.68 |
| 30:B4:40:HIS:CD2 | 30:B4:41:PRO:HA | 2.29 | 0.68 |
| 30:B4:8:LYS:O | 30:B4:9:LEU:HB2 | 1.93 | 0.68 |
| 31:B5:40:LYS:HZ1 | 31:B5:46:CYS:H | 1.37 | 0.68 |
| 36:BA:1230:C:H2' | 36:BA:1231:G:H8 | 1.58 | 0.68 |
| 36:BA:1497:U:H2' | 36:BA:1497:U:O2 | 1.92 | 0.68 |
| 36:BA:2163:C:H2' | 36:BA:2164:C:O4' | 1.94 | 0.68 |
| 36:BA:2554:U:H2' | 36:BA:2555:U:C6 | 2.29 | 0.68 |
| 36:BA:2723:C:H4' | 50:BR:2:ARG:HE | 1.57 | 0.68 |
| 36:BA:472:A:H2' | 36:BA:473:G:H5' | 1.75 | 0.68 |
| 42:BG:113:ARG:HA | 42:BG:113:ARG:NE | 2.09 | 0.68 |
| 52:BT:28:VAL:CG2 | 52:BT:46:GLU:HA | 2.24 | 0.68 |
| 53:BU:90:VAL:HG12 | 53:BU:91:ASP:H | 1.58 | 0.68 |
| 1:AA:1060:C:C5 | 3:AC:2:GLY:HA3 | 2.29 | 0.67 |
| 1:AA:158:G:H2' | 1:AA:159:G:H8 | 1.58 | 0.67 |
| 1:AA:650:G:O2' | 1:AA:651:C:H5' | 1.93 | 0.67 |
| 24:AY:75:C:H1' | 25:AZ:231:ILE:HD12 | 1.74 | 0.67 |
| 25:AZ:28:THR:HG23 | 25:AZ:79:HIS:ND1 | 2.09 | 0.67 |
| 25:AZ:363:MET:HB3 | 25:AZ:364:PRO:HD2 | 1.75 | 0.67 |
| 36:BA:1859:A:N6 | 36:BA:1883:G:H1' | 2.10 | 0.67 |
| 36:BA:2377:A:H2' | 36:BA:2378:A:C8 | 2.29 | 0.67 |
| 38:BC:6:ARG:HH11 | 38:BC:34:THR:HB | 1.57 | 0.67 |
| 42:BG:60:LEU:CD2 | 42:BG:63:ILE:HD11 | 2.17 | 0.67 |
| 49:BQ:60:ARG:HB3 | 49:BQ:60:ARG:NH1 | 2.08 | 0.67 |
| 52:BT:29:ARG:HB3 | 52:BT:85:LYS:HA | 1.75 | 0.67 |
| 56:BX:47:PHE:O | 56:BX:49:VAL:N | 2.25 | 0.67 |
| 57:BY:54:LYS:HE3 | 57:BY:55:TYR:CE1 | 2.30 | 0.67 |
| 1:AA:1008:C:H42 | 1:AA:1021:G:H1 | 1.41 | 0.67 |
| 1:AA:108:G:H5' | 1:AA:109:A:C5' | 2.23 | 0.67 |
| 4:AD:39:PRO:HD2 | 4:AD:44:GLY:O | 1.94 | 0.67 |
| 10:AJ:7:LYS:HB2 | 10:AJ:97:GLU:HB2 | 1.75 | 0.67 |
| 12:AL:6:THR:H | 12:AL:9:GLN:HE21 | 1.41 | 0.67 |
| 15:AO:70:LEU:HD23 | 15:AO:78:TYR:HA | 1.74 | 0.67 |
| 28:B2:51:ARG:HD3 | 28:B2:55:ARG:NH2 | 2.08 | 0.67 |
| 36:BA:1058:G:H2' | 36:BA:1059:G:C5' | 2.19 | 0.67 |
| 36:BA:1385:G:H4' | 36:BA:1386:C:OP1 | 1.93 | 0.67 |
| 36:BA:2672:G:C3' | 36:BA:2673:G:H5'' | 2.23 | 0.67 |
| 36:BA:287:C:H2' | 36:BA:288:C:C6 | 2.29 | 0.67 |
| 36:BA:590:A:H2' | 36:BA:591:C:C6 | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BF:34:TRP:HB2 | 48:BP:10:PRO:HB2 | 1.75 | 0.67 |
| 43:BH:167:GLU:CG | 43:BH:168:PRO:HD2 | 2.21 | 0.67 |
| 48:BP:23:PRO:CD | 48:BP:33:ARG:HE | 2.06 | 0.67 |
| 48:BP:31:ALA:O | 48:BP:33:ARG:N | 2.28 | 0.67 |
| 52:BT:51:ARG:HB2 | 52:BT:98:LYS:HG3 | 1.76 | 0.67 |
| 57:BY:13:VAL:HG11 | 57:BY:28:LYS:HZ3 | 1.59 | 0.67 |
| 3:AC:80:GLY:O | 3:AC:82:GLU:N | 2.27 | 0.67 |
| 10:AJ:90:LEU:N | 10:AJ:91:PRO:CD | 2.57 | 0.67 |
| 36:BA:1469:A:H2' | 36:BA:1470:G:O4' | 1.94 | 0.67 |
| 36:BA:1598:C:H5' | 56:BX:36:LYS:CG | 2.23 | 0.67 |
| 38:BC:47:LEU:HD11 | 38:BC:171:ILE:HB | 1.73 | 0.67 |
| 40:BE:179:GLU:O | 40:BE:179:GLU:HG3 | 1.94 | 0.67 |
| 52:BT:109:GLU:HG2 | 52:BT:112:ARG:CZ | 2.23 | 0.67 |
| 55:BW:14:PRO:HG3 | 55:BW:101:SER:CB | 2.20 | 0.67 |
| 55:BW:95:ILE:HG13 | 55:BW:95:ILE:O | 1.93 | 0.67 |
| 57:BY:31:LEU:HB2 | 57:BY:32:PRO:CA | 2.22 | 0.67 |
| 1:AA:1330:U:H5' | 1:AA:1331:G:OP2 | 1.95 | 0.67 |
| 1:AA:818:G:O2' | 1:AA:819:A:H5' | 1.94 | 0.67 |
| 2:AB:172:ILE:N | 2:AB:172:ILE:HD12 | 2.08 | 0.67 |
| 13:AM:23:TYR:HB3 | 13:AM:67:GLU:CB | 2.24 | 0.67 |
| 19:AS:44:MET:HA | 19:AS:47:HIS:HD2 | 1.57 | 0.67 |
| 1:AA:191:G:C4 | 20:AT:105:SER:HB3 | 2.30 | 0.67 |
| 26:B0:53:MET:HA | 26:B0:58:THR:O | 1.95 | 0.67 |
| 29:B3:8:LEU:CD2 | 29:B3:31:LEU:HG | 2.24 | 0.67 |
| 36:BA:1268:A:H2' | 36:BA:1269:A:O4' | 1.93 | 0.67 |
| 36:BA:2469:A:O2' | 49:BQ:56:ARG:HD2 | 1.94 | 0.67 |
| 36:BA:851:U:H3 | 36:BA:926:A:H61 | 1.42 | 0.67 |
| 53:BU:91:ASP:OD1 | 53:BU:96:ALA:HB2 | 1.95 | 0.67 |
| 53:BU:95:LEU:HD12 | 54:BV:11:GLN:HE21 | 1.59 | 0.67 |
| 57:BY:28:LYS:HA | 57:BY:38:ILE:HG22 | 1.75 | 0.67 |
| 1:AA:1234:C:O2' | 1:AA:1235:U:H5' | 1.95 | 0.67 |
| 1:AA:424:G:O2' | 1:AA:425:G:H5' | 1.94 | 0.67 |
| 2:AB:102:LEU:HD23 | 2:AB:182:ILE:HD12 | 1.76 | 0.67 |
| 2:AB:22:LYS:CA | 2:AB:22:LYS:HE2 | 2.25 | 0.67 |
| 1:AA:407:G:O2' | 4:AD:116:GLN:HG3 | 1.93 | 0.67 |
| 7:AG:115:ARG:O | 7:AG:118:VAL:HG22 | 1.95 | 0.67 |
| 25:AZ:185:ASN:HD21 | 25:AZ:188:THR:CB | 2.07 | 0.67 |
| 36:BA:2012:G:H4' | 55:BW:96:ILE:HD11 | 1.76 | 0.67 |
| 36:BA:2050:C:H1' | 40:BE:156:MET:CE | 2.25 | 0.67 |
| 36:BA:2147:G:H2' | 36:BA:2148:G:H5' | 1.77 | 0.67 |
| 36:BA:2716:U:O2' | 36:BA:2717:G:H5' | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:611:C:H2' | 36:BA:612:C:C6 | 2.30 | 0.67 |
| 53:BU:85:LYS:HD3 | 53:BU:117:GLN:HE22 | 1.58 | 0.67 |
| 54:BV:35:LEU:O | 54:BV:37:VAL:N | 2.28 | 0.67 |
| 55:BW:8:ARG:CA | 55:BW:102:HIS:HB3 | 2.12 | 0.67 |
| 1:AA:8:A:N6 | 4:AD:209:ARG:H | 1.93 | 0.67 |
| 5:AE:12:LEU:CD2 | 5:AE:13:ILE:N | 2.58 | 0.67 |
| 10:AJ:78:ASN:HD22 | 10:AJ:80:LYS:HB3 | 1.59 | 0.67 |
| 13:AM:116:THR:O | 13:AM:117:VAL:C | 2.31 | 0.67 |
| 18:AR:29:PHE:CE1 | 18:AR:31:LEU:HB3 | 2.30 | 0.67 |
| 36:BA:1681:G:O2' | 36:BA:1762:A:H2' | 1.95 | 0.67 |
| 36:BA:287:C:H42 | 36:BA:354:G:H1 | 1.43 | 0.67 |
| 36:BA:611:C:H2' | 36:BA:612:C:H6 | 1.58 | 0.67 |
| 42:BG:43:LEU:HB3 | 42:BG:45:GLU:HG2 | 1.77 | 0.67 |
| 42:BG:9:ARG:O | 42:BG:13:GLU:HG2 | 1.95 | 0.67 |
| 58:BZ:100:VAL:CG2 | 58:BZ:126:VAL:HG21 | 2.25 | 0.67 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:H8 | 1.59 | 0.67 |
| 1:AA:1368:G:OP2 | 9:AI:112:LYS:HD3 | 1.95 | 0.67 |
| 1:AA:393:A:O2' | 1:AA:394:G:H5' | 1.95 | 0.67 |
| 6:AF:8:ILE:HD12 | 6:AF:26:ILE:HD13 | 1.76 | 0.67 |
| 7:AG:14:PRO:HA | 7:AG:21:VAL:HG12 | 1.77 | 0.67 |
| 8:AH:125:ARG:HG3 | 8:AH:125:ARG:HH11 | 1.58 | 0.67 |
| 13:AM:11:ARG:HG2 | 13:AM:12:ASN:H | 1.59 | 0.67 |
| 22:AW:38:A:C2' | 22:AW:39:U:H5'' | 2.24 | 0.67 |
| 25:AZ:299:GLU:O | 25:AZ:302:GLN:HG2 | 1.94 | 0.67 |
| 25:AZ:371:THR:HG22 | 25:AZ:372:VAL:H | 1.59 | 0.67 |
| 29:B3:31:LEU:O | 29:B3:32:GLN:HB2 | 1.95 | 0.67 |
| 38:BC:68:LEU:O | 38:BC:177:LYS:HG2 | 1.94 | 0.67 |
| 39:BD:139:GLY:H | 39:BD:165:ILE:HB | 1.59 | 0.67 |
| 41:BF:22:ALA:O | 41:BF:26:ALA:HB2 | 1.95 | 0.67 |
| 3:AC:60:ALA:HB3 | 3:AC:63:ASN:HD21 | 1.59 | 0.67 |
| 20:AT:50:GLU:HB2 | 20:AT:100:ILE:HD13 | 1.77 | 0.67 |
| 25:AZ:241:ARG:HH11 | 25:AZ:241:ARG:HB3 | 1.59 | 0.67 |
| 27:B1:41:ARG:HH12 | 36:BA:1365:A:H5'' | 1.60 | 0.67 |
| 36:BA:2656:U:H2' | 36:BA:2657:A:H5'' | 1.76 | 0.67 |
| 38:BC:68:LEU:CD2 | 38:BC:176:GLY:HA2 | 2.24 | 0.67 |
| 48:BP:126:VAL:HG22 | 48:BP:145:PRO:CB | 2.24 | 0.67 |
| 48:BP:20:GLY:O | 48:BP:21:ARG:HB2 | 1.95 | 0.67 |
| 48:BP:77:ARG:HH11 | 48:BP:77:ARG:HG2 | 1.60 | 0.67 |
| 51:BS:66:ALA:O | 51:BS:70:GLY:N | 2.27 | 0.67 |
| 54:BV:52:VAL:CG1 | 54:BV:55:ALA:HB3 | 2.21 | 0.67 |
| 58:BZ:108:PRO:HA | 58:BZ:141:VAL:HG11 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:204:ASN:ND2 | 2:AB:204:ASN:C | 2.44 | 0.67 |
| 15:AO:43:LEU:HD11 | 15:AO:53:HIS:HA | 1.77 | 0.67 |
| 1:AA:1305:G:H5'' | 21:AU:4:GLY:C | 2.16 | 0.67 |
| 25:AZ:356:PRO:HG2 | 25:AZ:369:THR:O | 1.95 | 0.67 |
| 36:BA:524:U:H2' | 36:BA:525:U:H6 | 1.60 | 0.67 |
| 38:BC:47:LEU:HB3 | 38:BC:49:ILE:HG13 | 1.76 | 0.67 |
| 36:BA:2511:U:H4' | 40:BE:124:GLY:HA2 | 1.76 | 0.67 |
| 36:BA:797:C:OP2 | 41:BF:62:ARG:HG3 | 1.93 | 0.67 |
| 46:BN:6:PRO:HB3 | 46:BN:41:ASP:OD1 | 1.95 | 0.67 |
| 47:BO:19:ILE:HD12 | 47:BO:41:ALA:CB | 2.25 | 0.67 |
| 48:BP:108:LYS:C | 48:BP:110:TYR:H | 1.99 | 0.67 |
| 52:BT:39:ARG:N | 52:BT:39:ARG:HD2 | 2.07 | 0.67 |
| 1:AA:1170:A:H2' | 1:AA:1171:G:O4' | 1.95 | 0.67 |
| 1:AA:429:U:H1' | 1:AA:430:A:H5'' | 1.76 | 0.67 |
| 2:AB:204:ASN:ND2 | 2:AB:205:ASP:N | 2.43 | 0.67 |
| 2:AB:222:ILE:O | 2:AB:226:ARG:HB2 | 1.95 | 0.67 |
| 1:AA:1152:A:H5' | 10:AJ:70:ARG:NH2 | 2.09 | 0.67 |
| 26:B0:26:TYR:HE2 | 36:BA:857:C:H1' | 1.60 | 0.67 |
| 36:BA:18:C:O3' | 53:BU:23:GLY:HA2 | 1.95 | 0.67 |
| 39:BD:131:LEU:HB2 | 39:BD:136:ILE:HD11 | 1.76 | 0.67 |
| 41:BF:188:ARG:HA | 48:BP:7:ARG:CD | 2.21 | 0.67 |
| 41:BF:154:VAL:HG11 | 41:BF:193:VAL:HG23 | 1.77 | 0.67 |
| 42:BG:115:ARG:NH1 | 42:BG:137:GLU:HG3 | 2.10 | 0.67 |
| 43:BH:85:LYS:HZ3 | 43:BH:133:VAL:H | 1.41 | 0.67 |
| 48:BP:111:ARG:HA | 48:BP:128:HIS:CD2 | 2.30 | 0.67 |
| 53:BU:66:ASN:ND2 | 53:BU:76:TYR:H | 1.93 | 0.67 |
| 54:BV:88:ARG:O | 54:BV:90:PRO:HD3 | 1.95 | 0.67 |
| 58:BZ:155:LEU:HD23 | 58:BZ:155:LEU:N | 2.10 | 0.67 |
| 1:AA:980:C:H6 | 1:AA:980:C:C5' | 2.04 | 0.66 |
| 10:AJ:54:PHE:CE1 | 10:AJ:55:LYS:NZ | 2.63 | 0.66 |
| 24:AY:8:4SU:H5'' | 24:AY:8:4SU:H6 | 1.77 | 0.66 |
| 25:AZ:318:ALA:HB2 | 25:AZ:400:VAL:HA | 1.76 | 0.66 |
| 36:BA:1907:G:O2' | 36:BA:1908:C:H5' | 1.95 | 0.66 |
| 36:BA:2114:A:H2' | 36:BA:2115:G:H5' | 1.75 | 0.66 |
| 22:AW:19:G:C4 | 36:BA:2169:A:H1' | 2.30 | 0.66 |
| 36:BA:2688:U:H1' | 36:BA:2721:A:N6 | 2.10 | 0.66 |
| 36:BA:2842:G:O2' | 36:BA:2843:G:H5' | 1.95 | 0.66 |
| 38:BC:140:PRO:HA | 38:BC:145:VAL:HB | 1.76 | 0.66 |
| 38:BC:24:GLU:O | 38:BC:28:LEU:HB3 | 1.93 | 0.66 |
| 40:BE:4:ILE:HD12 | 40:BE:92:THR:O | 1.95 | 0.66 |
| 41:BF:10:PRO:HD2 | 41:BF:13:SER:O | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BF:124:LEU:HD12 | 41:BF:125:LEU:H | 1.59 | 0.66 |
| 49:BQ:131:ILE:HD12 | 49:BQ:131:ILE:H | 1.60 | 0.66 |
| 52:BT:27:THR:CG2 | 52:BT:49:VAL:HB | 2.25 | 0.66 |
| 3:AC:20:SER:HB2 | 3:AC:40:ARG:NH2 | 2.09 | 0.66 |
| 4:AD:31:CYS:SG | 60:AD:301:ZN:ZN | 1.82 | 0.66 |
| 12:AL:67:THR:HG21 | 12:AL:96:VAL:HG22 | 1.76 | 0.66 |
| 13:AM:88:ARG:HG3 | 13:AM:98:VAL:CG1 | 2.26 | 0.66 |
| 25:AZ:185:ASN:HD21 | 25:AZ:188:THR:HB | 1.60 | 0.66 |
| 27:B1:89:GLU:HG2 | 27:B1:92:LYS:NZ | 2.09 | 0.66 |
| 36:BA:2125:G:H21 | 36:BA:2173:A:N6 | 1.91 | 0.66 |
| 36:BA:2186:G:H2' | 36:BA:2187:G:C8 | 2.30 | 0.66 |
| 36:BA:812:C:H2' | 36:BA:813:U:H6 | 1.59 | 0.66 |
| 36:BA:607:U:OP1 | 41:BF:102:PRO:HA | 1.95 | 0.66 |
| 41:BF:17:ARG:HH11 | 41:BF:17:ARG:HG3 | 1.60 | 0.66 |
| 49:BQ:134:ARG:HA | 49:BQ:137:TYR:CD2 | 2.30 | 0.66 |
| 53:BU:6:THR:O | 53:BU:9:VAL:HG22 | 1.95 | 0.66 |
| 58:BZ:162:GLU:O | 58:BZ:163:LEU:HD23 | 1.96 | 0.66 |
| 1:AA:1529:G:H4' | 1:AA:1530:G:OP2 | 1.94 | 0.66 |
| 9:AI:53:VAL:HG11 | 9:AI:92:TYR:CD2 | 2.31 | 0.66 |
| 36:BA:1539:G:H2' | 36:BA:1540:U:O4' | 1.96 | 0.66 |
| 36:BA:2284:C:H2' | 36:BA:2285:C:H6 | 1.60 | 0.66 |
| 36:BA:833:U:H5'' | 48:BP:48:PRO:HB3 | 1.75 | 0.66 |
| 38:BC:6:ARG:NH1 | 38:BC:34:THR:HB | 2.11 | 0.66 |
| 46:BN:94:HIS:HB3 | 46:BN:97:ARG:HG3 | 1.78 | 0.66 |
| 50:BR:21:TYR:N | 50:BR:21:TYR:CD1 | 2.59 | 0.66 |
| 54:BV:16:PRO:O | 54:BV:96:ILE:HB | 1.95 | 0.66 |
| 57:BY:35:TYR:HD2 | 57:BY:68:HIS:HE1 | 1.42 | 0.66 |
| 1:AA:1321:C:O2' | 19:AS:77:THR:HG21 | 1.94 | 0.66 |
| 1:AA:723:U:H2' | 1:AA:723:U:O2 | 1.95 | 0.66 |
| 1:AA:979:C:H3' | 1:AA:980:C:H5'' | 1.77 | 0.66 |
| 2:AB:32:ILE:HD11 | 2:AB:40:HIS:CG | 2.30 | 0.66 |
| 3:AC:138:VAL:HG23 | 3:AC:149:ALA:HB3 | 1.77 | 0.66 |
| 14:AN:6:LEU:HB3 | 14:AN:23:ARG:HH22 | 1.60 | 0.66 |
| 15:AO:74:ASP:OD1 | 15:AO:77:ARG:HG2 | 1.95 | 0.66 |
| 25:AZ:143:ASP:HB3 | 25:AZ:146:LEU:CB | 2.22 | 0.66 |
| 25:AZ:371:THR:HG22 | 25:AZ:372:VAL:N | 2.10 | 0.66 |
| 26:B0:50:ASN:HD22 | 26:B0:63:VAL:HG21 | 1.61 | 0.66 |
| 36:BA:1494:A:N3 | 36:BA:1494:A:H3' | 2.10 | 0.66 |
| 36:BA:2293:C:H5'' | 51:BS:92:TYR:OH | 1.94 | 0.66 |
| 36:BA:648:G:H4' | 36:BA:2351:G:H5'' | 1.77 | 0.66 |
| 36:BA:654(U):A:O2' | 36:BA:654(V):A:H5' | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BE:111:ARG:HD3 | 40:BE:160:TYR:CE1 | 2.31 | 0.66 |
| 41:BF:175:THR:O | 41:BF:176:LEU:HD12 | 1.94 | 0.66 |
| 47:BO:97:ARG:NH2 | 47:BO:99:PHE:HE1 | 1.93 | 0.66 |
| 48:BP:7:ARG:HB3 | 48:BP:8:PRO:HD3 | 1.77 | 0.66 |
| 51:BS:24:LEU:CD1 | 51:BS:41:ASP:HB2 | 2.26 | 0.66 |
| 58:BZ:19:ARG:NH1 | 58:BZ:84:GLU:HA | 2.11 | 0.66 |
| 3:AC:8:ILE:HG12 | 3:AC:16:ARG:HG2 | 1.77 | 0.66 |
| 6:AF:3:ARG:HH11 | 6:AF:3:ARG:HG3 | 1.60 | 0.66 |
| 17:AQ:67:LYS:HA | 17:AQ:70:ARG:NH1 | 2.10 | 0.66 |
| 31:B5:16:ARG:HD2 | 31:B5:20:ARG:CZ | 2.26 | 0.66 |
| 32:B6:8:LYS:HG3 | 32:B6:25:LYS:HD3 | 1.78 | 0.66 |
| 36:BA:2249:U:H4' | 36:BA:2275:C:H5 | 1.60 | 0.66 |
| 36:BA:2370:G:H2' | 36:BA:2371:G:H8 | 1.58 | 0.66 |
| 43:BH:17:VAL:HG12 | 43:BH:18:GLU:N | 2.10 | 0.66 |
| 58:BZ:48:PHE:CD2 | 58:BZ:52:SER:HA | 2.31 | 0.66 |
| 3:AC:114:PRO:O | 3:AC:118:GLN:HG3 | 1.96 | 0.66 |
| 8:AH:101:PRO:C | 8:AH:102:ARG:HD3 | 2.15 | 0.66 |
| 8:AH:2:LEU:HD21 | 8:AH:8:ASP:HB2 | 1.76 | 0.66 |
| 9:AI:114:TYR:HE1 | 10:AJ:60:ARG:N | 1.90 | 0.66 |
| 9:AI:93:ARG:C | 9:AI:95:LYS:H | 1.99 | 0.66 |
| 34:B8:47:LYS:HZ2 | 34:B8:47:LYS:HB2 | 1.61 | 0.66 |
| 36:BA:1678:G:N2 | 36:BA:1989:G:N2 | 2.43 | 0.66 |
| 36:BA:2729:G:H1' | 40:BE:187:ALA:CB | 2.24 | 0.66 |
| 41:BF:5:ALA:H | 41:BF:19:GLU:HB3 | 1.61 | 0.66 |
| 41:BF:51:THR:HB | 41:BF:88:VAL:HG11 | 1.76 | 0.66 |
| 42:BG:52:ILE:HB | 42:BG:54:GLU:OE1 | 1.95 | 0.66 |
| 48:BP:111:ARG:HE | 48:BP:149:GLU:HG3 | 1.60 | 0.66 |
| 53:BU:52:ARG:NH1 | 53:BU:52:ARG:HB3 | 2.10 | 0.66 |
| 1:AA:1030(D):A:H2' | 1:AA:1031:G:H5' | 1.77 | 0.66 |
| 2:AB:19:HIS:O | 2:AB:39:ILE:HG23 | 1.95 | 0.66 |
| 35:B9:29:ASN:O | 35:B9:29:ASN:ND2 | 2.28 | 0.66 |
| 36:BA:2183:C:H2' | 36:BA:2184:G:H8 | 1.61 | 0.66 |
| 38:BC:45:ALA:O | 38:BC:47:LEU:HD12 | 1.96 | 0.66 |
| 41:BF:114:VAL:HG21 | 41:BF:202:PHE:CE1 | 2.30 | 0.66 |
| 48:BP:66:GLY:O | 48:BP:67:MET:CB | 2.44 | 0.66 |
| 50:BR:52:ILE:CD1 | 50:BR:79:LEU:HD21 | 2.26 | 0.66 |
| 52:BT:32:TYR:HB3 | 52:BT:81:PRO:HB3 | 1.78 | 0.66 |
| 53:BU:88:ILE:HB | 53:BU:90:VAL:HG23 | 1.78 | 0.66 |
| 56:BX:35:THR:HG22 | 56:BX:38:GLU:H | 1.60 | 0.66 |
| 57:BY:17:SER:HB2 | 57:BY:71:LYS:CE | 2.23 | 0.66 |
| 1:AA:1499:A:H1' | 1:AA:1520:G:H5' | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:991:U:O2 | 1:AA:991:U:H2' | 1.96 | 0.66 |
| 32:B6:19:ARG:CG | 32:B6:20:ASN:H | 1.96 | 0.66 |
| 36:BA:2476:A:C2 | 36:BA:2477:C:C5 | 2.81 | 0.66 |
| 37:BB:52:A:O2' | 37:BB:53:A:C8 | 2.49 | 0.66 |
| 38:BC:66:HIS:NE2 | 38:BC:184:LYS:HD3 | 2.11 | 0.66 |
| 46:BN:15:LEU:O | 46:BN:136:GLU:HA | 1.95 | 0.66 |
| 36:BA:1131:G:H21 | 46:BN:73:THR:HG21 | 1.60 | 0.66 |
| 53:BU:66:ASN:HD21 | 53:BU:76:TYR:H | 1.44 | 0.66 |
| 56:BX:35:THR:HG22 | 56:BX:37:THR:N | 2.11 | 0.66 |
| 2:AB:235:SER:HG | 2:AB:236:TYR:HD1 | 1.42 | 0.66 |
| 13:AM:97:PRO:HA | 13:AM:110:ARG:CD | 2.23 | 0.66 |
| 24:AY:20:H2U:H4' | 24:AY:21:A:H5'' | 1.77 | 0.66 |
| 25:AZ:159:ASN:HD21 | 25:AZ:166:ASP:N | 1.94 | 0.66 |
| 28:B2:11:GLU:O | 28:B2:15:LYS:HG2 | 1.96 | 0.66 |
| 36:BA:1362:C:O2' | 36:BA:1363:C:H5' | 1.96 | 0.66 |
| 36:BA:2193:G:H2' | 36:BA:2194:G:O4' | 1.95 | 0.66 |
| 37:BB:3:C:H42 | 37:BB:118:G:H1 | 1.44 | 0.66 |
| 39:BD:226:MET:HB3 | 39:BD:230:ASP:HB2 | 1.77 | 0.66 |
| 41:BF:125:LEU:HD23 | 41:BF:125:LEU:N | 2.11 | 0.66 |
| 36:BA:660:G:H5' | 41:BF:99:TYR:CE2 | 2.31 | 0.66 |
| 48:BP:83:VAL:CG1 | 48:BP:112:LEU:HD21 | 2.25 | 0.66 |
| 48:BP:16:ARG:CD | 48:BP:18:ARG:H | 2.07 | 0.66 |
| 47:BO:104:ARG:HE | 52:BT:33:LYS:HE3 | 1.61 | 0.66 |
| 53:BU:21:ALA:HB1 | 53:BU:24:TYR:CD1 | 2.30 | 0.66 |
| 54:BV:99:ILE:HD13 | 54:BV:99:ILE:N | 2.11 | 0.66 |
| 1:AA:1264:C:H2' | 1:AA:1265:G:C8 | 2.31 | 0.66 |
| 2:AB:9:GLU:N | 2:AB:9:GLU:OE2 | 2.29 | 0.66 |
| 4:AD:117:ALA:O | 4:AD:121:VAL:HG23 | 1.96 | 0.66 |
| 16:AP:67:THR:H | 16:AP:70:ALA:HB3 | 1.60 | 0.66 |
| 29:B3:35:ARG:NH1 | 29:B3:35:ARG:HB2 | 2.04 | 0.66 |
| 34:B8:33:ASN:CG | 34:B8:34:TRP:N | 2.50 | 0.66 |
| 36:BA:2248:C:C2' | 36:BA:2249:U:H5' | 2.25 | 0.66 |
| 36:BA:2416:C:H2' | 36:BA:2417:C:C6 | 2.31 | 0.66 |
| 36:BA:2476:A:H2 | 36:BA:2477:C:C6 | 2.13 | 0.66 |
| 36:BA:404:C:C4' | 36:BA:405:U:H5' | 2.26 | 0.66 |
| 36:BA:886:C:H2' | 36:BA:887:A:O4' | 1.95 | 0.66 |
| 41:BF:102:PRO:O | 41:BF:106:ARG:HG3 | 1.96 | 0.66 |
| 41:BF:114:VAL:HG21 | 41:BF:202:PHE:HE1 | 1.60 | 0.66 |
| 46:BN:65:LYS:HB3 | 46:BN:65:LYS:NZ | 2.11 | 0.66 |
| 53:BU:92:ARG:NH2 | 54:BV:10:LYS:HA | 2.10 | 0.66 |
| 3:AC:14:ILE:O | 3:AC:15:THR:HB | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:27:LEU:O | 12:AL:29:GLY:N | 2.29 | 0.65 |
| 13:AM:54:VAL:O | 13:AM:58:GLU:HG2 | 1.96 | 0.65 |
| 36:BA:2128:C:O2' | 36:BA:2129:C:H6 | 1.79 | 0.65 |
| 36:BA:2146:C:H4' | 36:BA:2147:G:N7 | 2.11 | 0.65 |
| 36:BA:2866:U:C6 | 36:BA:2868:A:H1' | 2.31 | 0.65 |
| 36:BA:650:C:H3' | 36:BA:651:G:H5'' | 1.78 | 0.65 |
| 38:BC:43:VAL:HG22 | 38:BC:214:VAL:HG22 | 1.77 | 0.65 |
| 51:BS:88:ASP:CG | 51:BS:89:ARG:H | 1.98 | 0.65 |
| 52:BT:3:ARG:HH11 | 52:BT:6:LEU:HD13 | 1.60 | 0.65 |
| 52:BT:89:VAL:CG1 | 52:BT:91:ARG:HG3 | 2.26 | 0.65 |
| 54:BV:18:LEU:HD23 | 54:BV:19:LYS:H | 1.60 | 0.65 |
| 49:BQ:135:ASP:HB2 | 58:BZ:81:ARG:HH22 | 1.60 | 0.65 |
| 1:AA:59:A:H3' | 1:AA:331:G:H22 | 1.60 | 0.65 |
| 6:AF:9:VAL:HB | 6:AF:87:ARG:HB2 | 1.78 | 0.65 |
| 19:AS:29:ARG:O | 19:AS:31:ILE:HG22 | 1.96 | 0.65 |
| 19:AS:53:ASN:OD1 | 19:AS:55:LYS:HB3 | 1.95 | 0.65 |
| 19:AS:40:ILE:HG21 | 19:AS:66:MET:O | 1.95 | 0.65 |
| 20:AT:36:LEU:HD13 | 20:AT:36:LEU:O | 1.97 | 0.65 |
| 21:AU:6:ARG:CD | 21:AU:15:ARG:NH1 | 2.60 | 0.65 |
| 22:AW:43:C:O2 | 22:AW:44:G:H1' | 1.96 | 0.65 |
| 31:B5:25:LEU:HD12 | 55:BW:19:LEU:O | 1.96 | 0.65 |
| 31:B5:3:LYS:HB2 | 36:BA:747:U:C5 | 2.31 | 0.65 |
| 36:BA:1188:U:O2' | 36:BA:1189:A:H5' | 1.96 | 0.65 |
| 36:BA:234:C:H2' | 36:BA:235:U:H6 | 1.59 | 0.65 |
| 36:BA:752:A:O2' | 36:BA:753:C:OP2 | 2.13 | 0.65 |
| 37:BB:20:C:C2' | 37:BB:21:G:H5'' | 2.24 | 0.65 |
| 40:BE:59:VAL:HG22 | 40:BE:63:LEU:HA | 1.76 | 0.65 |
| 43:BH:148:ILE:HG22 | 43:BH:162:ILE:HD11 | 1.78 | 0.65 |
| 54:BV:15:GLU:HB3 | 54:BV:16:PRO:HD2 | 1.79 | 0.65 |
| 1:AA:1265:G:C6 | 1:AA:1266:G:O6 | 2.49 | 0.65 |
| 1:AA:1266:G:N2 | 1:AA:1268:A:H5'' | 2.10 | 0.65 |
| 1:AA:453:A:O2' | 1:AA:454:C:H6 | 1.78 | 0.65 |
| 1:AA:80:G:C2' | 1:AA:81:U:H5' | 2.26 | 0.65 |
| 1:AA:979:C:H3' | 1:AA:980:C:C5' | 2.27 | 0.65 |
| 2:AB:69:LEU:HD22 | 2:AB:91:PRO:HB2 | 1.78 | 0.65 |
| 5:AE:11:ILE:HD11 | 5:AE:33:VAL:HG21 | 1.78 | 0.65 |
| 10:AJ:78:ASN:ND2 | 10:AJ:80:LYS:HB3 | 2.11 | 0.65 |
| 14:AN:50:LYS:HB2 | 14:AN:52:GLN:HG3 | 1.76 | 0.65 |
| 19:AS:51:VAL:HG23 | 19:AS:60:VAL:HG11 | 1.77 | 0.65 |
| 20:AT:89:ARG:HH21 | 20:AT:104:LEU:HD21 | 1.61 | 0.65 |
| 31:B5:39:MET:HG3 | 55:BW:34:ASN:OD1 | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BE:50:GLY:CA | 40:BE:78:LEU:HB3 | 2.23 | 0.65 |
| 41:BF:82:ILE:HG13 | 41:BF:83:PHE:N | 2.11 | 0.65 |
| 46:BN:56:ASN:H | 46:BN:125:GLY:CA | 2.08 | 0.65 |
| 48:BP:16:ARG:CB | 48:BP:16:ARG:HH11 | 2.10 | 0.65 |
| 50:BR:94:TYR:CD2 | 50:BR:94:TYR:N | 2.61 | 0.65 |
| 50:BR:94:TYR:HD2 | 50:BR:94:TYR:N | 1.95 | 0.65 |
| 51:BS:59:LYS:HG2 | 51:BS:60:GLY:H | 1.59 | 0.65 |
| 55:BW:1:MET:HG3 | 55:BW:64:MET:HE2 | 1.77 | 0.65 |
| 1:AA:1030(A):G:H1' | 1:AA:1031:G:H1 | 1.61 | 0.65 |
| 2:AB:10:LEU:O | 2:AB:13:ALA:HB3 | 1.97 | 0.65 |
| 2:AB:189:ASP:OD2 | 2:AB:190:THR:N | 2.28 | 0.65 |
| 25:AZ:145:GLU:O | 25:AZ:145:GLU:HG2 | 1.96 | 0.65 |
| 38:BC:149:ILE:O | 38:BC:153:ILE:HG13 | 1.96 | 0.65 |
| 39:BD:28:GLU:H | 39:BD:29:PRO:CD | 2.06 | 0.65 |
| 39:BD:30:GLU:HG3 | 39:BD:63:ARG:NH2 | 2.10 | 0.65 |
| 41:BF:84:VAL:HG12 | 41:BF:85:GLY:H | 1.60 | 0.65 |
| 48:BP:59:LEU:CA | 48:BP:61:ARG:HE | 2.09 | 0.65 |
| 51:BS:15:ARG:HH11 | 51:BS:15:ARG:CB | 2.09 | 0.65 |
| 51:BS:28:VAL:HG12 | 51:BS:29:PHE:H | 1.60 | 0.65 |
| 36:BA:1252:G:O4' | 53:BU:33:ARG:HD3 | 1.96 | 0.65 |
| 1:AA:1313:U:O4 | 19:AS:4:SER:HB2 | 1.97 | 0.65 |
| 7:AG:145:ALA:O | 7:AG:146:GLU:C | 2.34 | 0.65 |
| 5:AE:148:VAL:CG2 | 8:AH:107:LEU:HD13 | 2.24 | 0.65 |
| 22:AV:47:U:H3' | 22:AV:48:C:C5' | 2.26 | 0.65 |
| 25:AZ:149:LEU:O | 25:AZ:153:GLU:HG2 | 1.97 | 0.65 |
| 25:AZ:368:VAL:CG1 | 25:AZ:369:THR:H | 2.06 | 0.65 |
| 27:B1:48:LYS:NZ | 27:B1:61:ARG:HG2 | 2.11 | 0.65 |
| 30:B4:28:LYS:HE3 | 30:B4:28:LYS:HA | 1.78 | 0.65 |
| 34:B8:14:VAL:HG21 | 34:B8:22:VAL:CG1 | 2.27 | 0.65 |
| 36:BA:2398:U:H5' | 36:BA:2399:G:OP2 | 1.96 | 0.65 |
| 37:BB:105:A:H2' | 37:BB:106:G:O4' | 1.97 | 0.65 |
| 39:BD:30:GLU:CG | 39:BD:63:ARG:HE | 2.09 | 0.65 |
| 40:BE:31:CYS:HB3 | 40:BE:49:LEU:HB3 | 1.77 | 0.65 |
| 42:BG:72:ARG:CZ | 42:BG:86:MET:HA | 2.26 | 0.65 |
| 43:BH:20:ALA:HB1 | 43:BH:21:PRO:HD2 | 1.77 | 0.65 |
| 50:BR:38:VAL:O | 50:BR:41:ALA:HB3 | 1.96 | 0.65 |
| 51:BS:17:ARG:HA | 51:BS:20:ARG:NH1 | 2.12 | 0.65 |
| 57:BY:82:PRO:O | 57:BY:96:ILE:HG22 | 1.96 | 0.65 |
| 1:AA:404:U:H5'' | 4:AD:122:ARG:HD3 | 1.78 | 0.65 |
| 1:AA:573:A:H5' | 1:AA:573:A:C8 | 2.32 | 0.65 |
| 4:AD:148:VAL:HG11 | 4:AD:158:ILE:HG21 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:AF:15:ASP:OD1 | 6:AF:18:GLN:HG3 | 1.96 | 0.65 |
| 10:AJ:32:ALA:CB | 10:AJ:76:ASN:HB2 | 2.27 | 0.65 |
| 11:AK:82:VAL:CG1 | 11:AK:108:ILE:HA | 2.26 | 0.65 |
| 18:AR:37:VAL:HG12 | 18:AR:78:LEU:HB3 | 1.79 | 0.65 |
| 36:BA:1024:G:C3' | 36:BA:1025:G:H5'' | 2.20 | 0.65 |
| 36:BA:304:G:H1 | 36:BA:313:C:N4 | 1.93 | 0.65 |
| 36:BA:709:U:H2' | 36:BA:710:G:C8 | 2.31 | 0.65 |
| 50:BR:12:ARG:HB3 | 50:BR:16:HIS:HD2 | 1.60 | 0.65 |
| 52:BT:129:ARG:CZ | 52:BT:131:ALA:HB3 | 2.26 | 0.65 |
| 2:AB:72:GLY:HA2 | 2:AB:165:VAL:HG22 | 1.78 | 0.65 |
| 2:AB:212:GLN:O | 2:AB:216:SER:HB2 | 1.97 | 0.65 |
| 13:AM:120:LYS:HA | 13:AM:120:LYS:HE3 | 1.79 | 0.65 |
| 22:AW:16:U:H5' | 22:AW:17:C:OP2 | 1.97 | 0.65 |
| 36:BA:1019:U:O2' | 36:BA:1021:A:H2 | 1.79 | 0.65 |
| 36:BA:225:A:O2' | 36:BA:257:A:H4' | 1.97 | 0.65 |
| 36:BA:2667:C:H1' | 43:BH:109:PHE:CD1 | 2.30 | 0.65 |
| 36:BA:266:G:C2' | 36:BA:267:C:H5'' | 2.27 | 0.65 |
| 39:BD:166:GLN:HE21 | 39:BD:166:GLN:HA | 1.60 | 0.65 |
| 39:BD:273:ARG:O | 39:BD:274:ARG:HG3 | 1.97 | 0.65 |
| 43:BH:46:GLU:HB3 | 43:BH:50:VAL:HG22 | 1.77 | 0.65 |
| 1:AA:977:A:N3 | 1:AA:977:A:H2' | 2.11 | 0.65 |
| 9:AI:41:VAL:O | 9:AI:41:VAL:HG12 | 1.97 | 0.65 |
| 13:AM:22:ILE:HG21 | 13:AM:66:LEU:CD2 | 2.27 | 0.65 |
| 20:AT:89:ARG:HD2 | 20:AT:104:LEU:HD11 | 1.78 | 0.65 |
| 22:AV:59:U:O2' | 22:AV:60:U:H6 | 1.72 | 0.65 |
| 36:BA:1042:G:C2 | 36:BA:1043:C:H1' | 2.31 | 0.65 |
| 36:BA:2777:G:H5'' | 36:BA:2778:A:C5' | 2.27 | 0.65 |
| 38:BC:58:VAL:HG22 | 38:BC:201:PRO:CG | 2.27 | 0.65 |
| 41:BF:195:ASP:H | 41:BF:198:ALA:HB3 | 1.61 | 0.65 |
| 42:BG:145:THR:HG22 | 42:BG:147:ASP:H | 1.62 | 0.65 |
| 42:BG:76:SER:CB | 42:BG:83:ARG:HB3 | 2.27 | 0.65 |
| 43:BH:85:LYS:NZ | 43:BH:133:VAL:N | 2.38 | 0.65 |
| 43:BH:51:ARG:HG3 | 43:BH:52:VAL:H | 1.62 | 0.65 |
| 51:BS:57:LYS:O | 51:BS:57:LYS:HD2 | 1.97 | 0.65 |
| 53:BU:3:ARG:HH12 | 53:BU:5:LYS:HB3 | 1.60 | 0.65 |
| 3:AC:5:ILE:N | 3:AC:5:ILE:HD13 | 2.11 | 0.65 |
| 10:AJ:30:SER:HA | 10:AJ:80:LYS:CE | 2.27 | 0.65 |
| 10:AJ:30:SER:HA | 10:AJ:80:LYS:NZ | 2.11 | 0.65 |
| 30:B4:20:ASN:HD22 | 30:B4:21:VAL:N | 1.93 | 0.65 |
| 33:B7:8:ASN:ND2 | 33:B7:11:LYS:H | 1.95 | 0.65 |
| 36:BA:2289:G:H1' | 36:BA:2346:A:H2 | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:629:G:H1' | 36:BA:639:U:O2' | 1.96 | 0.65 |
| 38:BC:41:VAL:HB | 38:BC:175:VAL:HB | 1.79 | 0.65 |
| 40:BE:104:VAL:HG11 | 40:BE:188:VAL:CG2 | 2.27 | 0.65 |
| 43:BH:87:LEU:HD23 | 43:BH:164:TYR:HA | 1.79 | 0.65 |
| 48:BP:16:ARG:HD3 | 48:BP:16:ARG:C | 2.17 | 0.65 |
| 48:BP:39:LYS:HD3 | 48:BP:40:SER:H | 1.61 | 0.65 |
| 49:BQ:78:PRO:O | 49:BQ:81:VAL:HG12 | 1.97 | 0.65 |
| 1:AA:1002:G:H2' | 1:AA:1003:G:C8 | 2.32 | 0.65 |
| 22:AW:30:G:H2' | 22:AW:31:A:C8 | 2.32 | 0.65 |
| 25:AZ:322:VAL:HG13 | 25:AZ:395:VAL:O | 1.97 | 0.65 |
| 27:B1:89:GLU:HG2 | 27:B1:92:LYS:HZ1 | 1.60 | 0.65 |
| 36:BA:1782:C:H1' | 36:BA:2609:U:H5'' | 1.79 | 0.65 |
| 36:BA:2146:C:H4' | 36:BA:2147:G:C8 | 2.32 | 0.65 |
| 36:BA:2199:A:H5' | 36:BA:2200:C:OP2 | 1.97 | 0.65 |
| 36:BA:2760:C:C2' | 36:BA:2761:G:H5'' | 2.27 | 0.65 |
| 22:AW:56:C:C5' | 38:BC:137:LEU:HB2 | 2.27 | 0.65 |
| 46:BN:137:LYS:O | 46:BN:138:LEU:HG | 1.97 | 0.65 |
| 48:BP:83:VAL:O | 48:BP:114:ILE:HD12 | 1.97 | 0.65 |
| 3:AC:14:ILE:HG12 | 3:AC:14:ILE:O | 1.96 | 0.64 |
| 7:AG:20:ASP:HB3 | 7:AG:23:VAL:HG23 | 1.78 | 0.64 |
| 19:AS:19:VAL:HG11 | 19:AS:44:MET:HG3 | 1.77 | 0.64 |
| 25:AZ:129:PRO:O | 25:AZ:130:TYR:HB2 | 1.97 | 0.64 |
| 26:B0:7:LEU:HD22 | 49:BQ:85:LYS:CB | 2.26 | 0.64 |
| 33:B7:9:ARG:NE | 36:BA:1310:G:OP2 | 2.28 | 0.64 |
| 36:BA:20:C:H2' | 36:BA:21:A:H8 | 1.62 | 0.64 |
| 36:BA:2176:A:C2 | 38:BC:172:HIS:CE1 | 2.84 | 0.64 |
| 36:BA:2248:C:H2' | 36:BA:2249:U:H5' | 1.79 | 0.64 |
| 36:BA:2176:A:H2 | 38:BC:172:HIS:NE2 | 1.94 | 0.64 |
| 41:BF:3:GLU:O | 41:BF:19:GLU:HB2 | 1.96 | 0.64 |
| 43:BH:68:THR:C | 43:BH:70:THR:H | 2.00 | 0.64 |
| 46:BN:55:VAL:HG22 | 46:BN:126:PRO:HA | 1.79 | 0.64 |
| 53:BU:52:ARG:HB3 | 53:BU:52:ARG:HH11 | 1.62 | 0.64 |
| 1:AA:194:C:C2' | 1:AA:195:A:H5'' | 2.27 | 0.64 |
| 7:AG:113:GLU:HB2 | 7:AG:119:ARG:HG2 | 1.79 | 0.64 |
| 36:BA:270:A:O2' | 36:BA:271:A:H5' | 1.97 | 0.64 |
| 36:BA:894:C:H2' | 36:BA:895:U:H5' | 1.78 | 0.64 |
| 38:BC:128:GLY:HA2 | 38:BC:137:LEU:HD21 | 1.78 | 0.64 |
| 38:BC:70:LYS:HD2 | 38:BC:177:LYS:NZ | 2.08 | 0.64 |
| 39:BD:118:VAL:HG22 | 39:BD:119:ALA:N | 2.12 | 0.64 |
| 39:BD:130:ALA:C | 39:BD:131:LEU:HD12 | 2.18 | 0.64 |
| 36:BA:784:A:H5'' | 39:BD:227:ASN:CG | 2.18 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BA:1248:G:OP1 | 41:BF:92:PRO:HG3 | 1.96 | 0.64 |
| 46:BN:28:THR:HG23 | 46:BN:29:LYS:H | 1.59 | 0.64 |
| 12:AL:55:VAL:HG21 | 12:AL:67:THR:HG23 | 1.79 | 0.64 |
| 36:BA:1310:G:H2' | 36:BA:1311:G:H5' | 1.79 | 0.64 |
| 47:BO:86:ILE:HG22 | 47:BO:94:ARG:HG3 | 1.78 | 0.64 |
| 49:BQ:75:THR:HG22 | 49:BQ:75:THR:O | 1.97 | 0.64 |
| 51:BS:96:GLY:O | 51:BS:98:VAL:N | 2.24 | 0.64 |
| 58:BZ:37:VAL:HG23 | 58:BZ:38:TYR:N | 2.11 | 0.64 |
| 1:AA:1327:C:H2' | 1:AA:1328:C:H6 | 1.63 | 0.64 |
| 1:AA:943:U:C2' | 1:AA:944:G:H5' | 2.27 | 0.64 |
| 3:AC:11:ARG:O | 3:AC:14:ILE:O | 2.16 | 0.64 |
| 12:AL:32:PHE:HB3 | 12:AL:84:LEU:CD2 | 2.27 | 0.64 |
| 13:AM:15:VAL:HG22 | 13:AM:41:PRO:O | 1.97 | 0.64 |
| 19:AS:44:MET:SD | 19:AS:44:MET:N | 2.70 | 0.64 |
| 36:BA:1697:G:H3' | 36:BA:1698:A:C5' | 2.22 | 0.64 |
| 36:BA:780:G:H21 | 36:BA:783:A:H62 | 1.45 | 0.64 |
| 36:BA:922:U:H2' | 36:BA:923:C:C6 | 2.33 | 0.64 |
| 38:BC:68:LEU:HD23 | 38:BC:176:GLY:CA | 2.23 | 0.64 |
| 39:BD:94:LEU:HB2 | 39:BD:104:TYR:CE2 | 2.31 | 0.64 |
| 41:BF:7:TYR:HD2 | 41:BF:16:GLY:CA | 2.09 | 0.64 |
| 49:BQ:39:PRO:O | 49:BQ:40:ALA:HB2 | 1.97 | 0.64 |
| 1:AA:269:C:H2' | 1:AA:270:A:C8 | 2.32 | 0.64 |
| 1:AA:961:U:O2' | 1:AA:962:C:P | 2.56 | 0.64 |
| 13:AM:27:LYS:HE2 | 13:AM:31:LYS:HE3 | 1.80 | 0.64 |
| 27:B1:72:GLU:O | 27:B1:76:ARG:HG3 | 1.97 | 0.64 |
| 27:B1:84:GLY:O | 27:B1:86:SER:N | 2.29 | 0.64 |
| 36:BA:1386:C:H2' | 36:BA:1387:C:C6 | 2.32 | 0.64 |
| 36:BA:1416:G:HO2' | 36:BA:1417:C:H5 | 1.45 | 0.64 |
| 36:BA:2115:G:H5' | 36:BA:2167:U:O2' | 1.96 | 0.64 |
| 36:BA:2761:G:H2' | 36:BA:2762:G:C5' | 2.25 | 0.64 |
| 36:BA:471:A:H2' | 36:BA:472:A:C5' | 2.28 | 0.64 |
| 36:BA:605:C:O2' | 36:BA:606:U:H5' | 1.97 | 0.64 |
| 36:BA:892:G:H2' | 36:BA:893:C:C5 | 2.33 | 0.64 |
| 36:BA:2124:G:H21 | 38:BC:217:THR:C | 2.00 | 0.64 |
| 39:BD:31:LYS:HE3 | 39:BD:102:LYS:HD3 | 1.79 | 0.64 |
| 46:BN:57:ALA:CB | 46:BN:124:ALA:HA | 2.27 | 0.64 |
| 52:BT:66:VAL:HG12 | 52:BT:71:GLY:CA | 2.27 | 0.64 |
| 57:BY:88:LYS:HZ3 | 57:BY:93:GLY:N | 1.95 | 0.64 |
| 58:BZ:4:ARG:HG2 | 58:BZ:58:VAL:HB | 1.79 | 0.64 |
| 1:AA:108:G:H5' | 1:AA:109:A:H5' | 1.79 | 0.64 |
| 4:AD:124:GLY:O | 4:AD:126:ILE:N | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:AG:15:ASP:OD2 | 7:AG:16:LEU:N | 2.31 | 0.64 |
| 36:BA:1887:C:H3' | 36:BA:1888:G:H5'' | 1.77 | 0.64 |
| 34:B8:30:ARG:NH2 | 36:BA:2419:U:O4 | 2.30 | 0.64 |
| 36:BA:760:G:C2' | 36:BA:761:A:H5' | 2.28 | 0.64 |
| 36:BA:941:A:H4' | 48:BP:35:HIS:CE1 | 2.32 | 0.64 |
| 39:BD:186:HIS:HD2 | 39:BD:188:GLU:HB2 | 1.63 | 0.64 |
| 39:BD:35:LYS:HD2 | 39:BD:36:PRO:CA | 2.28 | 0.64 |
| 43:BH:52:VAL:HG21 | 43:BH:69:ARG:CB | 2.27 | 0.64 |
| 46:BN:115:ARG:HA | 46:BN:118:LYS:HE2 | 1.80 | 0.64 |
| 1:AA:452:A:O2' | 1:AA:453:A:H5' | 1.97 | 0.64 |
| 9:AI:93:ARG:O | 9:AI:95:LYS:N | 2.28 | 0.64 |
| 15:AO:26:GLU:OE1 | 15:AO:81:LEU:HD23 | 1.98 | 0.64 |
| 26:B0:25:ARG:HD2 | 26:B0:29:GLN:NE2 | 2.13 | 0.64 |
| 32:B6:12:GLU:HG3 | 32:B6:23:THR:HG22 | 1.80 | 0.64 |
| 36:BA:1222:C:H2' | 36:BA:1223:G:C5' | 2.21 | 0.64 |
| 36:BA:2066:C:O2' | 36:BA:2067:G:H5' | 1.98 | 0.64 |
| 36:BA:2444:G:OP2 | 41:BF:68:LYS:NZ | 2.29 | 0.64 |
| 36:BA:2465:C:O2' | 36:BA:2466:C:H5' | 1.98 | 0.64 |
| 36:BA:2713:A:H3' | 36:BA:2714:G:C5' | 2.27 | 0.64 |
| 36:BA:298:G:H8 | 36:BA:298:G:OP2 | 1.79 | 0.64 |
| 36:BA:907:U:OP1 | 49:BQ:24:GLY:N | 2.29 | 0.64 |
| 39:BD:76:PRO:HG2 | 39:BD:98:VAL:HG21 | 1.78 | 0.64 |
| 36:BA:2619:C:OP1 | 40:BE:152:LYS:HD3 | 1.98 | 0.64 |
| 43:BH:18:GLU:HB2 | 43:BH:25:LYS:H | 1.62 | 0.64 |
| 51:BS:28:VAL:HG12 | 51:BS:29:PHE:N | 2.12 | 0.64 |
| 51:BS:93:LYS:O | 51:BS:95:HIS:N | 2.31 | 0.64 |
| 52:BT:16:ARG:CB | 52:BT:16:ARG:HH11 | 2.07 | 0.64 |
| 52:BT:55:ASN:ND2 | 52:BT:58:ASN:HD21 | 1.94 | 0.64 |
| 54:BV:38:LEU:O | 54:BV:39:LEU:HD13 | 1.96 | 0.64 |
| 55:BW:76:VAL:HB | 55:BW:103:ILE:HG23 | 1.79 | 0.64 |
| 36:BA:81:G:N2 | 57:BY:2:ARG:HH12 | 1.95 | 0.64 |
| 58:BZ:108:PRO:CA | 58:BZ:141:VAL:HG11 | 2.27 | 0.64 |
| 1:AA:254:G:H21 | 17:AQ:16:GLN:NE2 | 1.96 | 0.64 |
| 1:AA:594:G:C2' | 1:AA:595:G:H5' | 2.27 | 0.64 |
| 2:AB:30:ARG:HG3 | 2:AB:31:TYR:CD2 | 2.33 | 0.64 |
| 4:AD:187:ARG:HH11 | 4:AD:187:ARG:HB3 | 1.62 | 0.64 |
| 8:AH:83:ILE:CD1 | 8:AH:137:VAL:HG22 | 2.28 | 0.64 |
| 25:AZ:355:LEU:CD2 | 25:AZ:359:VAL:HB | 2.26 | 0.64 |
| 26:B0:56:ASP:OD1 | 26:B0:58:THR:OG1 | 2.16 | 0.64 |
| 36:BA:1223:G:H5' | 36:BA:1223:G:H8 | 1.62 | 0.64 |
| 36:BA:587:C:C4 | 48:BP:33:ARG:HG2 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:598:G:H5' | 48:BP:15:ARG:CB | 2.27 | 0.64 |
| 38:BC:163:PHE:HB3 | 38:BC:173:ALA:CB | 2.25 | 0.64 |
| 42:BG:15:VAL:O | 42:BG:19:LEU:HG | 1.98 | 0.64 |
| 51:BS:12:PHE:O | 51:BS:14:VAL:HG23 | 1.97 | 0.64 |
| 51:BS:66:ALA:HA | 51:BS:69:VAL:CG1 | 2.27 | 0.64 |
| 54:BV:38:LEU:O | 54:BV:52:VAL:HG12 | 1.98 | 0.64 |
| 56:BX:27:THR:CG2 | 56:BX:80:ILE:HG22 | 2.27 | 0.64 |
| 4:AD:9:CYS:O | 4:AD:12:CYS:HB2 | 1.98 | 0.64 |
| 7:AG:77:SER:HB2 | 7:AG:84:ASN:HD21 | 1.62 | 0.64 |
| 13:AM:97:PRO:HB2 | 13:AM:101:GLN:NE2 | 2.12 | 0.64 |
| 15:AO:71:GLN:HG2 | 15:AO:71:GLN:O | 1.98 | 0.64 |
| 36:BA:1314:C:C6 | 36:BA:1314:C:H5' | 2.31 | 0.64 |
| 36:BA:1511:C:H2' | 36:BA:1512:U:C6 | 2.27 | 0.64 |
| 36:BA:2053:G:H5' | 40:BE:144:ARG:O | 1.97 | 0.64 |
| 36:BA:936:C:H2' | 36:BA:937:U:H6 | 1.61 | 0.64 |
| 39:BD:239:ARG:NH2 | 39:BD:239:ARG:HG2 | 1.96 | 0.64 |
| 53:BU:8:VAL:HG23 | 53:BU:11:ARG:NH2 | 2.11 | 0.64 |
| 25:AZ:265:THR:HG22 | 25:AZ:291:ARG:HB3 | 1.80 | 0.64 |
| 31:B5:59:GLU:O | 31:B5:59:GLU:HG3 | 1.98 | 0.64 |
| 32:B6:30:THR:O | 32:B6:32:ASN:N | 2.31 | 0.64 |
| 36:BA:1803:A:O2' | 39:BD:259:THR:HG21 | 1.98 | 0.64 |
| 36:BA:259:G:N2 | 36:BA:621:A:H8 | 1.93 | 0.64 |
| 37:BB:30:C:H2' | 37:BB:31:C:O4' | 1.98 | 0.64 |
| 38:BC:120:MET:CE | 38:BC:138:PRO:HB2 | 2.28 | 0.64 |
| 40:BE:113:PHE:HE1 | 40:BE:158:GLY:HA2 | 1.63 | 0.64 |
| 40:BE:199:ARG:HG2 | 40:BE:200:GLU:OE2 | 1.98 | 0.64 |
| 40:BE:199:ARG:NH1 | 40:BE:199:ARG:HB2 | 2.12 | 0.64 |
| 43:BH:12:PRO:HA | 43:BH:48:GLY:CA | 2.26 | 0.64 |
| 46:BN:63:THR:HB | 46:BN:66:LYS:NZ | 2.12 | 0.64 |
| 48:BP:107:LYS:C | 48:BP:109:GLY:H | 1.99 | 0.64 |
| 48:BP:111:ARG:H | 48:BP:111:ARG:HD2 | 1.62 | 0.64 |
| 54:BV:38:LEU:HD12 | 54:BV:57:VAL:HB | 1.80 | 0.64 |
| 1:AA:202:U:H5'' | 1:AA:203:U:OP2 | 1.98 | 0.63 |
| 1:AA:681:C:O2' | 1:AA:682:G:H5' | 1.97 | 0.63 |
| 12:AL:41:ARG:HH12 | 12:AL:57:LYS:NZ | 1.95 | 0.63 |
| 26:B0:42:GLY:HA3 | 36:BA:2331:G:O4' | 1.99 | 0.63 |
| 36:BA:2112:G:H2' | 36:BA:2112:G:N3 | 2.13 | 0.63 |
| 36:BA:2491:U:H5' | 36:BA:2570:G:C5' | 2.20 | 0.63 |
| 36:BA:271(U):G:O2' | 36:BA:271(V):G:H5' | 1.98 | 0.63 |
| 36:BA:558:G:P | 46:BN:111:PRO:HD2 | 2.38 | 0.63 |
| 36:BA:8:A:H2' | 36:BA:9:U:H5 | 1.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 38:BC:14:VAL:HG23 | 38:BC:32:LEU:HD11 | 1.79 | 0.63 |
| 41:BF:119:ARG:HH11 | 41:BF:119:ARG:HG2 | 1.63 | 0.63 |
| 43:BH:149:ARG:HG3 | 43:BH:162:ILE:O | 1.98 | 0.63 |
| 48:BP:30:THR:HG22 | 48:BP:31:ALA:N | 2.13 | 0.63 |
| 52:BT:25:GLY:O | 52:BT:49:VAL:HG12 | 1.95 | 0.63 |
| 52:BT:27:THR:O | 52:BT:28:VAL:HB | 1.97 | 0.63 |
| 58:BZ:91:LEU:HD13 | 58:BZ:130:PRO:HB3 | 1.79 | 0.63 |
| 58:BZ:177:PRO:C | 58:BZ:178:GLU:HG2 | 2.18 | 0.63 |
| 1:AA:1152:A:O2' | 1:AA:1153:C:H5' | 1.98 | 0.63 |
| 2:AB:32:ILE:HD11 | 2:AB:40:HIS:HB3 | 1.81 | 0.63 |
| 4:AD:30:LYS:C | 4:AD:32:ALA:H | 2.00 | 0.63 |
| 32:B6:45:LYS:O | 32:B6:46:HIS:HB3 | 1.97 | 0.63 |
| 36:BA:2657:A:O2' | 43:BH:160:LYS:HE2 | 1.96 | 0.63 |
| 36:BA:519:U:H2' | 36:BA:520:G:H8 | 1.63 | 0.63 |
| 36:BA:628:G:H2' | 36:BA:629:G:C5' | 2.28 | 0.63 |
| 36:BA:68:G:H2' | 36:BA:69:C:H6 | 1.62 | 0.63 |
| 42:BG:103:LEU:HD21 | 42:BG:178:PHE:CZ | 2.34 | 0.63 |
| 34:B8:59:LYS:HD3 | 48:BP:50:ARG:HB3 | 1.78 | 0.63 |
| 51:BS:25:ARG:HG2 | 51:BS:25:ARG:HH11 | 1.63 | 0.63 |
| 52:BT:58:ASN:H | 52:BT:58:ASN:ND2 | 1.96 | 0.63 |
| 1:AA:1275:A:O2' | 1:AA:1276:G:H5' | 1.97 | 0.63 |
| 1:AA:161:A:H2' | 1:AA:162:A:C8 | 2.33 | 0.63 |
| 2:AB:104:ASN:O | 2:AB:108:ILE:HG12 | 1.98 | 0.63 |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:CE2 | 2.32 | 0.63 |
| 13:AM:40:ASN:HD22 | 13:AM:43:THR:HG23 | 1.63 | 0.63 |
| 17:AQ:62:SER:CB | 17:AQ:72:ARG:HG3 | 2.28 | 0.63 |
| 25:AZ:315:LYS:HE3 | 25:AZ:373:GLU:HB2 | 1.81 | 0.63 |
| 26:B0:49:LYS:N | 26:B0:80:HIS:HD1 | 1.92 | 0.63 |
| 35:B9:30:PRO:HB2 | 36:BA:2527:C:C5' | 2.23 | 0.63 |
| 36:BA:1019:U:H3 | 36:BA:1142(A):A:H62 | 1.46 | 0.63 |
| 36:BA:1503:U:H2' | 36:BA:1504:C:H6 | 1.62 | 0.63 |
| 36:BA:1766:U:H2' | 36:BA:1767:C:H6 | 1.63 | 0.63 |
| 36:BA:2206:G:C2 | 36:BA:2207:G:H5' | 2.33 | 0.63 |
| 36:BA:2645:G:H3' | 36:BA:2646:C:C5' | 2.20 | 0.63 |
| 38:BC:165:ASN:HA | 38:BC:170:ALA:O | 1.98 | 0.63 |
| 40:BE:2:LYS:HB3 | 40:BE:95:ILE:HG22 | 1.80 | 0.63 |
| 41:BF:101:LEU:CD1 | 41:BF:102:PRO:HD2 | 2.27 | 0.63 |
| 41:BF:132:VAL:HG22 | 41:BF:133:ASN:N | 2.08 | 0.63 |
| 42:BG:152:LEU:HD23 | 42:BG:152:LEU:H | 1.63 | 0.63 |
| 47:BO:35:VAL:HG11 | 47:BO:103:ALA:HB3 | 1.80 | 0.63 |
| 1:AA:1230:C:O2' | 1:AA:1231:G:H5' | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:393:A:C2' | 1:AA:394:G:H5' | 2.29 | 0.63 |
| 2:AB:7:VAL:HA | 2:AB:11:LEU:HG | 1.80 | 0.63 |
| 10:AJ:54:PHE:CZ | 10:AJ:55:LYS:NZ | 2.66 | 0.63 |
| 10:AJ:61:GLU:OE2 | 14:AN:45:ARG:HD2 | 1.98 | 0.63 |
| 10:AJ:30:SER:HA | 10:AJ:80:LYS:HZ2 | 1.63 | 0.63 |
| 10:AJ:96:ILE:H | 10:AJ:96:ILE:CD1 | 2.10 | 0.63 |
| 18:AR:44:LEU:CD2 | 18:AR:79:LEU:HD22 | 2.28 | 0.63 |
| 20:AT:53:LEU:HD22 | 20:AT:100:ILE:O | 1.98 | 0.63 |
| 22:AW:38:A:C3' | 22:AW:39:U:H5'' | 2.28 | 0.63 |
| 36:BA:1150:C:O2' | 36:BA:1151:G:H5' | 1.98 | 0.63 |
| 36:BA:1993:U:H4' | 40:BE:128:SER:OG | 1.99 | 0.63 |
| 36:BA:612:C:H2' | 36:BA:613:G:H5' | 1.81 | 0.63 |
| 36:BA:718:A:H2' | 36:BA:719:C:O4' | 1.98 | 0.63 |
| 37:BB:16:G:HO2' | 37:BB:17:C:H6 | 1.46 | 0.63 |
| 37:BB:31:C:H42 | 37:BB:51:G:H1 | 1.45 | 0.63 |
| 37:BB:65:C:H2' | 37:BB:66:A:H5' | 1.79 | 0.63 |
| 38:BC:150:GLY:HA2 | 38:BC:153:ILE:HD12 | 1.81 | 0.63 |
| 39:BD:35:LYS:C | 39:BD:35:LYS:HD2 | 2.18 | 0.63 |
| 42:BG:91:ARG:HD2 | 42:BG:91:ARG:C | 2.18 | 0.63 |
| 43:BH:12:PRO:CD | 43:BH:15:VAL:HG21 | 2.25 | 0.63 |
| 48:BP:107:LYS:O | 48:BP:109:GLY:N | 2.30 | 0.63 |
| 1:AA:64:G:H4' | 1:AA:65:U:H5'' | 1.81 | 0.63 |
| 4:AD:74:GLN:NE2 | 4:AD:100:ARG:HH22 | 1.97 | 0.63 |
| 19:AS:50:ALA:HA | 19:AS:58:VAL:O | 1.98 | 0.63 |
| 22:AV:4:C:C2' | 22:AV:5:G:H5'' | 2.26 | 0.63 |
| 36:BA:1291:C:C2' | 36:BA:1292:U:H5' | 2.27 | 0.63 |
| 36:BA:1594:G:H2' | 36:BA:1595:G:H8 | 1.63 | 0.63 |
| 36:BA:1948:G:H5' | 36:BA:1948:G:C8 | 2.31 | 0.63 |
| 36:BA:2466:C:O2' | 36:BA:2467:C:H5' | 1.98 | 0.63 |
| 43:BH:50:VAL:HG12 | 43:BH:51:ARG:N | 2.12 | 0.63 |
| 49:BQ:22:LYS:O | 49:BQ:22:LYS:HG3 | 1.99 | 0.63 |
| 53:BU:13:LYS:HA | 53:BU:16:LYS:HD2 | 1.80 | 0.63 |
| 57:BY:64:GLU:O | 57:BY:65:ALA:HB2 | 1.97 | 0.63 |
| 2:AB:8:LYS:HB2 | 2:AB:9:GLU:OE2 | 1.98 | 0.63 |
| 3:AC:68:VAL:HG12 | 3:AC:70:VAL:CG2 | 2.27 | 0.63 |
| 10:AJ:54:PHE:CD2 | 10:AJ:55:LYS:HD2 | 2.34 | 0.63 |
| 22:AW:55:U:C5 | 22:AW:57:G:H5'' | 2.34 | 0.63 |
| 31:B5:50:GLY:HA3 | 31:B5:56:LYS:CD | 2.29 | 0.63 |
| 36:BA:1217:C:H2' | 36:BA:1218:C:H6 | 1.63 | 0.63 |
| 36:BA:1590:U:H2' | 36:BA:1591:G:C5' | 2.28 | 0.63 |
| 36:BA:35:G:O2' | 36:BA:36:G:H5' | 1.97 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:658:C:H2' | 36:BA:659:C:C6 | 2.34 | 0.63 |
| 38:BC:137:LEU:HD13 | 38:BC:138:PRO:N | 2.14 | 0.63 |
| 42:BG:85:GLY:O | 42:BG:86:MET:HB3 | 1.99 | 0.63 |
| 53:BU:92:ARG:HB3 | 54:BV:11:GLN:NE2 | 2.14 | 0.63 |
| 1:AA:1304:G:H1' | 1:AA:1334:G:N2 | 2.13 | 0.63 |
| 2:AB:194:PRO:O | 2:AB:196:LEU:HD12 | 1.99 | 0.63 |
| 25:AZ:355:LEU:HD23 | 25:AZ:356:PRO:CD | 2.25 | 0.63 |
| 36:BA:1528:A:H2' | 36:BA:1528:A:N3 | 2.14 | 0.63 |
| 36:BA:195:A:H5'' | 36:BA:196:A:OP2 | 1.98 | 0.63 |
| 36:BA:2190:G:H2' | 36:BA:2190:G:N3 | 2.12 | 0.63 |
| 38:BC:200:LYS:HA | 38:BC:208:PHE:CZ | 2.34 | 0.63 |
| 42:BG:172:LEU:O | 42:BG:176:LEU:HB2 | 1.98 | 0.63 |
| 43:BH:54:ARG:HB2 | 43:BH:55:PRO:HD2 | 1.81 | 0.63 |
| 48:BP:126:VAL:HG22 | 48:BP:145:PRO:HB2 | 1.80 | 0.63 |
| 52:BT:102:ILE:HD12 | 52:BT:110:ILE:HD12 | 1.80 | 0.63 |
| 56:BX:18:TYR:O | 56:BX:20:GLY:N | 2.32 | 0.63 |
| 1:AA:1459:C:H2' | 1:AA:1460:A:C8 | 2.34 | 0.63 |
| 4:AD:61:LYS:HA | 4:AD:203:VAL:HG22 | 1.81 | 0.63 |
| 6:AF:67:MET:HB2 | 6:AF:68:PRO:CD | 2.27 | 0.63 |
| 11:AK:124:LYS:HD2 | 11:AK:125:PHE:CE1 | 2.34 | 0.63 |
| 22:AV:75:C:H2' | 22:AV:76:A:O4' | 1.99 | 0.63 |
| 25:AZ:9:LYS:HB3 | 25:AZ:10:PRO:HD2 | 1.81 | 0.63 |
| 25:AZ:181:GLN:CD | 25:AZ:193:ASN:HD21 | 2.02 | 0.63 |
| 25:AZ:19:HIS:CD2 | 25:AZ:20:VAL:N | 2.66 | 0.63 |
| 36:BA:2423:U:H5' | 36:BA:2423:U:H6 | 1.62 | 0.63 |
| 36:BA:2512:C:H2' | 36:BA:2513:G:O4' | 1.99 | 0.63 |
| 38:BC:100:ILE:HD13 | 38:BC:126:LYS:HB3 | 1.81 | 0.63 |
| 38:BC:44:HIS:O | 38:BC:212:VAL:HG13 | 1.97 | 0.63 |
| 41:BF:5:ALA:HB2 | 41:BF:24:LEU:CD1 | 2.28 | 0.63 |
| 42:BG:109:VAL:O | 42:BG:112:PRO:HD2 | 1.97 | 0.63 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:C6 | 2.34 | 0.63 |
| 2:AB:209:ARG:HH11 | 2:AB:239:VAL:CG1 | 2.01 | 0.63 |
| 15:AO:62:GLN:HE21 | 15:AO:62:GLN:HA | 1.64 | 0.63 |
| 1:AA:1503:A:N7 | 23:AX:15:A:C5 | 2.67 | 0.63 |
| 36:BA:1092:C:H42 | 36:BA:1100:C:H42 | 1.46 | 0.63 |
| 36:BA:2306:C:H4' | 42:BG:136:ARG:HH22 | 1.64 | 0.63 |
| 34:B8:32:LEU:HD22 | 36:BA:2392:A:OP1 | 1.99 | 0.63 |
| 36:BA:2491:U:H4' | 36:BA:2570:G:OP1 | 1.99 | 0.63 |
| 36:BA:2656:U:C2' | 36:BA:2657:A:H5'' | 2.28 | 0.63 |
| 36:BA:606:U:H4' | 36:BA:658:C:H4' | 1.81 | 0.63 |
| 38:BC:120:MET:CE | 38:BC:123:VAL:HG11 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:87:ARG:HH11 | 2:AB:223:ILE:CD1 | 2.12 | 0.62 |
| 12:AL:46:LYS:CG | 12:AL:47:LYS:H | 2.02 | 0.62 |
| 13:AM:12:ASN:H | 13:AM:12:ASN:ND2 | 1.94 | 0.62 |
| 26:B0:27:GLU:CD | 36:BA:856:C:H1' | 2.19 | 0.62 |
| 28:B2:21:LEU:HD11 | 28:B2:63:VAL:HG12 | 1.79 | 0.62 |
| 28:B2:47:ASN:HA | 28:B2:50:ILE:HD13 | 1.81 | 0.62 |
| 36:BA:2639:A:H2' | 36:BA:2640:G:O4' | 1.99 | 0.62 |
| 38:BC:120:MET:HE1 | 38:BC:123:VAL:HG21 | 1.81 | 0.62 |
| 40:BE:111:ARG:HD3 | 40:BE:160:TYR:CD1 | 2.34 | 0.62 |
| 42:BG:113:ARG:HE | 42:BG:113:ARG:HA | 1.63 | 0.62 |
| 42:BG:64:THR:OG1 | 42:BG:94:LEU:HD11 | 1.99 | 0.62 |
| 49:BQ:131:ILE:HD12 | 49:BQ:131:ILE:N | 2.15 | 0.62 |
| 50:BR:99:LYS:N | 50:BR:99:LYS:HD2 | 2.12 | 0.62 |
| 51:BS:17:ARG:C | 51:BS:19:LYS:N | 2.51 | 0.62 |
| 53:BU:79:PHE:O | 53:BU:83:LEU:HD13 | 1.99 | 0.62 |
| 56:BX:26:TYR:HB2 | 56:BX:81:VAL:HG23 | 1.81 | 0.62 |
| 2:AB:115:LEU:HB2 | 2:AB:145:LEU:HD12 | 1.81 | 0.62 |
| 4:AD:125:HIS:C | 4:AD:126:ILE:HD12 | 2.19 | 0.62 |
| 7:AG:71:PRO:O | 7:AG:91:VAL:HG11 | 1.98 | 0.62 |
| 9:AI:16:ARG:HG3 | 9:AI:16:ARG:HH11 | 1.63 | 0.62 |
| 25:AZ:194:GLU:HG3 | 25:AZ:195:TRP:N | 2.14 | 0.62 |
| 32:B6:26:ASN:ND2 | 32:B6:32:ASN:ND2 | 2.42 | 0.62 |
| 32:B6:45:LYS:N | 32:B6:45:LYS:CD | 2.58 | 0.62 |
| 36:BA:1087:G:H8 | 36:BA:1088:A:H4' | 1.64 | 0.62 |
| 36:BA:1921:G:O2' | 36:BA:1922:G:H5' | 1.99 | 0.62 |
| 36:BA:234:C:H2' | 36:BA:235:U:C6 | 2.34 | 0.62 |
| 36:BA:287:C:H2' | 36:BA:288:C:H6 | 1.64 | 0.62 |
| 36:BA:631:A:H5'' | 48:BP:65:ARG:NH1 | 2.13 | 0.62 |
| 41:BF:103:LYS:O | 41:BF:107:LYS:HG2 | 1.98 | 0.62 |
| 47:BO:111:PHE:HB3 | 47:BO:114:ILE:HD13 | 1.81 | 0.62 |
| 1:AA:339:C:H2' | 1:AA:340:U:C6 | 2.34 | 0.62 |
| 2:AB:60:ASP:HB3 | 2:AB:64:ARG:HH21 | 1.63 | 0.62 |
| 9:AI:88:TYR:O | 9:AI:89:ASN:ND2 | 2.32 | 0.62 |
| 12:AL:20:LYS:N | 12:AL:20:LYS:HD3 | 2.08 | 0.62 |
| 36:BA:1386:C:OP2 | 36:BA:1396:U:H5 | 1.82 | 0.62 |
| 36:BA:2630:G:H1' | 36:BA:2894:G:H1' | 1.81 | 0.62 |
| 40:BE:59:VAL:CG2 | 40:BE:63:LEU:HA | 2.28 | 0.62 |
| 30:B4:9:LEU:HG | 42:BG:98:ARG:NH1 | 2.13 | 0.62 |
| 50:BR:2:ARG:NH1 | 50:BR:2:ARG:N | 2.47 | 0.62 |
| 56:BX:26:TYR:O | 56:BX:81:VAL:HG22 | 1.99 | 0.62 |
| 58:BZ:100:VAL:HG23 | 58:BZ:126:VAL:CG2 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:163:C:H2' | 1:AA:164:U:C6 | 2.34 | 0.62 |
| 1:AA:178:C:O2' | 1:AA:179:A:H5' | 2.00 | 0.62 |
| 1:AA:388:G:O2' | 1:AA:389:A:P | 2.57 | 0.62 |
| 3:AC:113:ALA:HB3 | 3:AC:114:PRO:HD3 | 1.80 | 0.62 |
| 9:AI:53:VAL:HG13 | 9:AI:95:LYS:NZ | 2.14 | 0.62 |
| 11:AK:50:TYR:HH | 11:AK:59:TYR:HE2 | 1.42 | 0.62 |
| 10:AJ:61:GLU:OE2 | 14:AN:45:ARG:NH1 | 2.31 | 0.62 |
| 20:AT:23:ARG:HH11 | 20:AT:23:ARG:HG2 | 1.65 | 0.62 |
| 1:AA:192:U:H4' | 20:AT:57:ARG:HD3 | 1.80 | 0.62 |
| 25:AZ:318:ALA:CB | 25:AZ:400:VAL:HA | 2.28 | 0.62 |
| 36:BA:145:G:C3' | 36:BA:146:G:H5'' | 2.29 | 0.62 |
| 36:BA:2756:U:H1' | 36:BA:2757:A:C5' | 2.24 | 0.62 |
| 36:BA:2787:C:O2 | 40:BE:61:ARG:NH1 | 2.33 | 0.62 |
| 46:BN:18:ALA:HB3 | 46:BN:26:LEU:HD22 | 1.80 | 0.62 |
| 47:BO:107:ARG:HH12 | 52:BT:35:LYS:HD2 | 1.64 | 0.62 |
| 55:BW:73:ALA:HB3 | 55:BW:106:ILE:CG1 | 2.30 | 0.62 |
| 58:BZ:71:VAL:HG11 | 58:BZ:74:VAL:CG2 | 2.29 | 0.62 |
| 1:AA:397:A:N7 | 1:AA:547:A:O2' | 2.29 | 0.62 |
| 1:AA:757:U:H2' | 1:AA:758:G:O4' | 2.00 | 0.62 |
| 1:AA:838:G:H2' | 1:AA:839:U:H5'' | 1.82 | 0.62 |
| 4:AD:3:ARG:O | 4:AD:5:ILE:HG13 | 2.00 | 0.62 |
| 11:AK:120:ARG:HG3 | 11:AK:120:ARG:HH11 | 1.64 | 0.62 |
| 13:AM:3:ARG:HD3 | 42:BG:113:ARG:HH11 | 1.64 | 0.62 |
| 20:AT:89:ARG:NH2 | 20:AT:104:LEU:HD21 | 2.14 | 0.62 |
| 25:AZ:223:MET:HE3 | 25:AZ:240:GLY:HA3 | 1.81 | 0.62 |
| 36:BA:1057:A:H2 | 36:BA:1082:U:H3 | 1.47 | 0.62 |
| 36:BA:1387:C:H5' | 36:BA:1469:A:H4' | 1.82 | 0.62 |
| 36:BA:2781:A:H5' | 36:BA:2782:G:C5' | 2.19 | 0.62 |
| 36:BA:534:U:O2' | 53:BU:49:HIS:HD2 | 1.83 | 0.62 |
| 37:BB:65:C:C2' | 37:BB:66:A:H5' | 2.30 | 0.62 |
| 41:BF:7:TYR:HD2 | 41:BF:16:GLY:HA3 | 1.63 | 0.62 |
| 42:BG:78:SER:O | 42:BG:80:PHE:N | 2.32 | 0.62 |
| 49:BQ:97:VAL:HG11 | 49:BQ:103:MET:CE | 2.29 | 0.62 |
| 53:BU:12:ARG:O | 53:BU:16:LYS:HG3 | 1.98 | 0.62 |
| 1:AA:170:U:O2' | 1:AA:171:A:H5' | 1.99 | 0.62 |
| 1:AA:405:U:O2 | 1:AA:498:U:H2' | 1.98 | 0.62 |
| 2:AB:87:ARG:NH1 | 2:AB:220:ASP:OD1 | 2.31 | 0.62 |
| 5:AE:20:GLN:NE2 | 5:AE:25:ARG:CZ | 2.62 | 0.62 |
| 10:AJ:55:LYS:H | 10:AJ:55:LYS:HE3 | 1.61 | 0.62 |
| 11:AK:97:ALA:O | 11:AK:101:SER:HB3 | 1.99 | 0.62 |
| 13:AM:86:CYS:HA | 19:AS:73:GLU:O | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BA:1199:U:H1' | 53:BU:4:ALA:HB2 | 1.82 | 0.62 |
| 36:BA:1851:U:O2' | 36:BA:1852:C:H5' | 1.99 | 0.62 |
| 36:BA:1902:C:H4' | 39:BD:244:ARG:HA | 1.81 | 0.62 |
| 38:BC:141:LYS:HB2 | 38:BC:141:LYS:NZ | 2.14 | 0.62 |
| 39:BD:261:LYS:NZ | 39:BD:263:ARG:CZ | 2.62 | 0.62 |
| 39:BD:77:ALA:HB2 | 39:BD:97:TYR:CD2 | 2.34 | 0.62 |
| 48:BP:50:ARG:HG2 | 48:BP:50:ARG:NH2 | 2.15 | 0.62 |
| 49:BQ:108:GLY:HA3 | 58:BZ:116:VAL:CG1 | 2.29 | 0.62 |
| 52:BT:19:LEU:HD13 | 52:BT:78:LEU:HD23 | 1.82 | 0.62 |
| 52:BT:50:ILE:HD11 | 52:BT:64:ARG:HB2 | 1.82 | 0.62 |
| 52:BT:91:ARG:HA | 52:BT:117:ASP:H | 1.63 | 0.62 |
| 1:AA:977:A:C2' | 1:AA:977:A:N3 | 2.63 | 0.62 |
| 1:AA:992:U:H1' | 1:AA:993:G:C2 | 2.34 | 0.62 |
| 2:AB:116:GLU:C | 2:AB:118:LEU:H | 2.01 | 0.62 |
| 2:AB:138:LEU:C | 2:AB:140:HIS:H | 2.00 | 0.62 |
| 3:AC:90:GLU:O | 3:AC:93:LYS:HB3 | 1.99 | 0.62 |
| 4:AD:28:SER:HB3 | 4:AD:29:PRO:HD2 | 1.80 | 0.62 |
| 8:AH:33:GLU:HG2 | 8:AH:48:TYR:CE1 | 2.35 | 0.62 |
| 17:AQ:22:LEU:HD12 | 17:AQ:41:LYS:HG2 | 1.81 | 0.62 |
| 23:AX:20:U:O2' | 23:AX:21:C:H5' | 1.99 | 0.62 |
| 25:AZ:104:LEU:HD12 | 25:AZ:105:VAL:N | 2.14 | 0.62 |
| 29:B3:4:LEU:O | 29:B3:36:VAL:HA | 2.00 | 0.62 |
| 36:BA:2124:G:H3' | 36:BA:2125:G:H8 | 1.65 | 0.62 |
| 36:BA:2208:A:H1' | 36:BA:2219:G:C6 | 2.34 | 0.62 |
| 36:BA:473:G:H5'' | 36:BA:508:G:H22 | 1.64 | 0.62 |
| 36:BA:588:U:H2' | 36:BA:589:C:C6 | 2.35 | 0.62 |
| 37:BB:104:U:O2' | 37:BB:105:A:H5' | 1.98 | 0.62 |
| 38:BC:14:VAL:HG13 | 38:BC:20:TYR:CE1 | 2.34 | 0.62 |
| 39:BD:46:GLN:N | 39:BD:46:GLN:OE1 | 2.33 | 0.62 |
| 39:BD:27:THR:HG23 | 39:BD:83:GLU:HG2 | 1.81 | 0.62 |
| 36:BA:2632:A:H2 | 40:BE:61:ARG:HD2 | 1.64 | 0.62 |
| 46:BN:132:ALA:O | 46:BN:133:GLN:HB2 | 2.00 | 0.62 |
| 46:BN:134:ARG:NH2 | 46:BN:136:GLU:HB2 | 2.13 | 0.62 |
| 47:BO:22:ILE:HB | 47:BO:40:VAL:O | 1.99 | 0.62 |
| 49:BQ:17:LEU:CD2 | 49:BQ:96:VAL:HG13 | 2.29 | 0.62 |
| 51:BS:49:VAL:HG13 | 51:BS:76:LYS:HD2 | 1.80 | 0.62 |
| 58:BZ:17:ALA:HA | 58:BZ:20:ARG:CG | 2.30 | 0.62 |
| 5:AE:11:ILE:HD11 | 5:AE:33:VAL:CG2 | 2.30 | 0.62 |
| 10:AJ:83:GLU:O | 10:AJ:85:LEU:N | 2.32 | 0.62 |
| 11:AK:51:LYS:HA | 11:AK:55:LYS:HE2 | 1.80 | 0.62 |
| 17:AQ:67:LYS:O | 17:AQ:69:LYS:N | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:AZ:342:PHE:HB2 | 25:AZ:344:PHE:HE1 | 1.65 | 0.62 |
| 26:B0:17:GLN:O | 26:B0:19:LYS:HG3 | 1.99 | 0.62 |
| 29:B3:56:VAL:HG12 | 29:B3:57:GLU:H | 1.64 | 0.62 |
| 34:B8:43:GLN:C | 34:B8:44:LYS:HD2 | 2.20 | 0.62 |
| 34:B8:56:GLU:OE1 | 34:B8:56:GLU:N | 2.23 | 0.62 |
| 36:BA:1193:G:H2' | 36:BA:1194:A:O4' | 1.99 | 0.62 |
| 36:BA:1198:U:H2' | 36:BA:1199:U:H6 | 1.65 | 0.62 |
| 36:BA:142:A:C8 | 36:BA:1408:C:H1' | 2.34 | 0.62 |
| 36:BA:2310:A:O2' | 36:BA:2311:A:H5' | 1.98 | 0.62 |
| 36:BA:657:U:H2' | 36:BA:658:C:C6 | 2.35 | 0.62 |
| 36:BA:944:G:H5' | 36:BA:945:A:O5' | 2.00 | 0.62 |
| 41:BF:157:VAL:CG2 | 41:BF:194:MET:HG2 | 2.30 | 0.62 |
| 46:BN:34:LEU:HD21 | 46:BN:120:LEU:HD23 | 1.81 | 0.62 |
| 46:BN:129:PRO:O | 46:BN:130:HIS:HB3 | 1.99 | 0.62 |
| 48:BP:16:ARG:HD3 | 48:BP:18:ARG:N | 2.08 | 0.62 |
| 48:BP:23:PRO:O | 48:BP:33:ARG:HD2 | 2.00 | 0.62 |
| 53:BU:101:ARG:O | 53:BU:103:PRO:CD | 2.47 | 0.62 |
| 54:BV:51:VAL:HG12 | 54:BV:52:VAL:H | 1.64 | 0.62 |
| 57:BY:27:VAL:HG12 | 57:BY:28:LYS:N | 2.15 | 0.62 |
| 57:BY:39:VAL:HG12 | 57:BY:40:GLU:N | 2.15 | 0.62 |
| 58:BZ:156:LYS:O | 58:BZ:158:PRO:HD3 | 2.00 | 0.62 |
| 58:BZ:26:GLY:HA2 | 58:BZ:85:HIS:CD2 | 2.34 | 0.62 |
| 58:BZ:48:PHE:CZ | 58:BZ:74:VAL:HG21 | 2.34 | 0.62 |
| 4:AD:107:ARG:HH12 | 4:AD:114:ARG:NH2 | 1.97 | 0.62 |
| 4:AD:187:ARG:NH1 | 4:AD:187:ARG:HB3 | 2.15 | 0.62 |
| 22:AV:56:C:O4' | 42:BG:76:SER:HB2 | 2.00 | 0.62 |
| 22:AW:18:G:H22 | 22:AW:55:U:H6 | 1.47 | 0.62 |
| 25:AZ:138:VAL:C | 25:AZ:140:MET:H | 2.01 | 0.62 |
| 28:B2:35:LEU:HD11 | 28:B2:50:ILE:CG1 | 2.13 | 0.62 |
| 29:B3:5:LYS:HD2 | 29:B3:57:GLU:HB3 | 1.81 | 0.62 |
| 35:B9:7:VAL:HG22 | 35:B9:34:GLN:HG3 | 1.81 | 0.62 |
| 36:BA:105:C:H2' | 36:BA:106:C:H6 | 1.64 | 0.62 |
| 36:BA:1499:C:O2' | 36:BA:1500:G:H5' | 1.99 | 0.62 |
| 36:BA:1677:A:H2' | 36:BA:1678:G:C8 | 2.35 | 0.62 |
| 36:BA:1688:U:H1' | 36:BA:1701:A:C6 | 2.35 | 0.62 |
| 36:BA:1854:A:H62 | 36:BA:1888:G:H8 | 1.48 | 0.62 |
| 34:B8:34:TRP:HA | 36:BA:2420:C:OP1 | 2.00 | 0.62 |
| 36:BA:596:G:H2' | 36:BA:597:U:O4' | 2.00 | 0.62 |
| 36:BA:80:G:O2' | 36:BA:81:G:H5' | 2.00 | 0.62 |
| 36:BA:1952:A:C6 | 47:BO:22:ILE:HD12 | 2.35 | 0.62 |
| 52:BT:75:ILE:N | 52:BT:75:ILE:HD12 | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:BU:112:ARG:O | 53:BU:115:ALA:HB3 | 1.99 | 0.62 |
| 1:AA:858:G:H8 | 1:AA:858:G:O5' | 1.82 | 0.62 |
| 4:AD:70:ILE:HG22 | 4:AD:71:SER:N | 2.15 | 0.62 |
| 16:AP:45:THR:HG22 | 16:AP:47:ASP:HB3 | 1.81 | 0.62 |
| 19:AS:31:ILE:CG2 | 19:AS:49:ILE:HA | 2.26 | 0.62 |
| 20:AT:20:LEU:O | 20:AT:23:ARG:HB3 | 1.99 | 0.62 |
| 21:AU:6:ARG:HD3 | 21:AU:15:ARG:HH12 | 1.63 | 0.62 |
| 22:AW:20:U:H5' | 36:BA:2112:G:N1 | 2.15 | 0.62 |
| 36:BA:1498:C:H2' | 36:BA:1499:C:C5' | 2.30 | 0.62 |
| 36:BA:1498:C:H2' | 36:BA:1499:C:H5' | 1.81 | 0.62 |
| 36:BA:612:C:C2' | 36:BA:613:G:C5' | 2.76 | 0.62 |
| 36:BA:2052:G:H4' | 40:BE:143:ASN:O | 2.00 | 0.62 |
| 41:BF:29:ASN:ND2 | 41:BF:32:LEU:H | 1.98 | 0.62 |
| 42:BG:86:MET:N | 42:BG:87:PRO:CD | 2.63 | 0.62 |
| 51:BS:29:PHE:C | 51:BS:29:PHE:HD2 | 2.04 | 0.62 |
| 54:BV:72:VAL:HG23 | 54:BV:85:LYS:CB | 2.29 | 0.62 |
| 55:BW:5:ALA:HB2 | 55:BW:54:ALA:HB2 | 1.81 | 0.62 |
| 58:BZ:141:VAL:O | 58:BZ:141:VAL:HG12 | 2.00 | 0.62 |
| 58:BZ:40:ASP:OD1 | 58:BZ:42:VAL:HG12 | 2.00 | 0.62 |
| 1:AA:1447:A:H2' | 1:AA:1447:A:N3 | 2.14 | 0.61 |
| 1:AA:309:G:O2' | 1:AA:310:G:H5' | 2.00 | 0.61 |
| 5:AE:20:GLN:HG2 | 5:AE:21:ALA:H | 1.65 | 0.61 |
| 7:AG:22:LEU:HD23 | 7:AG:22:LEU:O | 2.00 | 0.61 |
| 16:AP:74:LEU:O | 16:AP:79:VAL:HG23 | 2.00 | 0.61 |
| 25:AZ:34:VAL:HG11 | 25:AZ:199:ILE:CG2 | 2.30 | 0.61 |
| 25:AZ:75:ARG:HH12 | 25:AZ:210:ILE:HG22 | 1.65 | 0.61 |
| 26:B0:7:LEU:CB | 49:BQ:85:LYS:HG3 | 2.30 | 0.61 |
| 36:BA:1151:G:H2' | 36:BA:1152:C:C6 | 2.34 | 0.61 |
| 36:BA:1400:G:H2' | 36:BA:1401:G:C8 | 2.35 | 0.61 |
| 36:BA:1591:G:O2' | 36:BA:1592:C:H5' | 2.00 | 0.61 |
| 36:BA:1914:C:H2' | 36:BA:1915:U:O4' | 2.00 | 0.61 |
| 36:BA:330:A:O2' | 36:BA:331:A:H8 | 1.83 | 0.61 |
| 36:BA:442:G:H4' | 41:BF:46:ARG:HB2 | 1.81 | 0.61 |
| 48:BP:7:ARG:O | 48:BP:10:PRO:HD2 | 2.00 | 0.61 |
| 50:BR:99:LYS:CD | 50:BR:99:LYS:H | 2.10 | 0.61 |
| 52:BT:115:ARG:HH11 | 52:BT:115:ARG:HG3 | 1.63 | 0.61 |
| 53:BU:95:LEU:C | 53:BU:97:ASP:N | 2.53 | 0.61 |
| 54:BV:39:LEU:CD1 | 54:BV:47:VAL:HG11 | 2.29 | 0.61 |
| 54:BV:19:LYS:HG2 | 54:BV:94:LEU:HB2 | 1.82 | 0.61 |
| 55:BW:69:LEU:HD23 | 55:BW:108:GLY:O | 1.99 | 0.61 |
| 4:AD:61:LYS:HE2 | 4:AD:62:GLN:HE21 | 1.63 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:AG:78:ARG:O | 7:AG:78:ARG:HG3 | 2.00 | 0.61 |
| 10:AJ:17:ASP:OD1 | 10:AJ:70:ARG:NE | 2.33 | 0.61 |
| 10:AJ:5:ARG:HG3 | 10:AJ:71:LEU:HD11 | 1.82 | 0.61 |
| 26:B0:20:ARG:HD2 | 26:B0:20:ARG:H | 1.65 | 0.61 |
| 35:B9:11:CYS:SG | 35:B9:12:ASP:N | 2.73 | 0.61 |
| 36:BA:1141:U:H2' | 46:BN:63:THR:CG2 | 2.29 | 0.61 |
| 36:BA:1324:G:H4' | 36:BA:1616:A:C2 | 2.35 | 0.61 |
| 26:B0:36:ILE:HD11 | 36:BA:2355:C:O4' | 1.99 | 0.61 |
| 36:BA:524:U:H4' | 36:BA:555:U:H4' | 1.80 | 0.61 |
| 36:BA:1803:A:H4' | 39:BD:259:THR:CG2 | 2.30 | 0.61 |
| 39:BD:33:LEU:O | 39:BD:36:PRO:HG3 | 2.00 | 0.61 |
| 43:BH:37:VAL:HG12 | 43:BH:38:SER:N | 2.15 | 0.61 |
| 43:BH:44:VAL:HG12 | 43:BH:45:VAL:N | 2.14 | 0.61 |
| 48:BP:56:SER:O | 48:BP:57:THR:CG2 | 2.47 | 0.61 |
| 52:BT:30:VAL:HA | 52:BT:43:GLN:O | 2.00 | 0.61 |
| 57:BY:12:THR:HG22 | 57:BY:75:ILE:HG21 | 1.81 | 0.61 |
| 57:BY:35:TYR:HD2 | 57:BY:68:HIS:CE1 | 2.17 | 0.61 |
| 57:BY:7:VAL:HG11 | 57:BY:8:LYS:HZ1 | 1.65 | 0.61 |
| 57:BY:85:VAL:HG12 | 57:BY:86:ARG:N | 2.14 | 0.61 |
| 1:AA:1128:C:O2' | 1:AA:1130:A:C8 | 2.53 | 0.61 |
| 17:AQ:91:ARG:HH11 | 17:AQ:91:ARG:HB2 | 1.66 | 0.61 |
| 19:AS:44:MET:O | 19:AS:47:HIS:HB2 | 2.00 | 0.61 |
| 36:BA:1963:U:H2' | 36:BA:1963:U:O2 | 1.99 | 0.61 |
| 36:BA:2801:A:O2' | 36:BA:2895:U:H5' | 1.99 | 0.61 |
| 38:BC:208:PHE:C | 38:BC:209:LEU:HD23 | 2.20 | 0.61 |
| 39:BD:261:LYS:HZ1 | 39:BD:263:ARG:HH21 | 1.48 | 0.61 |
| 39:BD:75:ILE:HD13 | 39:BD:75:ILE:N | 2.15 | 0.61 |
| 40:BE:186:GLY:O | 40:BE:187:ALA:HB3 | 2.00 | 0.61 |
| 58:BZ:10:ARG:NH2 | 58:BZ:36:LYS:HB2 | 2.12 | 0.61 |
| 58:BZ:119:GLU:H | 58:BZ:119:GLU:CD | 2.02 | 0.61 |
| 1:AA:1007:C:O2' | 1:AA:1008:C:H5' | 1.98 | 0.61 |
| 1:AA:1429:C:H2' | 1:AA:1430:C:C6 | 2.35 | 0.61 |
| 1:AA:189(I):G:H2' | 1:AA:189(J):G:H8 | 1.63 | 0.61 |
| 2:AB:111:ARG:HH11 | 2:AB:111:ARG:HG2 | 1.64 | 0.61 |
| 4:AD:102:ASP:HA | 4:AD:121:VAL:HG21 | 1.83 | 0.61 |
| 10:AJ:29:ARG:HG2 | 10:AJ:29:ARG:HH11 | 1.65 | 0.61 |
| 13:AM:87:TYR:O | 13:AM:90:LEU:O | 2.18 | 0.61 |
| 22:AW:29:G:H1 | 22:AW:41:C:H42 | 1.46 | 0.61 |
| 25:AZ:309:SER:O | 25:AZ:310:ILE:HB | 2.00 | 0.61 |
| 36:BA:2097:C:H2' | 36:BA:2098:U:O4' | 2.00 | 0.61 |
| 36:BA:20:C:H2' | 36:BA:21:A:C8 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BA:2886:G:H2' | 36:BA:2887:U:H6 | 1.65 | 0.61 |
| 36:BA:311:A:H5' | 36:BA:332:A:C2 | 2.35 | 0.61 |
| 36:BA:742:G:H2' | 36:BA:743:G:C8 | 2.35 | 0.61 |
| 36:BA:935:C:O2' | 36:BA:936:C:H5' | 2.01 | 0.61 |
| 38:BC:180:PHE:HD2 | 38:BC:184:LYS:HG3 | 1.64 | 0.61 |
| 42:BG:34:LEU:O | 42:BG:34:LEU:HD12 | 2.00 | 0.61 |
| 42:BG:61:ALA:HA | 42:BG:66:GLN:O | 1.99 | 0.61 |
| 45:BK:59:UNK:HA | 45:BK:64:UNK:O | 2.00 | 0.61 |
| 48:BP:23:PRO:HD2 | 48:BP:33:ARG:NE | 2.11 | 0.61 |
| 53:BU:17:ILE:HG23 | 53:BU:39:LEU:HD11 | 1.81 | 0.61 |
| 57:BY:8:LYS:HE3 | 57:BY:74:PRO:HD3 | 1.83 | 0.61 |
| 58:BZ:10:ARG:HB2 | 58:BZ:37:VAL:O | 2.00 | 0.61 |
| 1:AA:148:G:H2' | 1:AA:149:A:C8 | 2.34 | 0.61 |
| 1:AA:274:A:O2' | 1:AA:275:G:H8 | 1.83 | 0.61 |
| 1:AA:368:U:OP1 | 25:AZ:291:ARG:NH1 | 2.33 | 0.61 |
| 1:AA:627:G:H2' | 1:AA:628:G:C8 | 2.34 | 0.61 |
| 1:AA:679:C:H2' | 1:AA:680:C:C6 | 2.35 | 0.61 |
| 21:AU:24:ARG:O | 21:AU:25:LYS:HB2 | 1.99 | 0.61 |
| 34:B8:32:LEU:HB3 | 34:B8:36:LYS:HE2 | 1.82 | 0.61 |
| 36:BA:1532:C:O2' | 36:BA:1533:G:H5' | 2.00 | 0.61 |
| 36:BA:1887:C:C3' | 36:BA:1888:G:H5'' | 2.31 | 0.61 |
| 36:BA:2102:U:H2' | 36:BA:2103:C:O4' | 2.01 | 0.61 |
| 36:BA:2377:A:O2' | 36:BA:2378:A:H5' | 2.00 | 0.61 |
| 36:BA:524:U:H2' | 36:BA:525:U:C6 | 2.35 | 0.61 |
| 39:BD:10:THR:HG23 | 39:BD:13:ARG:CB | 2.31 | 0.61 |
| 39:BD:160:GLY:HA2 | 39:BD:197:GLY:H | 1.66 | 0.61 |
| 46:BN:96:GLU:O | 46:BN:100:GLU:HG3 | 2.00 | 0.61 |
| 47:BO:35:VAL:HG21 | 47:BO:69:ILE:HD11 | 1.81 | 0.61 |
| 52:BT:27:THR:OG1 | 52:BT:28:VAL:N | 2.33 | 0.61 |
| 58:BZ:59:LEU:O | 58:BZ:66:SER:HA | 2.00 | 0.61 |
| 1:AA:346:G:H2' | 1:AA:346:G:N3 | 2.13 | 0.61 |
| 12:AL:18:VAL:HG23 | 12:AL:19:ARG:N | 2.10 | 0.61 |
| 16:AP:44:THR:O | 16:AP:45:THR:CB | 2.48 | 0.61 |
| 25:AZ:204:ASP:O | 25:AZ:208:GLU:HG2 | 2.00 | 0.61 |
| 36:BA:1771:C:C1' | 36:BA:1786:A:C8 | 2.83 | 0.61 |
| 36:BA:2364:C:O2' | 36:BA:2365:G:H5' | 2.01 | 0.61 |
| 37:BB:25:A:H2' | 37:BB:25:A:N3 | 2.14 | 0.61 |
| 39:BD:267:SER:HA | 39:BD:270:ILE:CG1 | 2.31 | 0.61 |
| 39:BD:33:LEU:O | 39:BD:36:PRO:CG | 2.49 | 0.61 |
| 43:BH:76:VAL:O | 43:BH:79:VAL:HG22 | 1.99 | 0.61 |
| 50:BR:97:VAL:HA | 50:BR:113:LEU:O | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:2839:G:H21 | 50:BR:92:GLY:HA3 | 1.66 | 0.61 |
| 54:BV:72:VAL:CG2 | 54:BV:85:LYS:HB2 | 2.28 | 0.61 |
| 49:BQ:140:ALA:HB1 | 58:BZ:99:TYR:HB2 | 1.82 | 0.61 |
| 1:AA:119:A:H4' | 1:AA:120:A:O5' | 2.00 | 0.61 |
| 1:AA:1319:A:H5' | 1:AA:1320:C:OP1 | 2.00 | 0.61 |
| 1:AA:1327:C:H2' | 1:AA:1328:C:C6 | 2.36 | 0.61 |
| 1:AA:1531:A:O5' | 1:AA:1531:A:H8 | 1.84 | 0.61 |
| 5:AE:84:PHE:HB2 | 5:AE:134:ALA:HB2 | 1.83 | 0.61 |
| 8:AH:102:ARG:N | 8:AH:102:ARG:HD3 | 2.15 | 0.61 |
| 14:AN:57:ARG:HG2 | 14:AN:57:ARG:NH1 | 2.15 | 0.61 |
| 25:AZ:72:THR:C | 25:AZ:74:LYS:H | 2.03 | 0.61 |
| 26:B0:10:THR:HG22 | 26:B0:12:ASN:N | 2.13 | 0.61 |
| 36:BA:1859:A:H2' | 36:BA:1860:G:O4' | 2.00 | 0.61 |
| 36:BA:2672:G:H3' | 36:BA:2673:G:H5'' | 1.82 | 0.61 |
| 38:BC:94:VAL:CG1 | 38:BC:95:GLY:N | 2.64 | 0.61 |
| 40:BE:107:THR:HA | 40:BE:163:GLU:O | 2.00 | 0.61 |
| 41:BF:155:LEU:CD1 | 41:BF:176:LEU:HD13 | 2.30 | 0.61 |
| 36:BA:1139:G:H5'' | 46:BN:70:LYS:NZ | 2.15 | 0.61 |
| 50:BR:69:ASP:O | 50:BR:71:GLN:N | 2.33 | 0.61 |
| 51:BS:104:GLY:O | 51:BS:106:ARG:N | 2.34 | 0.61 |
| 53:BU:57:PHE:O | 53:BU:59:ARG:N | 2.34 | 0.61 |
| 7:AG:22:LEU:HD22 | 7:AG:62:PHE:CE2 | 2.35 | 0.61 |
| 19:AS:29:ARG:HB3 | 19:AS:48:THR:N | 2.14 | 0.61 |
| 20:AT:10:LEU:HD12 | 20:AT:11:SER:H | 1.66 | 0.61 |
| 25:AZ:21:ASP:H | 61:AZ:501:GCP:H3B2 | 1.65 | 0.61 |
| 34:B8:32:LEU:HD12 | 34:B8:36:LYS:HZ1 | 1.64 | 0.61 |
| 36:BA:2127:G:H5' | 38:BC:37:PHE:HB3 | 1.81 | 0.61 |
| 36:BA:2189:U:H2' | 36:BA:2190:G:O4' | 2.00 | 0.61 |
| 36:BA:2628:C:H1' | 36:BA:2781:A:H2' | 1.83 | 0.61 |
| 36:BA:709:U:H2' | 36:BA:710:G:H8 | 1.64 | 0.61 |
| 39:BD:25:THR:O | 39:BD:26:LYS:O | 2.19 | 0.61 |
| 39:BD:270:ILE:H | 39:BD:270:ILE:CD1 | 2.03 | 0.61 |
| 42:BG:111:LEU:HD21 | 42:BG:179:PRO:HG2 | 1.83 | 0.61 |
| 43:BH:121:ILE:HD11 | 43:BH:140:LYS:HB3 | 1.83 | 0.61 |
| 46:BN:57:ALA:H | 46:BN:124:ALA:HA | 1.66 | 0.61 |
| 48:BP:80:TYR:CD1 | 48:BP:111:ARG:HB3 | 2.35 | 0.61 |
| 50:BR:101:ALA:O | 50:BR:102:GLU:HB2 | 1.98 | 0.61 |
| 52:BT:28:VAL:HG22 | 52:BT:46:GLU:HA | 1.82 | 0.61 |
| 53:BU:54:LYS:O | 53:BU:58:ARG:HG3 | 2.00 | 0.61 |
| 1:AA:490:G:H2' | 1:AA:491:G:C8 | 2.35 | 0.61 |
| 7:AG:149:ARG:HG2 | 7:AG:149:ARG:HH11 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:73:HIS:HB3 | 20:AT:74:LYS:CD | 2.28 | 0.61 |
| 36:BA:1718:G:H5' | 36:BA:1718:G:H8 | 1.66 | 0.61 |
| 26:B0:20:ARG:HD3 | 36:BA:2356:C:O3' | 2.01 | 0.61 |
| 36:BA:2641:G:C5' | 36:BA:2641:G:H8 | 2.12 | 0.61 |
| 36:BA:289:A:H2' | 36:BA:290:G:C8 | 2.36 | 0.61 |
| 36:BA:335:C:H2' | 36:BA:336:C:C6 | 2.36 | 0.61 |
| 36:BA:875:G:H2' | 36:BA:876:C:C6 | 2.35 | 0.61 |
| 37:BB:5:C:O2' | 37:BB:6:C:H5' | 2.01 | 0.61 |
| 38:BC:62:VAL:HG11 | 38:BC:192:PHE:CD1 | 2.36 | 0.61 |
| 38:BC:82:LYS:HD3 | 38:BC:85:GLU:OE1 | 2.01 | 0.61 |
| 39:BD:44:ASN:HB2 | 39:BD:48:ARG:O | 1.99 | 0.61 |
| 40:BE:27:LEU:HD12 | 40:BE:180:ASN:O | 2.01 | 0.61 |
| 40:BE:182:LEU:C | 40:BE:183:LEU:HD12 | 2.21 | 0.61 |
| 42:BG:125:PHE:HB3 | 42:BG:130:ASN:O | 2.01 | 0.61 |
| 43:BH:52:VAL:CB | 43:BH:69:ARG:HD3 | 2.26 | 0.61 |
| 49:BQ:101:ARG:HH11 | 49:BQ:101:ARG:HG3 | 1.65 | 0.61 |
| 51:BS:34:HIS:HB2 | 51:BS:36:TYR:HE1 | 1.65 | 0.61 |
| 57:BY:46:LYS:H | 57:BY:62:GLU:HG2 | 1.66 | 0.61 |
| 58:BZ:11:GLU:H | 58:BZ:11:GLU:CD | 2.03 | 0.61 |
| 58:BZ:26:GLY:HA2 | 58:BZ:85:HIS:HD2 | 1.65 | 0.61 |
| 1:AA:1134:G:N2 | 1:AA:1141:C:C2 | 2.69 | 0.61 |
| 1:AA:80:G:H1 | 1:AA:90:U:H5' | 1.66 | 0.61 |
| 1:AA:80:G:N1 | 1:AA:90:U:H5' | 2.16 | 0.61 |
| 2:AB:17:PHE:O | 2:AB:18:GLY:O | 2.18 | 0.61 |
| 5:AE:11:ILE:HG21 | 5:AE:105:VAL:HG22 | 1.83 | 0.61 |
| 5:AE:147:ASP:HA | 5:AE:150:ARG:NH1 | 2.16 | 0.61 |
| 13:AM:49:THR:C | 13:AM:51:ALA:N | 2.55 | 0.61 |
| 31:B5:36:CYS:SG | 31:B5:48:GLU:O | 2.59 | 0.61 |
| 36:BA:1013:C:O2' | 36:BA:1014:U:H5' | 2.01 | 0.61 |
| 38:BC:30:LYS:HD3 | 38:BC:185:LEU:CD1 | 2.30 | 0.61 |
| 39:BD:96:HIS:CE1 | 39:BD:102:LYS:HZ1 | 2.18 | 0.61 |
| 40:BE:116:VAL:HG21 | 40:BE:122:PHE:CD2 | 2.36 | 0.61 |
| 41:BF:4:VAL:HA | 41:BF:19:GLU:CG | 2.31 | 0.61 |
| 36:BA:558:G:OP1 | 46:BN:111:PRO:HD2 | 2.01 | 0.61 |
| 48:BP:84:ASN:ND2 | 48:BP:116:GLY:HA2 | 2.16 | 0.61 |
| 37:BB:50:G:OP2 | 51:BS:62:LYS:HD3 | 2.01 | 0.61 |
| 52:BT:109:GLU:O | 52:BT:112:ARG:HG2 | 2.01 | 0.61 |
| 52:BT:93:ARG:HG2 | 52:BT:117:ASP:HB2 | 1.82 | 0.61 |
| 52:BT:96:ARG:HB2 | 52:BT:96:ARG:CZ | 2.30 | 0.61 |
| 55:BW:51:LEU:O | 55:BW:51:LEU:HD22 | 2.01 | 0.61 |
| 57:BY:86:ARG:NH2 | 57:BY:95:LYS:NZ | 2.49 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:166:SER:HB2 | 58:BZ:167:PRO:C | 2.21 | 0.61 |
| 4:AD:145:GLU:HG2 | 4:AD:184:LYS:HG2 | 1.83 | 0.60 |
| 6:AF:80:ARG:NH1 | 6:AF:88:VAL:HB | 2.16 | 0.60 |
| 13:AM:40:ASN:HD21 | 13:AM:42:ALA:HB3 | 1.66 | 0.60 |
| 19:AS:47:HIS:O | 19:AS:62:ILE:HG22 | 2.01 | 0.60 |
| 34:B8:55:ALA:HB1 | 48:BP:49:ARG:O | 2.01 | 0.60 |
| 36:BA:1023:U:O2' | 36:BA:1122:G:H5'' | 2.01 | 0.60 |
| 36:BA:2463:C:O2' | 36:BA:2464:C:H5' | 2.01 | 0.60 |
| 36:BA:348:G:H2' | 36:BA:349:G:C8 | 2.36 | 0.60 |
| 36:BA:680:G:H2' | 36:BA:681:G:C8 | 2.36 | 0.60 |
| 42:BG:67:LYS:CD | 42:BG:67:LYS:H | 2.10 | 0.60 |
| 52:BT:48:ILE:O | 52:BT:63:VAL:HG13 | 2.00 | 0.60 |
| 52:BT:65:LYS:HA | 52:BT:65:LYS:HZ1 | 1.64 | 0.60 |
| 55:BW:24:ILE:HG21 | 55:BW:36:LEU:HD21 | 1.81 | 0.60 |
| 56:BX:12:VAL:CG2 | 56:BX:13:LEU:H | 2.14 | 0.60 |
| 56:BX:8:ILE:C | 56:BX:9:LEU:HD23 | 2.20 | 0.60 |
| 58:BZ:108:PRO:N | 58:BZ:141:VAL:HG11 | 2.16 | 0.60 |
| 49:BQ:141:GLN:CD | 58:BZ:72:ARG:HD3 | 2.22 | 0.60 |
| 3:AC:108:ASN:HB3 | 3:AC:111:LEU:HD12 | 1.83 | 0.60 |
| 3:AC:150:LYS:HG3 | 3:AC:169:ALA:HB2 | 1.82 | 0.60 |
| 11:AK:33:THR:HB | 11:AK:38:ASN:N | 2.16 | 0.60 |
| 13:AM:11:ARG:O | 13:AM:13:LYS:N | 2.34 | 0.60 |
| 22:AW:55:U:OP1 | 38:BC:59:ARG:NH1 | 2.34 | 0.60 |
| 25:AZ:25:THR:O | 25:AZ:28:THR:HB | 2.00 | 0.60 |
| 36:BA:1594:G:H2' | 36:BA:1595:G:C8 | 2.36 | 0.60 |
| 36:BA:152:G:H1 | 36:BA:174:C:H42 | 1.48 | 0.60 |
| 36:BA:2183:C:H2' | 36:BA:2184:G:C8 | 2.36 | 0.60 |
| 34:B8:41:ILE:HD12 | 36:BA:2419:U:OP1 | 2.00 | 0.60 |
| 36:BA:614(B):G:H2' | 41:BF:44:ARG:HH11 | 1.66 | 0.60 |
| 39:BD:126:GLN:HG2 | 39:BD:129:ASN:ND2 | 2.16 | 0.60 |
| 42:BG:110:ALA:CB | 42:BG:140:ILE:HD13 | 2.31 | 0.60 |
| 42:BG:52:ILE:HG12 | 42:BG:53:LEU:N | 2.13 | 0.60 |
| 43:BH:40:GLU:O | 43:BH:41:MET:HB3 | 2.01 | 0.60 |
| 47:BO:65:THR:HA | 47:BO:82:ASN:OD1 | 2.01 | 0.60 |
| 48:BP:85:LEU:HA | 48:BP:88:LEU:HB3 | 1.83 | 0.60 |
| 53:BU:79:PHE:HD1 | 53:BU:80:ILE:HD13 | 1.66 | 0.60 |
| 1:AA:614:A:O2' | 1:AA:615:C:H5' | 2.00 | 0.60 |
| 1:AA:67:C:H2' | 1:AA:68:G:C8 | 2.35 | 0.60 |
| 1:AA:697:U:H2' | 1:AA:698:G:H5' | 1.82 | 0.60 |
| 1:AA:996:A:H2' | 1:AA:997:U:C6 | 2.36 | 0.60 |
| 10:AJ:78:ASN:HD22 | 10:AJ:80:LYS:CB | 2.13 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AW:42:C:H2' | 22:AW:43:C:C6 | 2.37 | 0.60 |
| 24:AY:61:C:H2' | 24:AY:62:U:C5' | 2.30 | 0.60 |
| 26:B0:40:GLN:OE1 | 26:B0:44:ARG:HB2 | 2.00 | 0.60 |
| 32:B6:6:ARG:CB | 32:B6:6:ARG:HH11 | 2.12 | 0.60 |
| 36:BA:2692:C:H2' | 36:BA:2693:A:H8 | 1.65 | 0.60 |
| 36:BA:298:G:H5' | 36:BA:299:A:OP1 | 2.01 | 0.60 |
| 38:BC:120:MET:HE1 | 38:BC:138:PRO:HB2 | 1.83 | 0.60 |
| 46:BN:67:LEU:O | 46:BN:68:GLU:HB2 | 2.01 | 0.60 |
| 48:BP:122:PRO:HB3 | 48:BP:141:ALA:CB | 2.31 | 0.60 |
| 50:BR:87:TYR:OH | 50:BR:116:LEU:O | 2.18 | 0.60 |
| 58:BZ:166:SER:HB2 | 58:BZ:167:PRO:CA | 2.31 | 0.60 |
| 1:AA:345:C:H1' | 1:AA:346:G:N2 | 2.16 | 0.60 |
| 2:AB:142:LEU:O | 2:AB:142:LEU:HD23 | 2.02 | 0.60 |
| 5:AE:137:GLU:O | 5:AE:141:GLN:HG3 | 2.00 | 0.60 |
| 8:AH:82:HIS:HD2 | 8:AH:138:TRP:NE1 | 1.99 | 0.60 |
| 17:AQ:92:ARG:HA | 17:AQ:95:TYR:CE2 | 2.36 | 0.60 |
| 20:AT:100:ILE:HD12 | 20:AT:100:ILE:N | 2.15 | 0.60 |
| 34:B8:41:ILE:HG12 | 34:B8:41:ILE:O | 2.01 | 0.60 |
| 35:B9:17:ILE:HG21 | 35:B9:19:ARG:NH2 | 2.09 | 0.60 |
| 36:BA:2167:U:H3 | 36:BA:2171:A:N6 | 1.98 | 0.60 |
| 36:BA:2538:C:H2' | 36:BA:2539:C:H6 | 1.65 | 0.60 |
| 38:BC:42:GLU:CB | 38:BC:215:THR:HG23 | 2.23 | 0.60 |
| 39:BD:215:LEU:HD13 | 39:BD:217:ARG:HH21 | 1.65 | 0.60 |
| 40:BE:132:HIS:HA | 40:BE:135:HIS:CE1 | 2.36 | 0.60 |
| 40:BE:14:ILE:HD11 | 40:BE:173:VAL:CG1 | 2.28 | 0.60 |
| 40:BE:4:ILE:CD1 | 40:BE:28:ALA:HB1 | 2.31 | 0.60 |
| 47:BO:1:MET:HB3 | 47:BO:32:TYR:CD2 | 2.35 | 0.60 |
| 50:BR:96:ARG:NH2 | 50:BR:117:VAL:HG23 | 2.16 | 0.60 |
| 50:BR:38:VAL:CB | 50:BR:39:PRO:HD3 | 2.25 | 0.60 |
| 51:BS:56:LEU:HD23 | 51:BS:56:LEU:O | 2.01 | 0.60 |
| 55:BW:24:ILE:O | 55:BW:27:LYS:HG3 | 2.02 | 0.60 |
| 55:BW:29:LEU:HD21 | 55:BW:33:ARG:HH11 | 1.66 | 0.60 |
| 56:BX:23:GLU:O | 56:BX:25:LYS:N | 2.33 | 0.60 |
| 1:AA:1003:G:N2 | 1:AA:1038:C:C4 | 2.69 | 0.60 |
| 1:AA:197:A:O2' | 1:AA:198:G:C8 | 2.55 | 0.60 |
| 3:AC:16:ARG:CB | 3:AC:16:ARG:HH11 | 2.15 | 0.60 |
| 5:AE:36:ASP:OD1 | 5:AE:38:GLN:N | 2.33 | 0.60 |
| 7:AG:113:GLU:CB | 7:AG:119:ARG:HG2 | 2.31 | 0.60 |
| 11:AK:38:ASN:HD22 | 11:AK:38:ASN:N | 2.00 | 0.60 |
| 11:AK:61:ALA:HB2 | 11:AK:90:GLY:HA3 | 1.84 | 0.60 |
| 12:AL:41:ARG:HH22 | 12:AL:57:LYS:HZ3 | 1.50 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:AW:43:C:C2 | 22:AW:44:G:H1' | 2.37 | 0.60 |
| 28:B2:2:LYS:HB2 | 36:BA:97:C:H5'' | 1.84 | 0.60 |
| 31:B5:48:GLU:O | 31:B5:49:CYS:SG | 2.60 | 0.60 |
| 36:BA:116:C:O2' | 36:BA:117:G:H5' | 2.01 | 0.60 |
| 36:BA:1526:G:O2' | 36:BA:1527:G:H5' | 2.02 | 0.60 |
| 36:BA:1643:G:H2' | 36:BA:1644:C:H6 | 1.67 | 0.60 |
| 36:BA:2668:G:O2' | 36:BA:2669:G:H5' | 2.00 | 0.60 |
| 36:BA:2730:C:O2' | 36:BA:2731:G:H5' | 2.01 | 0.60 |
| 29:B3:17:LYS:HG2 | 36:BA:969:U:OP1 | 2.02 | 0.60 |
| 38:BC:42:GLU:HB2 | 38:BC:215:THR:O | 2.01 | 0.60 |
| 41:BF:32:LEU:O | 41:BF:32:LEU:HD23 | 2.01 | 0.60 |
| 42:BG:115:ARG:HH12 | 42:BG:137:GLU:HG3 | 1.66 | 0.60 |
| 51:BS:88:ASP:CG | 51:BS:89:ARG:N | 2.55 | 0.60 |
| 53:BU:111:GLU:O | 53:BU:115:ALA:HB2 | 2.02 | 0.60 |
| 53:BU:90:VAL:HG12 | 53:BU:91:ASP:N | 2.15 | 0.60 |
| 55:BW:97:LYS:HE3 | 55:BW:99:ARG:CZ | 2.31 | 0.60 |
| 3:AC:84:ILE:HG12 | 3:AC:84:ILE:O | 2.00 | 0.60 |
| 7:AG:75:VAL:HA | 7:AG:88:PRO:HA | 1.83 | 0.60 |
| 10:AJ:5:ARG:O | 10:AJ:99:LYS:HB2 | 2.01 | 0.60 |
| 22:AV:20:U:H5' | 22:AV:21:A:OP2 | 2.02 | 0.60 |
| 25:AZ:32:THR:CG2 | 25:AZ:44:VAL:HA | 2.31 | 0.60 |
| 25:AZ:55:GLU:O | 25:AZ:59:ARG:HB3 | 2.01 | 0.60 |
| 32:B6:53:LYS:O | 32:B6:54:ILE:HG22 | 2.01 | 0.60 |
| 36:BA:1328:G:H2' | 36:BA:1330:C:C5 | 2.37 | 0.60 |
| 36:BA:2681:C:H2' | 36:BA:2681:C:O2 | 2.01 | 0.60 |
| 36:BA:659:C:H4' | 41:BF:100:THR:O | 2.01 | 0.60 |
| 37:BB:54:G:O2' | 37:BB:55:U:H5' | 2.02 | 0.60 |
| 40:BE:116:VAL:O | 40:BE:117:MET:CB | 2.49 | 0.60 |
| 40:BE:82:ARG:HG3 | 40:BE:82:ARG:HH11 | 1.66 | 0.60 |
| 40:BE:8:LYS:O | 40:BE:193:GLY:HA2 | 2.01 | 0.60 |
| 42:BG:73:ALA:O | 42:BG:85:GLY:HA2 | 2.02 | 0.60 |
| 47:BO:26:LYS:HB2 | 47:BO:30:ALA:CB | 2.31 | 0.60 |
| 54:BV:5:VAL:HG23 | 54:BV:37:VAL:O | 2.01 | 0.60 |
| 28:B2:30:ARG:HB2 | 56:BX:5:TYR:CE1 | 2.37 | 0.60 |
| 1:AA:161:A:H2' | 1:AA:162:A:H8 | 1.65 | 0.60 |
| 1:AA:80:G:C3' | 1:AA:81:U:H5' | 2.32 | 0.60 |
| 3:AC:17:ASP:OD1 | 3:AC:18:TRP:N | 2.34 | 0.60 |
| 9:AI:49:PRO:HB3 | 9:AI:101:PHE:CD2 | 2.35 | 0.60 |
| 10:AJ:51:ARG:NH1 | 10:AJ:60:ARG:O | 2.35 | 0.60 |
| 17:AQ:8:GLY:HA3 | 17:AQ:21:VAL:CG1 | 2.31 | 0.60 |
| 25:AZ:35:THR:HG22 | 25:AZ:203:LEU:CD1 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:B0:43:THR:O | 26:B0:43:THR:CG2 | 2.49 | 0.60 |
| 36:BA:1529:G:O2' | 36:BA:1530:C:H5' | 2.02 | 0.60 |
| 36:BA:1866:C:H2' | 36:BA:1876:A:O4' | 2.02 | 0.60 |
| 36:BA:2163:C:H3' | 36:BA:2164:C:C6 | 2.36 | 0.60 |
| 36:BA:2223:G:C2' | 36:BA:2224:G:H5' | 2.32 | 0.60 |
| 36:BA:672:C:C2' | 36:BA:673:C:C5' | 2.78 | 0.60 |
| 36:BA:860:U:C5 | 36:BA:917:A:N7 | 2.67 | 0.60 |
| 38:BC:155:GLU:O | 38:BC:160:ARG:HB2 | 2.01 | 0.60 |
| 38:BC:94:VAL:CG1 | 38:BC:95:GLY:H | 2.14 | 0.60 |
| 39:BD:32:SER:O | 39:BD:36:PRO:HG3 | 2.02 | 0.60 |
| 41:BF:5:ALA:HB3 | 41:BF:18:ARG:O | 2.01 | 0.60 |
| 42:BG:133:LEU:HD11 | 42:BG:157:ILE:HB | 1.82 | 0.60 |
| 43:BH:54:ARG:HG2 | 43:BH:54:ARG:HH11 | 1.65 | 0.60 |
| 48:BP:112:LEU:HD22 | 48:BP:113:LYS:N | 2.17 | 0.60 |
| 48:BP:23:PRO:CB | 48:BP:33:ARG:HG3 | 2.29 | 0.60 |
| 48:BP:33:ARG:O | 48:BP:34:GLY:C | 2.40 | 0.60 |
| 50:BR:55:ALA:HB2 | 50:BR:79:LEU:CD1 | 2.32 | 0.60 |
| 53:BU:62:ILE:HG23 | 53:BU:76:TYR:CE1 | 2.37 | 0.60 |
| 53:BU:68:ALA:HB1 | 53:BU:106:PHE:HE2 | 1.67 | 0.60 |
| 57:BY:60:PHE:HA | 57:BY:62:GLU:OE2 | 2.01 | 0.60 |
| 1:AA:1003:G:H2' | 1:AA:1004:A:C4' | 2.28 | 0.60 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.36 | 0.60 |
| 1:AA:353:A:C8 | 1:AA:353:A:H5' | 2.37 | 0.60 |
| 6:AF:30:LEU:HB3 | 6:AF:35:ALA:HB3 | 1.83 | 0.60 |
| 9:AI:104:ARG:HD3 | 9:AI:105:ASP:N | 2.16 | 0.60 |
| 25:AZ:185:ASN:ND2 | 25:AZ:188:THR:HB | 2.16 | 0.60 |
| 36:BA:1718:G:O2' | 36:BA:1719:G:H5' | 2.02 | 0.60 |
| 36:BA:2147:G:C2' | 36:BA:2148:G:H5' | 2.32 | 0.60 |
| 36:BA:30:G:H2' | 36:BA:31:C:H6 | 1.67 | 0.60 |
| 36:BA:729:G:OP2 | 39:BD:13:ARG:NH1 | 2.35 | 0.60 |
| 36:BA:2580:U:H5' | 40:BE:131:ALA:H | 1.67 | 0.60 |
| 41:BF:126:VAL:HG11 | 41:BF:142:TRP:HH2 | 1.66 | 0.60 |
| 41:BF:95:ARG:HG3 | 41:BF:95:ARG:O | 2.02 | 0.60 |
| 42:BG:172:LEU:HD23 | 42:BG:176:LEU:HD12 | 1.82 | 0.60 |
| 30:B4:9:LEU:CG | 42:BG:98:ARG:HH12 | 2.15 | 0.60 |
| 46:BN:57:ALA:HB3 | 46:BN:124:ALA:CA | 2.30 | 0.60 |
| 46:BN:5:VAL:CG1 | 46:BN:7:LYS:HG3 | 2.28 | 0.60 |
| 47:BO:20:MET:HE3 | 47:BO:44:LYS:HE3 | 1.83 | 0.60 |
| 47:BO:98:VAL:CG1 | 47:BO:117:LEU:HB3 | 2.32 | 0.60 |
| 48:BP:7:ARG:HB3 | 48:BP:8:PRO:CD | 2.31 | 0.60 |
| 1:AA:1050:G:O2' | 1:AA:1051:C:P | 2.60 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1151:A:HO2' | 1:AA:1152:A:H8 | 1.50 | 0.60 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:C8 | 2.70 | 0.60 |
| 1:AA:190:U:O2' | 1:AA:191:G:H5' | 2.02 | 0.60 |
| 2:AB:61:LEU:O | 2:AB:64:ARG:HG2 | 2.02 | 0.60 |
| 14:AN:55:GLY:O | 14:AN:56:VAL:C | 2.40 | 0.60 |
| 20:AT:18:GLN:O | 20:AT:22:ARG:HG3 | 2.02 | 0.60 |
| 24:AY:15:A:H3' | 24:AY:16:H2U:H5'' | 1.83 | 0.60 |
| 25:AZ:163:PHE:O | 25:AZ:165:GLY:N | 2.31 | 0.60 |
| 32:B6:22:ALA:C | 32:B6:23:THR:HG23 | 2.21 | 0.60 |
| 36:BA:1106:G:C2 | 36:BA:1107:G:H1' | 2.36 | 0.60 |
| 36:BA:1170:G:N2 | 36:BA:1179:C:H42 | 1.93 | 0.60 |
| 36:BA:1773:A:H2' | 36:BA:1774:C:H5' | 1.83 | 0.60 |
| 36:BA:2138:C:H2' | 36:BA:2139:C:H6 | 1.66 | 0.60 |
| 36:BA:2502:G:H5'' | 36:BA:2503:A:H5'' | 1.84 | 0.60 |
| 40:BE:94:GLU:OE2 | 40:BE:177:PRO:HB3 | 2.02 | 0.60 |
| 41:BF:118:ALA:HA | 41:BF:123:LEU:HB2 | 1.83 | 0.60 |
| 42:BG:97:ASP:H | 42:BG:100:TRP:HD1 | 1.49 | 0.60 |
| 48:BP:9:ASN:H | 48:BP:10:PRO:CD | 2.05 | 0.60 |
| 49:BQ:101:ARG:HG3 | 49:BQ:101:ARG:NH1 | 2.17 | 0.60 |
| 53:BU:13:LYS:N | 53:BU:13:LYS:HD3 | 2.17 | 0.60 |
| 53:BU:5:LYS:HG3 | 53:BU:7:GLY:N | 2.16 | 0.60 |
| 1:AA:1320:C:H6 | 1:AA:1320:C:C5' | 2.13 | 0.60 |
| 5:AE:20:GLN:NE2 | 5:AE:25:ARG:NE | 2.49 | 0.60 |
| 5:AE:7:GLU:O | 5:AE:8:GLU:HB3 | 2.02 | 0.60 |
| 9:AI:114:TYR:O | 9:AI:114:TYR:CD2 | 2.54 | 0.60 |
| 13:AM:49:THR:C | 13:AM:51:ALA:H | 2.05 | 0.60 |
| 20:AT:13:LEU:HD23 | 20:AT:13:LEU:N | 2.17 | 0.60 |
| 25:AZ:201:GLU:O | 25:AZ:205:ALA:HB2 | 2.02 | 0.60 |
| 25:AZ:310:ILE:HG22 | 25:AZ:310:ILE:O | 2.02 | 0.60 |
| 25:AZ:324:LYS:HD3 | 25:AZ:326:GLU:H | 1.65 | 0.60 |
| 25:AZ:21:ASP:N | 61:AZ:501:GCP:H3B1 | 2.17 | 0.60 |
| 36:BA:2257:U:O2' | 36:BA:2258:C:H5' | 2.01 | 0.60 |
| 36:BA:2579:C:O3' | 40:BE:131:ALA:HB2 | 2.02 | 0.60 |
| 36:BA:8:A:H2' | 36:BA:9:U:C5 | 2.37 | 0.60 |
| 22:AW:55:U:C5' | 38:BC:164:ARG:HH22 | 2.11 | 0.60 |
| 38:BC:186:ALA:O | 38:BC:190:ARG:HG3 | 2.02 | 0.60 |
| 36:BA:2175:C:O2 | 38:BC:44:HIS:NE2 | 2.35 | 0.60 |
| 39:BD:148:GLU:HB2 | 39:BD:151:LYS:HD2 | 1.82 | 0.60 |
| 39:BD:72:LYS:HZ3 | 39:BD:75:ILE:HG13 | 1.67 | 0.60 |
| 41:BF:120:GLU:HB3 | 41:BF:122:LYS:HE3 | 1.83 | 0.60 |
| 46:BN:56:ASN:N | 46:BN:125:GLY:H | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:BS:17:ARG:O | 51:BS:19:LYS:N | 2.35 | 0.60 |
| 51:BS:49:VAL:HG12 | 51:BS:50:SER:N | 2.12 | 0.60 |
| 51:BS:96:GLY:C | 51:BS:98:VAL:H | 2.03 | 0.60 |
| 56:BX:10:ALA:HB3 | 56:BX:29:TRP:HD1 | 1.66 | 0.60 |
| 58:BZ:57:ILE:HD12 | 58:BZ:57:ILE:N | 2.17 | 0.60 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:C8 | 2.36 | 0.59 |
| 8:AH:39:LEU:HB3 | 8:AH:45:ILE:HG12 | 1.84 | 0.59 |
| 8:AH:68:ARG:NH1 | 8:AH:68:ARG:HG2 | 2.15 | 0.59 |
| 19:AS:42:PRO:O | 19:AS:44:MET:SD | 2.60 | 0.59 |
| 19:AS:61:TYR:O | 19:AS:62:ILE:HB | 2.01 | 0.59 |
| 20:AT:22:ARG:O | 20:AT:26:ASN:ND2 | 2.35 | 0.59 |
| 22:AW:44:G:H2' | 22:AW:44:G:N3 | 2.16 | 0.59 |
| 36:BA:1257:C:H4' | 41:BF:83:PHE:CD2 | 2.36 | 0.59 |
| 36:BA:1899:G:H22 | 36:BA:1902:C:N4 | 1.97 | 0.59 |
| 36:BA:2185:C:C2' | 36:BA:2186:G:H5' | 2.31 | 0.59 |
| 36:BA:585:G:H2' | 36:BA:586:A:N7 | 2.17 | 0.59 |
| 36:BA:621:A:C2' | 36:BA:622:G:H5' | 2.29 | 0.59 |
| 39:BD:33:LEU:HD23 | 39:BD:33:LEU:C | 2.22 | 0.59 |
| 41:BF:52:LYS:O | 41:BF:88:VAL:HG12 | 2.02 | 0.59 |
| 51:BS:14:VAL:O | 51:BS:15:ARG:C | 2.39 | 0.59 |
| 52:BT:106:SER:O | 52:BT:107:ASP:OD1 | 2.20 | 0.59 |
| 52:BT:27:THR:O | 52:BT:28:VAL:CB | 2.50 | 0.59 |
| 52:BT:19:LEU:HD13 | 52:BT:78:LEU:CD2 | 2.32 | 0.59 |
| 1:AA:1281:U:H4' | 1:AA:1282:C:OP2 | 2.00 | 0.59 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:H8 | 2.00 | 0.59 |
| 1:AA:176:C:H2' | 1:AA:177:C:H6 | 1.67 | 0.59 |
| 1:AA:524:G:H2' | 1:AA:525:C:C6 | 2.37 | 0.59 |
| 2:AB:172:ILE:H | 2:AB:172:ILE:CD1 | 2.12 | 0.59 |
| 14:AN:57:ARG:HH11 | 14:AN:57:ARG:CG | 2.15 | 0.59 |
| 18:AR:67:ALA:O | 18:AR:71:LYS:HG3 | 2.02 | 0.59 |
| 26:B0:36:ILE:HD11 | 36:BA:2355:C:H1' | 1.83 | 0.59 |
| 31:B5:50:GLY:CA | 31:B5:56:LYS:HD3 | 2.32 | 0.59 |
| 36:BA:1047:G:C2 | 36:BA:1110:G:H2' | 2.37 | 0.59 |
| 36:BA:1048:A:H2 | 36:BA:1112:G:H21 | 1.47 | 0.59 |
| 36:BA:2068:U:H3 | 36:BA:2430:A:H2 | 1.50 | 0.59 |
| 36:BA:272(J):C:C3' | 36:BA:274:G:H5'' | 2.32 | 0.59 |
| 36:BA:2869:G:H2' | 36:BA:2870:C:O4' | 2.02 | 0.59 |
| 36:BA:291:C:H2' | 36:BA:292:C:H6 | 1.67 | 0.59 |
| 36:BA:614:U:H2' | 36:BA:614(A):U:H5' | 1.84 | 0.59 |
| 36:BA:93:G:H2' | 36:BA:94:C:C6 | 2.37 | 0.59 |
| 37:BB:114:C:H2' | 37:BB:115:G:C8 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 38:BC:212:VAL:O | 38:BC:224:ILE:HG12 | 2.02 | 0.59 |
| 43:BH:44:VAL:HG12 | 43:BH:45:VAL:H | 1.67 | 0.59 |
| 47:BO:19:ILE:HD12 | 47:BO:41:ALA:HB3 | 1.84 | 0.59 |
| 4:AD:133:VAL:HG12 | 4:AD:135:LEU:H | 1.66 | 0.59 |
| 6:AF:19:LEU:HD11 | 6:AF:59:TYR:CZ | 2.38 | 0.59 |
| 9:AI:104:ARG:HG3 | 9:AI:104:ARG:HH11 | 1.67 | 0.59 |
| 12:AL:119:LYS:O | 12:AL:120:TYR:CB | 2.49 | 0.59 |
| 25:AZ:150:VAL:O | 25:AZ:154:VAL:HG23 | 2.02 | 0.59 |
| 25:AZ:211:PRO:HG2 | 25:AZ:213:PRO:HD3 | 1.84 | 0.59 |
| 27:B1:48:LYS:HZ2 | 27:B1:61:ARG:HG2 | 1.67 | 0.59 |
| 36:BA:1188:U:C2' | 36:BA:1189:A:H5' | 2.32 | 0.59 |
| 36:BA:1509(A):A:H2' | 36:BA:1509(B):A:C8 | 2.37 | 0.59 |
| 36:BA:1644:C:O2 | 36:BA:1644:C:H2' | 2.01 | 0.59 |
| 36:BA:2423:U:C6 | 36:BA:2423:U:H5' | 2.37 | 0.59 |
| 36:BA:2791:C:N4 | 36:BA:2801(A):A:H62 | 1.99 | 0.59 |
| 36:BA:419:C:H2' | 36:BA:420:C:H6 | 1.67 | 0.59 |
| 36:BA:94:C:H5' | 36:BA:94(A):G:OP2 | 2.02 | 0.59 |
| 38:BC:180:PHE:CD2 | 38:BC:184:LYS:HG3 | 2.37 | 0.59 |
| 40:BE:10:GLY:HA2 | 40:BE:192:ASN:OD1 | 2.02 | 0.59 |
| 41:BF:192:LEU:HD23 | 41:BF:192:LEU:C | 2.23 | 0.59 |
| 46:BN:42:TRP:CZ2 | 46:BN:44:PRO:HB3 | 2.37 | 0.59 |
| 48:BP:85:LEU:HA | 48:BP:88:LEU:CB | 2.32 | 0.59 |
| 51:BS:67:ARG:HH21 | 51:BS:100:ALA:HB3 | 1.66 | 0.59 |
| 51:BS:77:ALA:HB1 | 51:BS:82:ILE:O | 2.03 | 0.59 |
| 53:BU:29:SER:O | 53:BU:30:LYS:HD3 | 2.02 | 0.59 |
| 55:BW:88:ARG:HB3 | 55:BW:92:ARG:HB2 | 1.84 | 0.59 |
| 57:BY:95:LYS:CG | 57:BY:100:ALA:HA | 2.31 | 0.59 |
| 58:BZ:76:LEU:O | 58:BZ:77:ASP:HB2 | 2.01 | 0.59 |
| 18:AR:53:ARG:C | 18:AR:55:ARG:H | 2.05 | 0.59 |
| 22:AW:43:C:H3' | 22:AW:44:G:O4' | 2.03 | 0.59 |
| 25:AZ:122:LEU:O | 25:AZ:126:VAL:HG23 | 2.03 | 0.59 |
| 25:AZ:130:TYR:CD2 | 25:AZ:211:PRO:HD3 | 2.37 | 0.59 |
| 34:B8:50:LEU:H | 34:B8:53:PRO:CD | 2.15 | 0.59 |
| 34:B8:52:LYS:N | 34:B8:53:PRO:CD | 2.66 | 0.59 |
| 36:BA:1771:C:C1' | 36:BA:1786:A:H8 | 2.14 | 0.59 |
| 36:BA:2115:G:H4' | 36:BA:2167:U:O2 | 2.02 | 0.59 |
| 36:BA:214:G:H1' | 36:BA:216:A:O2' | 2.02 | 0.59 |
| 36:BA:2184:G:H2' | 36:BA:2185:C:O4' | 2.02 | 0.59 |
| 36:BA:2327:A:H2' | 36:BA:2328:A:C8 | 2.37 | 0.59 |
| 36:BA:2386:C:H2' | 36:BA:2387:U:C6 | 2.36 | 0.59 |
| 36:BA:2496:C:O2' | 36:BA:2497:A:H5' | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:310:A:OP1 | 57:BY:17:SER:O | 2.19 | 0.59 |
| 36:BA:363(A):A:N3 | 36:BA:363(A):A:H2' | 2.16 | 0.59 |
| 36:BA:672:C:O2' | 36:BA:673:C:H5'' | 2.00 | 0.59 |
| 38:BC:58:VAL:O | 38:BC:59:ARG:HB2 | 2.03 | 0.59 |
| 42:BG:36:LYS:HG2 | 42:BG:37:VAL:N | 2.16 | 0.59 |
| 43:BH:30:LYS:HA | 43:BH:30:LYS:HE2 | 1.84 | 0.59 |
| 43:BH:51:ARG:O | 43:BH:52:VAL:HB | 2.03 | 0.59 |
| 47:BO:104:ARG:CZ | 47:BO:104:ARG:HB3 | 2.32 | 0.59 |
| 47:BO:87:ILE:HG22 | 47:BO:88:ASN:N | 2.17 | 0.59 |
| 50:BR:92:GLY:N | 50:BR:94:TYR:HE2 | 2.00 | 0.59 |
| 51:BS:89:ARG:HB3 | 51:BS:92:TYR:HB3 | 1.83 | 0.59 |
| 58:BZ:28:MET:CE | 58:BZ:33:LEU:HD21 | 2.32 | 0.59 |
| 1:AA:1016:A:H2' | 1:AA:1017:G:O4' | 2.02 | 0.59 |
| 1:AA:1117:G:H5' | 1:AA:1117:G:H8 | 1.67 | 0.59 |
| 1:AA:337:C:H2' | 1:AA:338:A:C8 | 2.38 | 0.59 |
| 1:AA:404:U:H2' | 1:AA:405:U:C6 | 2.37 | 0.59 |
| 1:AA:591:U:H2' | 1:AA:592:G:H8 | 1.67 | 0.59 |
| 10:AJ:46:ARG:HG2 | 10:AJ:46:ARG:HH11 | 1.67 | 0.59 |
| 12:AL:8:ASN:HD22 | 17:AQ:34:LYS:HE2 | 1.68 | 0.59 |
| 19:AS:78:ARG:H | 19:AS:81:ARG:HH12 | 1.50 | 0.59 |
| 24:AY:65:C:C5' | 25:AZ:341:GLN:HG2 | 2.32 | 0.59 |
| 24:AY:75:C:H5 | 25:AZ:232:THR:N | 1.97 | 0.59 |
| 25:AZ:113:MET:HB3 | 25:AZ:114:PRO:HD2 | 1.84 | 0.59 |
| 31:B5:57:VAL:HG12 | 31:B5:58:LEU:CD1 | 2.28 | 0.59 |
| 36:BA:850:C:H2' | 36:BA:851:U:H6 | 1.67 | 0.59 |
| 36:BA:90:U:H2' | 36:BA:90:U:O2 | 2.01 | 0.59 |
| 40:BE:38:THR:HG22 | 40:BE:40:GLU:H | 1.67 | 0.59 |
| 41:BF:39:TRP:CH2 | 41:BF:106:ARG:HD2 | 2.38 | 0.59 |
| 41:BF:24:LEU:CB | 41:BF:25:PRO:HD2 | 2.15 | 0.59 |
| 42:BG:95:ARG:O | 42:BG:96:ARG:O | 2.18 | 0.59 |
| 43:BH:68:THR:HA | 43:BH:71:LEU:HB2 | 1.84 | 0.59 |
| 57:BY:50:ARG:HD2 | 57:BY:53:PRO:HA | 1.82 | 0.59 |
| 1:AA:1175:G:O2' | 1:AA:1176:A:H5' | 2.03 | 0.59 |
| 1:AA:1269:A:C2 | 1:AA:1313:U:C2 | 2.90 | 0.59 |
| 1:AA:837:G:H22 | 1:AA:850:U:H1' | 1.66 | 0.59 |
| 2:AB:235:SER:OG | 2:AB:236:TYR:HD1 | 1.85 | 0.59 |
| 3:AC:5:ILE:CD1 | 3:AC:5:ILE:H | 2.12 | 0.59 |
| 1:AA:195:A:OP1 | 20:AT:65:LYS:HE2 | 2.03 | 0.59 |
| 25:AZ:16:THR:CG2 | 25:AZ:81:ASP:HA | 2.32 | 0.59 |
| 32:B6:18:ARG:HG3 | 32:B6:19:ARG:N | 2.17 | 0.59 |
| 31:B5:4:HIS:O | 36:BA:2056:G:N2 | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:2873:A:H1' | 50:BR:6:SER:OG | 2.02 | 0.59 |
| 39:BD:72:LYS:HD2 | 39:BD:103:ARG:NH1 | 2.17 | 0.59 |
| 39:BD:72:LYS:HB3 | 39:BD:72:LYS:NZ | 2.17 | 0.59 |
| 43:BH:125:VAL:O | 43:BH:125:VAL:HG12 | 2.03 | 0.59 |
| 46:BN:46:VAL:O | 46:BN:47:ALA:HB3 | 2.02 | 0.59 |
| 49:BQ:67:ARG:HB3 | 49:BQ:67:ARG:NH1 | 2.18 | 0.59 |
| 55:BW:1:MET:HG3 | 55:BW:64:MET:CE | 2.32 | 0.59 |
| 1:AA:1145:C:O2' | 1:AA:1146:A:H8 | 1.86 | 0.59 |
| 1:AA:1202:G:H2' | 1:AA:1203:C:H5' | 1.84 | 0.59 |
| 1:AA:346:G:O2' | 1:AA:347:G:H8 | 1.85 | 0.59 |
| 1:AA:878:G:H1' | 8:AH:3:THR:HG21 | 1.85 | 0.59 |
| 2:AB:223:ILE:HG21 | 2:AB:230:VAL:HG22 | 1.83 | 0.59 |
| 4:AD:105:VAL:HG21 | 4:AD:121:VAL:HG22 | 1.83 | 0.59 |
| 8:AH:112:LEU:HB2 | 8:AH:132:GLU:O | 2.02 | 0.59 |
| 9:AI:10:ARG:HG3 | 9:AI:75:ASP:CB | 2.33 | 0.59 |
| 1:AA:972:C:O2 | 10:AJ:55:LYS:HG3 | 2.03 | 0.59 |
| 12:AL:110:VAL:CG2 | 12:AL:120:TYR:HB3 | 2.33 | 0.59 |
| 15:AO:9:GLN:NE2 | 15:AO:12:ILE:HD12 | 2.17 | 0.59 |
| 19:AS:43:GLU:C | 19:AS:45:VAL:H | 2.05 | 0.59 |
| 36:BA:1301:A:H4' | 36:BA:1302:A:OP1 | 2.02 | 0.59 |
| 36:BA:133:C:N3 | 36:BA:146:G:O6 | 2.35 | 0.59 |
| 36:BA:1688:U:H5' | 36:BA:1689:A:OP1 | 2.03 | 0.59 |
| 36:BA:2308:G:N7 | 36:BA:2310:A:H5' | 2.17 | 0.59 |
| 36:BA:2555:U:H2' | 36:BA:2556:C:H5' | 1.83 | 0.59 |
| 36:BA:2653:U:H5' | 36:BA:2654:A:OP2 | 2.02 | 0.59 |
| 36:BA:2674:G:H2' | 36:BA:2675:A:C8 | 2.38 | 0.59 |
| 36:BA:2852:G:H2' | 36:BA:2853:C:C6 | 2.37 | 0.59 |
| 38:BC:149:ILE:HG23 | 38:BC:150:GLY:N | 2.16 | 0.59 |
| 36:BA:1654:A:N3 | 40:BE:113:PHE:HD2 | 2.01 | 0.59 |
| 1:AA:1441:G:H4' | 1:AA:1442:G:C4 | 2.37 | 0.59 |
| 1:AA:475:G:H2' | 1:AA:476:G:H8 | 1.66 | 0.59 |
| 2:AB:193:ASP:C | 2:AB:193:ASP:OD2 | 2.41 | 0.59 |
| 3:AC:22:TRP:CG | 3:AC:59:ARG:HG3 | 2.38 | 0.59 |
| 5:AE:12:LEU:HD21 | 5:AE:14:ARG:HB3 | 1.84 | 0.59 |
| 8:AH:44:PHE:CE2 | 8:AH:109:ILE:HG21 | 2.38 | 0.59 |
| 15:AO:69:TYR:CE1 | 15:AO:73:GLU:HG3 | 2.36 | 0.59 |
| 24:AY:77:TRP:N | 25:AZ:272:MET:HA | 2.17 | 0.59 |
| 34:B8:39:LYS:HE3 | 36:BA:2365:G:O6 | 2.02 | 0.59 |
| 36:BA:2115:G:C3' | 36:BA:2116:G:H5'' | 2.33 | 0.59 |
| 36:BA:89:G:H3' | 36:BA:90:U:H5'' | 1.83 | 0.59 |
| 39:BD:62:TYR:CE1 | 39:BD:64:ILE:HA | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:BO:8:LEU:N | 47:BO:8:LEU:CD1 | 2.65 | 0.59 |
| 34:B8:25:MET:CE | 48:BP:64:LYS:HD3 | 2.33 | 0.59 |
| 49:BQ:52:VAL:O | 49:BQ:55:VAL:HG13 | 2.03 | 0.59 |
| 53:BU:85:LYS:C | 53:BU:87:GLY:H | 2.05 | 0.59 |
| 1:AA:770:C:O2' | 1:AA:771:G:H5' | 2.03 | 0.59 |
| 1:AA:542:G:H5' | 4:AD:41:GLY:HA3 | 1.85 | 0.59 |
| 10:AJ:4:ILE:O | 10:AJ:74:ILE:HG12 | 2.02 | 0.59 |
| 22:AW:40:C:H2' | 22:AW:41:C:H6 | 1.68 | 0.59 |
| 24:AY:7:G:H3' | 24:AY:8:4SU:H5' | 1.85 | 0.59 |
| 25:AZ:75:ARG:HH12 | 25:AZ:210:ILE:CG2 | 2.16 | 0.59 |
| 36:BA:1799:G:H5' | 36:BA:1819:A:H61 | 1.68 | 0.59 |
| 36:BA:1997:G:O2' | 36:BA:1998:G:H5' | 2.03 | 0.59 |
| 36:BA:2163:C:H3' | 36:BA:2164:C:H6 | 1.68 | 0.59 |
| 36:BA:2824:C:H2' | 36:BA:2825:C:O4' | 2.02 | 0.59 |
| 36:BA:2854:G:H2' | 36:BA:2855:C:C6 | 2.38 | 0.59 |
| 36:BA:481:G:H1' | 36:BA:506:G:H21 | 1.66 | 0.59 |
| 36:BA:672:C:H2' | 36:BA:673:C:H5' | 1.83 | 0.59 |
| 36:BA:876:C:H2' | 36:BA:877:U:O4' | 2.03 | 0.59 |
| 36:BA:2124:G:H1' | 38:BC:42:GLU:CG | 2.33 | 0.59 |
| 41:BF:116:ASP:O | 41:BF:120:GLU:HG2 | 2.03 | 0.59 |
| 48:BP:47:ASP:CB | 48:BP:48:PRO:CA | 2.80 | 0.59 |
| 49:BQ:45:GLN:H | 49:BQ:45:GLN:HE21 | 1.50 | 0.59 |
| 50:BR:29:LEU:CD2 | 50:BR:70:LEU:HD11 | 2.33 | 0.59 |
| 3:AC:58:GLU:HB2 | 3:AC:65:ALA:HB2 | 1.85 | 0.59 |
| 4:AD:170:VAL:CG1 | 4:AD:174:LEU:HB2 | 2.33 | 0.59 |
| 11:AK:84:VAL:HG22 | 11:AK:110:ASP:HA | 1.84 | 0.59 |
| 19:AS:66:MET:HA | 19:AS:69:HIS:HD2 | 1.67 | 0.59 |
| 25:AZ:96:ALA:HA | 25:AZ:99:MET:SD | 2.42 | 0.59 |
| 36:BA:1047:G:H2' | 36:BA:1110:G:H21 | 1.68 | 0.59 |
| 36:BA:1464:C:O2' | 36:BA:1528:A:C8 | 2.52 | 0.59 |
| 36:BA:1967:C:H2' | 36:BA:1968:G:H5' | 1.85 | 0.59 |
| 36:BA:2572:A:C8 | 40:BE:144:ARG:HD3 | 2.37 | 0.59 |
| 36:BA:2713:A:H3' | 36:BA:2714:G:H5' | 1.84 | 0.59 |
| 36:BA:360:G:H2' | 36:BA:361:G:H8 | 1.68 | 0.59 |
| 36:BA:486:C:H2' | 36:BA:487:C:H6 | 1.67 | 0.59 |
| 38:BC:7:TYR:CE1 | 38:BC:220:PRO:HD3 | 2.38 | 0.59 |
| 40:BE:113:PHE:CE1 | 40:BE:158:GLY:HA2 | 2.37 | 0.59 |
| 40:BE:169:ASN:ND2 | 40:BE:169:ASN:O | 2.32 | 0.59 |
| 41:BF:62:ARG:HG2 | 41:BF:62:ARG:HH11 | 1.67 | 0.59 |
| 42:BG:82:LEU:HD22 | 42:BG:87:PRO:HB3 | 1.85 | 0.59 |
| 46:BN:76:SER:OG | 46:BN:77:GLY:N | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 48:BP:90:ARG:HD2 | 48:BP:91:PHE:HD1 | 1.67 | 0.59 |
| 49:BQ:67:ARG:HH11 | 49:BQ:67:ARG:HB3 | 1.68 | 0.59 |
| 52:BT:83:ILE:HG13 | 52:BT:84:GLN:HG2 | 1.85 | 0.59 |
| 1:AA:1004:A:H5'' | 1:AA:1025:U:O4 | 2.02 | 0.58 |
| 1:AA:1503:A:N3 | 23:AX:16:A:C6 | 2.71 | 0.58 |
| 4:AD:70:ILE:HG22 | 4:AD:71:SER:O | 2.03 | 0.58 |
| 7:AG:52:GLU:O | 7:AG:54:THR:N | 2.36 | 0.58 |
| 10:AJ:23:ILE:HG23 | 10:AJ:85:LEU:CD2 | 2.33 | 0.58 |
| 11:AK:18:ARG:NH2 | 11:AK:35:PRO:O | 2.36 | 0.58 |
| 27:B1:44:PRO:HA | 36:BA:396:G:O3' | 2.03 | 0.58 |
| 29:B3:11:SER:HB3 | 36:BA:988:A:P | 2.43 | 0.58 |
| 41:BF:148:LEU:HB3 | 41:BF:172:TRP:HZ3 | 1.67 | 0.58 |
| 41:BF:82:ILE:O | 41:BF:83:PHE:HB2 | 2.02 | 0.58 |
| 47:BO:4:PRO:O | 47:BO:5:GLN:CB | 2.51 | 0.58 |
| 48:BP:6:LEU:N | 48:BP:6:LEU:HD23 | 2.14 | 0.58 |
| 49:BQ:10:ARG:HH11 | 49:BQ:10:ARG:HB2 | 1.67 | 0.58 |
| 53:BU:92:ARG:HD2 | 54:BV:11:GLN:HG2 | 1.85 | 0.58 |
| 1:AA:321:A:C2 | 1:AA:333:G:C2 | 2.91 | 0.58 |
| 2:AB:61:LEU:HA | 2:AB:64:ARG:CZ | 2.32 | 0.58 |
| 9:AI:10:ARG:HG3 | 9:AI:75:ASP:HB3 | 1.85 | 0.58 |
| 10:AJ:20:ALA:C | 10:AJ:22:LYS:H | 2.07 | 0.58 |
| 10:AJ:5:ARG:CG | 10:AJ:71:LEU:HD11 | 2.32 | 0.58 |
| 20:AT:74:LYS:HG2 | 20:AT:75:ASN:N | 2.17 | 0.58 |
| 25:AZ:35:THR:HG22 | 25:AZ:203:LEU:HD11 | 1.85 | 0.58 |
| 36:BA:1165:U:H2' | 36:BA:1166:C:C6 | 2.38 | 0.58 |
| 36:BA:1331:A:C2' | 36:BA:1332:G:H5'' | 2.33 | 0.58 |
| 36:BA:1902:C:H2' | 36:BA:1903:G:O5' | 2.02 | 0.58 |
| 36:BA:2631:G:N2 | 40:BE:61:ARG:NH1 | 2.48 | 0.58 |
| 36:BA:2801(A):A:H4' | 36:BA:2802:G:C5' | 2.27 | 0.58 |
| 36:BA:744:G:O2' | 36:BA:745:G:H5' | 2.03 | 0.58 |
| 49:BQ:36:ALA:O | 49:BQ:37:LEU:HD23 | 2.03 | 0.58 |
| 49:BQ:6:ARG:O | 49:BQ:7:MET:HG3 | 2.03 | 0.58 |
| 49:BQ:97:VAL:HG11 | 49:BQ:103:MET:HE3 | 1.84 | 0.58 |
| 51:BS:104:GLY:C | 51:BS:106:ARG:H | 2.06 | 0.58 |
| 51:BS:74:ALA:HB1 | 51:BS:103:GLU:CG | 2.32 | 0.58 |
| 51:BS:89:ARG:O | 51:BS:92:TYR:HB3 | 2.03 | 0.58 |
| 58:BZ:171:ILE:HG13 | 58:BZ:172:ALA:N | 2.19 | 0.58 |
| 3:AC:20:SER:CB | 3:AC:40:ARG:HH22 | 2.13 | 0.58 |
| 1:AA:585:G:H4' | 12:AL:8:ASN:HD21 | 1.68 | 0.58 |
| 14:AN:57:ARG:HG2 | 14:AN:57:ARG:HH11 | 1.68 | 0.58 |
| 1:AA:333:G:H4' | 20:AT:16:HIS:CE1 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:AZ:19:HIS:CG | 25:AZ:20:VAL:H | 2.21 | 0.58 |
| 25:AZ:96:ALA:C | 25:AZ:98:GLN:H | 2.05 | 0.58 |
| 34:B8:61:LEU:N | 34:B8:61:LEU:HD12 | 2.19 | 0.58 |
| 36:BA:1494:A:N3 | 36:BA:1494:A:H5' | 2.18 | 0.58 |
| 36:BA:1636:C:H2' | 36:BA:1637:A:C8 | 2.38 | 0.58 |
| 36:BA:2138:C:H2' | 36:BA:2139:C:C6 | 2.37 | 0.58 |
| 36:BA:2292:C:O2' | 36:BA:2293:C:H5' | 2.03 | 0.58 |
| 36:BA:6:A:H2' | 36:BA:7:G:C8 | 2.38 | 0.58 |
| 37:BB:56:G:O2' | 37:BB:57:A:OP2 | 2.21 | 0.58 |
| 38:BC:26:ALA:O | 38:BC:185:LEU:HD12 | 2.03 | 0.58 |
| 36:BA:1813:G:H1' | 39:BD:50:THR:OG1 | 2.03 | 0.58 |
| 39:BD:35:LYS:HG3 | 39:BD:63:ARG:HG3 | 1.86 | 0.58 |
| 39:BD:77:ALA:CB | 39:BD:95:LEU:HD13 | 2.32 | 0.58 |
| 40:BE:32:PRO:O | 40:BE:34:VAL:N | 2.36 | 0.58 |
| 41:BF:10:PRO:HG2 | 41:BF:13:SER:OG | 2.02 | 0.58 |
| 43:BH:137:ASP:OD1 | 43:BH:138:LYS:N | 2.26 | 0.58 |
| 48:BP:71:VAL:N | 48:BP:72:PRO:CD | 2.61 | 0.58 |
| 57:BY:46:LYS:N | 57:BY:62:GLU:HG2 | 2.18 | 0.58 |
| 57:BY:52:SER:O | 57:BY:54:LYS:N | 2.37 | 0.58 |
| 11:AK:99:GLN:HG2 | 11:AK:105:VAL:HG21 | 1.85 | 0.58 |
| 13:AM:15:VAL:HG23 | 13:AM:16:ASP:N | 2.18 | 0.58 |
| 16:AP:28:ARG:HG2 | 16:AP:29:ASP:OD2 | 2.03 | 0.58 |
| 16:AP:45:THR:CG2 | 16:AP:47:ASP:HB3 | 2.33 | 0.58 |
| 29:B3:54:VAL:HG12 | 29:B3:55:ARG:N | 2.17 | 0.58 |
| 33:B7:22:MET:O | 33:B7:28:ARG:NH1 | 2.37 | 0.58 |
| 33:B7:9:ARG:HG3 | 33:B7:9:ARG:HH11 | 1.68 | 0.58 |
| 36:BA:2584:U:H2' | 36:BA:2585:U:H2' | 1.85 | 0.58 |
| 36:BA:845:G:OP2 | 36:BA:845:G:H8 | 1.87 | 0.58 |
| 28:B2:46:GLN:OE1 | 36:BA:95:G:H4' | 2.03 | 0.58 |
| 39:BD:27:THR:O | 39:BD:27:THR:CG2 | 2.50 | 0.58 |
| 36:BA:2787:C:O2 | 40:BE:61:ARG:HD3 | 2.02 | 0.58 |
| 1:AA:1050:G:HO2' | 1:AA:1051:C:H6 | 1.48 | 0.58 |
| 1:AA:1283:G:O2' | 1:AA:1284:C:P | 2.61 | 0.58 |
| 3:AC:61:ALA:N | 3:AC:63:ASN:OD1 | 2.35 | 0.58 |
| 4:AD:158:ILE:O | 4:AD:162:LEU:HB2 | 2.04 | 0.58 |
| 12:AL:113:ARG:HB3 | 12:AL:122:THR:HG21 | 1.83 | 0.58 |
| 24:AY:63:C:H2' | 24:AY:64:U:C6 | 2.38 | 0.58 |
| 26:B0:27:GLU:HB3 | 26:B0:68:GLU:CA | 2.25 | 0.58 |
| 32:B6:5:VAL:HG11 | 36:BA:2283:C:H5' | 1.85 | 0.58 |
| 36:BA:1536:C:H2' | 36:BA:1537:G:C4' | 2.34 | 0.58 |
| 36:BA:1799:G:H5' | 36:BA:1819:A:N6 | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:270:A:C2' | 36:BA:271:A:H5' | 2.33 | 0.58 |
| 36:BA:603:A:H1' | 36:BA:604:G:OP2 | 2.03 | 0.58 |
| 39:BD:28:GLU:N | 39:BD:29:PRO:CD | 2.64 | 0.58 |
| 48:BP:50:ARG:HH21 | 48:BP:50:ARG:HG2 | 1.69 | 0.58 |
| 34:B8:27:THR:HG22 | 48:BP:62:LEU:HD22 | 1.86 | 0.58 |
| 52:BT:24:PRO:HA | 52:BT:49:VAL:HG13 | 1.84 | 0.58 |
| 1:AA:1321:C:H3' | 1:AA:1322:C:H5' | 1.84 | 0.58 |
| 1:AA:149:A:O2' | 1:AA:150:C:H5' | 2.03 | 0.58 |
| 1:AA:722:A:N3 | 1:AA:722:A:H2' | 2.18 | 0.58 |
| 7:AG:8:GLU:HG3 | 7:AG:9:VAL:N | 2.17 | 0.58 |
| 10:AJ:58:ASP:O | 10:AJ:59:SER:C | 2.41 | 0.58 |
| 11:AK:34:ASP:OD2 | 11:AK:36:ASP:N | 2.37 | 0.58 |
| 25:AZ:171:ILE:HG22 | 25:AZ:172:ARG:N | 2.18 | 0.58 |
| 34:B8:33:ASN:CG | 34:B8:34:TRP:H | 2.07 | 0.58 |
| 34:B8:50:LEU:O | 34:B8:51:ALA:HB3 | 2.02 | 0.58 |
| 36:BA:2125:G:H21 | 36:BA:2173:A:H61 | 1.49 | 0.58 |
| 36:BA:2356:C:O2' | 36:BA:2357:U:H5' | 2.02 | 0.58 |
| 38:BC:216:THR:O | 38:BC:217:THR:C | 2.41 | 0.58 |
| 38:BC:22:ILE:HD12 | 38:BC:228:SER:O | 2.03 | 0.58 |
| 40:BE:104:VAL:HG11 | 40:BE:188:VAL:HG23 | 1.86 | 0.58 |
| 40:BE:115:GLY:HA2 | 40:BE:157:ALA:HB1 | 1.85 | 0.58 |
| 41:BF:158:THR:C | 41:BF:160:ASN:H | 2.06 | 0.58 |
| 42:BG:83:ARG:HB2 | 42:BG:84:LYS:HD2 | 1.84 | 0.58 |
| 46:BN:126:PRO:O | 46:BN:127:ASP:HB2 | 2.04 | 0.58 |
| 48:BP:123:LEU:H | 48:BP:123:LEU:HD23 | 1.69 | 0.58 |
| 48:BP:111:ARG:HH11 | 48:BP:149:GLU:HG3 | 1.67 | 0.58 |
| 52:BT:65:LYS:CE | 52:BT:66:VAL:H | 2.06 | 0.58 |
| 1:AA:1327:C:OP1 | 21:AU:20:LYS:N | 2.36 | 0.58 |
| 1:AA:1371:G:O3' | 9:AI:69:GLY:HA3 | 2.03 | 0.58 |
| 1:AA:642:A:H2' | 1:AA:643:C:C6 | 2.39 | 0.58 |
| 1:AA:673:G:H2' | 1:AA:674:G:C8 | 2.38 | 0.58 |
| 17:AQ:9:VAL:HG12 | 17:AQ:56:VAL:HG22 | 1.86 | 0.58 |
| 21:AU:23:PRO:C | 21:AU:25:LYS:H | 2.07 | 0.58 |
| 25:AZ:303:VAL:CG1 | 25:AZ:304:LEU:H | 2.13 | 0.58 |
| 25:AZ:56:GLU:HG3 | 25:AZ:63:ILE:HB | 1.85 | 0.58 |
| 27:B1:51:VAL:HG11 | 27:B1:74:VAL:HG21 | 1.86 | 0.58 |
| 28:B2:31:GLU:HB3 | 28:B2:53:LEU:HD11 | 1.85 | 0.58 |
| 32:B6:14:THR:CG2 | 32:B6:50:ARG:HB2 | 2.31 | 0.58 |
| 35:B9:24:TYR:O | 35:B9:25:VAL:HG23 | 2.03 | 0.58 |
| 35:B9:36:GLN:OE1 | 36:BA:1124:C:H1' | 2.03 | 0.58 |
| 36:BA:1170:G:H22 | 36:BA:1179:C:N4 | 1.93 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:BA:1916:A:H2' | 36:BA:1917:U:O4' | 2.02 | 0.58 |
| 36:BA:2030:A:H5'' | 36:BA:2031:A:OP1 | 2.03 | 0.58 |
| 40:BE:111:ARG:HA | 50:BR:2:ARG:HG3 | 1.84 | 0.58 |
| 41:BF:122:LYS:HG3 | 41:BF:191:ARG:HG3 | 1.85 | 0.58 |
| 56:BX:26:TYR:HB2 | 56:BX:81:VAL:CG2 | 2.34 | 0.58 |
| 1:AA:1143:G:H2' | 1:AA:1144:G:C8 | 2.39 | 0.58 |
| 1:AA:1308:U:H2' | 1:AA:1309:G:H8 | 1.69 | 0.58 |
| 2:AB:187:LEU:HD13 | 2:AB:205:ASP:HB3 | 1.84 | 0.58 |
| 5:AE:100:VAL:HG23 | 5:AE:100:VAL:O | 2.04 | 0.58 |
| 9:AI:40:LEU:C | 9:AI:42:ARG:H | 2.06 | 0.58 |
| 10:AJ:89:ASP:CB | 10:AJ:91:PRO:HD3 | 2.34 | 0.58 |
| 11:AK:82:VAL:HG11 | 11:AK:108:ILE:HG23 | 1.85 | 0.58 |
| 25:AZ:157:LEU:O | 25:AZ:160:GLN:HB3 | 2.04 | 0.58 |
| 34:B8:17:THR:OG1 | 34:B8:21:LYS:HB2 | 2.04 | 0.58 |
| 36:BA:1060:U:H1' | 36:BA:1061:U:O5' | 2.04 | 0.58 |
| 36:BA:2360:A:O2' | 36:BA:2361:A:O4' | 2.20 | 0.58 |
| 36:BA:736:C:H2' | 36:BA:737:C:H6 | 1.69 | 0.58 |
| 36:BA:761:A:H8 | 36:BA:761:A:H3' | 1.66 | 0.58 |
| 39:BD:97:TYR:CE1 | 39:BD:103:ARG:HD3 | 2.38 | 0.58 |
| 39:BD:70:TRP:CZ3 | 39:BD:146:GLU:OE2 | 2.57 | 0.58 |
| 36:BA:1569:A:O2' | 39:BD:38:LYS:HE2 | 2.04 | 0.58 |
| 39:BD:70:TRP:HZ3 | 39:BD:146:GLU:OE2 | 1.86 | 0.58 |
| 42:BG:41:GLN:HG2 | 42:BG:154:GLY:O | 2.04 | 0.58 |
| 43:BH:34:GLU:O | 43:BH:36:PRO:HD3 | 2.02 | 0.58 |
| 48:BP:31:ALA:C | 48:BP:33:ARG:N | 2.51 | 0.58 |
| 52:BT:128:GLU:O | 52:BT:129:ARG:C | 2.41 | 0.58 |
| 54:BV:95:LEU:HD23 | 54:BV:96:ILE:N | 2.18 | 0.58 |
| 58:BZ:96:VAL:HG22 | 58:BZ:97:GLU:H | 1.67 | 0.58 |
| 3:AC:95:THR:HG22 | 3:AC:97:LYS:HB2 | 1.85 | 0.58 |
| 5:AE:51:VAL:HB | 5:AE:52:PRO:CD | 2.32 | 0.58 |
| 9:AI:10:ARG:O | 9:AI:11:LYS:HB3 | 2.03 | 0.58 |
| 19:AS:16:LEU:C | 19:AS:18:LYS:H | 2.08 | 0.58 |
| 24:AY:15:A:H61 | 24:AY:48:U:H3 | 1.50 | 0.58 |
| 28:B2:35:LEU:HD13 | 28:B2:35:LEU:C | 2.24 | 0.58 |
| 32:B6:15:GLU:HG2 | 32:B6:18:ARG:NH1 | 2.19 | 0.58 |
| 36:BA:1310:G:C2' | 36:BA:1311:G:H5' | 2.33 | 0.58 |
| 36:BA:2801(A):A:H5' | 36:BA:2802:G:C8 | 2.29 | 0.58 |
| 36:BA:57:C:O2' | 36:BA:58:G:H5' | 2.03 | 0.58 |
| 39:BD:35:LYS:HZ2 | 39:BD:35:LYS:CB | 2.16 | 0.58 |
| 40:BE:198:VAL:HG12 | 40:BE:199:ARG:N | 2.18 | 0.58 |
| 46:BN:26:LEU:HG | 46:BN:30:ILE:HD11 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 46:BN:78:TYR:N | 46:BN:78:TYR:CD1 | 2.72 | 0.58 |
| 48:BP:136:GLU:O | 48:BP:139:LYS:HB3 | 2.03 | 0.58 |
| 49:BQ:134:ARG:NH2 | 58:BZ:122:ARG:NE | 2.50 | 0.58 |
| 50:BR:74:LYS:CD | 50:BR:77:ARG:HH21 | 2.17 | 0.58 |
| 51:BS:102:ALA:HB3 | 51:BS:103:GLU:OE1 | 2.04 | 0.58 |
| 51:BS:85:VAL:HG23 | 51:BS:106:ARG:CG | 2.34 | 0.58 |
| 58:BZ:166:SER:HB2 | 58:BZ:168:GLU:H | 1.68 | 0.58 |
| 59:AA:1601:PAR:H43 | 59:AA:1601:PAR:H642 | 1.85 | 0.58 |
| 1:AA:197:A:C6 | 1:AA:221:C:H4' | 2.39 | 0.58 |
| 1:AA:67:C:H2' | 1:AA:68:G:H8 | 1.68 | 0.58 |
| 2:AB:20:GLU:HG3 | 2:AB:191:ASP:HB2 | 1.86 | 0.58 |
| 3:AC:16:ARG:CA | 3:AC:16:ARG:HH11 | 2.16 | 0.58 |
| 3:AC:86:VAL:O | 3:AC:89:GLU:HB3 | 2.03 | 0.58 |
| 4:AD:110:PHE:HZ | 4:AD:182:LYS:O | 1.87 | 0.58 |
| 4:AD:53:ASP:O | 4:AD:57:ARG:HG3 | 2.03 | 0.58 |
| 4:AD:73:ARG:O | 4:AD:77:ASN:HB2 | 2.04 | 0.58 |
| 5:AE:147:ASP:HB3 | 5:AE:150:ARG:HH12 | 1.69 | 0.58 |
| 24:AY:54:5MU:H71 | 24:AY:54:5MU:OP2 | 2.04 | 0.58 |
| 25:AZ:36:ALA:O | 25:AZ:39:ASN:O | 2.22 | 0.58 |
| 36:BA:1155:A:O2' | 36:BA:1156:A:H2' | 2.04 | 0.58 |
| 36:BA:145:G:H2' | 36:BA:146:G:H5'' | 1.84 | 0.58 |
| 36:BA:1462:C:H4' | 36:BA:2703:C:C5' | 2.30 | 0.58 |
| 36:BA:528:A:C2 | 36:BA:2043:C:H4' | 2.38 | 0.58 |
| 36:BA:614(A):U:H4' | 36:BA:614(B):G:C5' | 2.34 | 0.58 |
| 36:BA:886:C:O2' | 36:BA:887:A:H4' | 2.04 | 0.58 |
| 36:BA:898:C:C2' | 36:BA:899:A:H5' | 2.32 | 0.58 |
| 39:BD:241:PRO:O | 39:BD:243:GLY:N | 2.37 | 0.58 |
| 40:BE:108:SER:OG | 40:BE:163:GLU:HG2 | 2.04 | 0.58 |
| 42:BG:34:LEU:N | 42:BG:172:LEU:HD11 | 2.19 | 0.58 |
| 42:BG:57:ALA:CA | 42:BG:90:LEU:HD21 | 2.34 | 0.58 |
| 43:BH:37:VAL:HG12 | 43:BH:38:SER:H | 1.68 | 0.58 |
| 47:BO:120:GLU:HG2 | 47:BO:122:LEU:HD21 | 1.84 | 0.58 |
| 48:BP:81:GLN:NE2 | 48:BP:106:LEU:HA | 2.19 | 0.58 |
| 51:BS:88:ASP:OD2 | 51:BS:89:ARG:N | 2.36 | 0.58 |
| 53:BU:90:VAL:CG1 | 53:BU:91:ASP:H | 2.14 | 0.58 |
| 54:BV:19:LYS:HA | 54:BV:19:LYS:HE2 | 1.85 | 0.58 |
| 1:AA:382:A:H2' | 1:AA:383:A:H8 | 1.69 | 0.57 |
| 8:AH:103:VAL:HG21 | 8:AH:110:ALA:HB2 | 1.85 | 0.57 |
| 9:AI:65:VAL:HG21 | 9:AI:73:GLN:HB3 | 1.86 | 0.57 |
| 17:AQ:10:VAL:HA | 17:AQ:20:THR:O | 2.03 | 0.57 |
| 25:AZ:130:TYR:CE2 | 25:AZ:211:PRO:HD3 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:2129:C:OP1 | 38:BC:4:GLY:HA3 | 2.04 | 0.57 |
| 36:BA:2136:C:O2' | 36:BA:2137:C:H5' | 2.04 | 0.57 |
| 36:BA:2291:U:H2' | 36:BA:2292:C:C6 | 2.39 | 0.57 |
| 36:BA:266:G:C3' | 36:BA:267:C:H5'' | 2.34 | 0.57 |
| 37:BB:30:C:H1' | 37:BB:57:A:H61 | 1.68 | 0.57 |
| 49:BQ:136:ALA:C | 49:BQ:138:ASP:H | 2.07 | 0.57 |
| 49:BQ:51:ARG:O | 49:BQ:55:VAL:HG12 | 2.04 | 0.57 |
| 58:BZ:17:ALA:HA | 58:BZ:20:ARG:HD3 | 1.85 | 0.57 |
| 1:AA:1033:G:H2' | 1:AA:1034:G:O4' | 2.04 | 0.57 |
| 1:AA:1299:A:H5'' | 1:AA:1299:A:N3 | 2.19 | 0.57 |
| 2:AB:112:VAL:O | 2:AB:116:GLU:HG2 | 2.04 | 0.57 |
| 2:AB:17:PHE:CB | 2:AB:44:LEU:HD11 | 2.35 | 0.57 |
| 8:AH:82:HIS:CD2 | 8:AH:138:TRP:NE1 | 2.72 | 0.57 |
| 22:AW:30:G:H2' | 22:AW:31:A:H8 | 1.69 | 0.57 |
| 25:AZ:55:GLU:O | 25:AZ:59:ARG:N | 2.37 | 0.57 |
| 28:B2:47:ASN:O | 28:B2:49:LYS:N | 2.37 | 0.57 |
| 31:B5:40:LYS:HZ1 | 31:B5:46:CYS:N | 2.00 | 0.57 |
| 31:B5:50:GLY:HA3 | 31:B5:56:LYS:HB3 | 1.85 | 0.57 |
| 36:BA:104:U:H2' | 36:BA:105:C:H5' | 1.85 | 0.57 |
| 36:BA:1069:A:H1' | 36:BA:1070:A:P | 2.45 | 0.57 |
| 36:BA:1403:C:H5'' | 36:BA:1471:A:C1' | 2.28 | 0.57 |
| 36:BA:1647:G:OP2 | 36:BA:1647:G:H3' | 2.05 | 0.57 |
| 36:BA:1890:A:H2' | 36:BA:1891:G:H5' | 1.86 | 0.57 |
| 36:BA:2720:U:H2' | 36:BA:2720:U:O2 | 2.03 | 0.57 |
| 36:BA:92:A:O2' | 36:BA:93:G:H5' | 2.04 | 0.57 |
| 22:AW:55:U:C5' | 38:BC:164:ARG:HH12 | 2.12 | 0.57 |
| 39:BD:32:SER:O | 39:BD:36:PRO:CG | 2.51 | 0.57 |
| 41:BF:175:THR:C | 41:BF:176:LEU:HD12 | 2.24 | 0.57 |
| 41:BF:31:HIS:ND1 | 48:BP:13:ASN:HB2 | 2.18 | 0.57 |
| 51:BS:29:PHE:C | 51:BS:29:PHE:CD2 | 2.75 | 0.57 |
| 51:BS:89:ARG:HB3 | 51:BS:92:TYR:CB | 2.34 | 0.57 |
| 55:BW:5:ALA:HB2 | 55:BW:54:ALA:CB | 2.34 | 0.57 |
| 56:BX:84:ALA:HB1 | 56:BX:85:PRO:HD2 | 1.85 | 0.57 |
| 58:BZ:149:SER:CB | 58:BZ:173:ALA:HA | 2.34 | 0.57 |
| 1:AA:1014:A:H4' | 19:AS:14:HIS:CE1 | 2.39 | 0.57 |
| 1:AA:1310:G:O2' | 1:AA:1311:G:H5' | 2.03 | 0.57 |
| 6:AF:33:TYR:HD2 | 6:AF:75:LEU:HA | 1.69 | 0.57 |
| 13:AM:49:THR:HB | 13:AM:52:GLU:H | 1.69 | 0.57 |
| 19:AS:62:ILE:O | 19:AS:62:ILE:HG23 | 2.03 | 0.57 |
| 25:AZ:24:LYS:NZ | 25:AZ:24:LYS:HB2 | 2.18 | 0.57 |
| 26:B0:20:ARG:NH1 | 26:B0:20:ARG:CG | 2.65 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:B2:47:ASN:O | 28:B2:50:ILE:HD13 | 2.04 | 0.57 |
| 29:B3:45:GLY:HA2 | 29:B3:48:GLU:HG3 | 1.85 | 0.57 |
| 36:BA:1092:C:N4 | 36:BA:1100:C:H42 | 2.00 | 0.57 |
| 36:BA:1274:A:N3 | 36:BA:1297:C:H1' | 2.19 | 0.57 |
| 36:BA:2373:G:H2' | 36:BA:2374:C:C6 | 2.38 | 0.57 |
| 36:BA:473:G:H5'' | 36:BA:508:G:N2 | 2.18 | 0.57 |
| 37:BB:80:U:H2' | 37:BB:81:G:N2 | 2.16 | 0.57 |
| 38:BC:152:ILE:O | 38:BC:152:ILE:HG22 | 2.05 | 0.57 |
| 41:BF:140:LEU:O | 41:BF:143:ALA:HB3 | 2.05 | 0.57 |
| 41:BF:177:ALA:HB1 | 41:BF:178:PRO:HD2 | 1.86 | 0.57 |
| 42:BG:14:GLU:O | 42:BG:17:PRO:HG2 | 2.03 | 0.57 |
| 43:BH:41:MET:O | 43:BH:42:ARG:HB3 | 2.05 | 0.57 |
| 46:BN:86:PRO:HG2 | 46:BN:89:LYS:CG | 2.30 | 0.57 |
| 50:BR:56:LYS:HE3 | 50:BR:94:TYR:CE1 | 2.39 | 0.57 |
| 52:BT:134:GLU:O | 52:BT:135:ALA:HB3 | 2.04 | 0.57 |
| 53:BU:112:ARG:NH1 | 54:BV:46:VAL:HG21 | 2.20 | 0.57 |
| 36:BA:1598:C:H5' | 56:BX:36:LYS:CD | 2.35 | 0.57 |
| 57:BY:90:LEU:HG | 57:BY:90:LEU:O | 2.04 | 0.57 |
| 58:BZ:28:MET:O | 58:BZ:29:TYR:HB3 | 2.02 | 0.57 |
| 1:AA:1498:U:H4' | 1:AA:1519:A:H2 | 1.65 | 0.57 |
| 1:AA:594:G:H2' | 1:AA:595:G:H5' | 1.85 | 0.57 |
| 1:AA:767:A:H2' | 1:AA:768:A:O4' | 2.04 | 0.57 |
| 8:AH:1:MET:N | 8:AH:1:MET:HE2 | 2.19 | 0.57 |
| 1:AA:958:A:N6 | 19:AS:77:THR:O | 2.37 | 0.57 |
| 25:AZ:404:LEU:HD12 | 25:AZ:405:GLU:HG3 | 1.85 | 0.57 |
| 28:B2:4:SER:HA | 28:B2:7:ARG:HH11 | 1.70 | 0.57 |
| 32:B6:41:PRO:HG3 | 32:B6:49:HIS:HE1 | 1.69 | 0.57 |
| 36:BA:1547:C:O2' | 36:BA:1548:C:H5' | 2.05 | 0.57 |
| 36:BA:2121:G:H2' | 36:BA:2122:U:C6 | 2.39 | 0.57 |
| 36:BA:2307:G:H3' | 36:BA:2307:G:N3 | 2.19 | 0.57 |
| 36:BA:2648:C:H2' | 36:BA:2649:U:H6 | 1.67 | 0.57 |
| 36:BA:438:G:O2' | 36:BA:440:G:H5' | 2.03 | 0.57 |
| 36:BA:88:G:N3 | 36:BA:88:G:H2' | 2.19 | 0.57 |
| 47:BO:71:ARG:NH1 | 47:BO:71:ARG:HG3 | 2.17 | 0.57 |
| 48:BP:90:ARG:HD2 | 48:BP:91:PHE:CD1 | 2.39 | 0.57 |
| 26:B0:7:LEU:CD2 | 49:BQ:81:VAL:HG23 | 2.33 | 0.57 |
| 51:BS:54:LEU:HD22 | 51:BS:58:LEU:O | 2.04 | 0.57 |
| 57:BY:31:LEU:HD22 | 57:BY:31:LEU:N | 2.19 | 0.57 |
| 57:BY:75:ILE:O | 57:BY:76:CYS:HB2 | 2.04 | 0.57 |
| 1:AA:1441:G:H5'' | 1:AA:1442:G:O4' | 2.04 | 0.57 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:C6 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:192:U:O4' | 20:AT:103:GLY:HA2 | 2.05 | 0.57 |
| 1:AA:655:A:H2' | 1:AA:656:C:H6 | 1.70 | 0.57 |
| 4:AD:33:MET:O | 4:AD:37:PRO:HG3 | 2.04 | 0.57 |
| 8:AH:82:HIS:CD2 | 8:AH:138:TRP:HE1 | 2.23 | 0.57 |
| 22:AW:55:U:H5'' | 38:BC:164:ARG:NH1 | 2.10 | 0.57 |
| 32:B6:13:CYS:HB2 | 32:B6:22:ALA:CB | 2.33 | 0.57 |
| 36:BA:1055:G:H1' | 36:BA:1084:A:N6 | 2.20 | 0.57 |
| 36:BA:1999:C:H4' | 36:BA:2723:C:O2 | 2.03 | 0.57 |
| 36:BA:2345:G:H5' | 36:BA:2347:C:O4' | 2.05 | 0.57 |
| 36:BA:2529:G:OP2 | 36:BA:2530:A:H8 | 1.87 | 0.57 |
| 38:BC:53:ARG:HH11 | 38:BC:53:ARG:CB | 2.14 | 0.57 |
| 38:BC:6:ARG:HD2 | 38:BC:34:THR:O | 2.05 | 0.57 |
| 39:BD:26:LYS:O | 39:BD:27:THR:HG22 | 2.04 | 0.57 |
| 39:BD:70:TRP:HB3 | 39:BD:190:TYR:CE1 | 2.39 | 0.57 |
| 36:BA:1255:U:C5 | 41:BF:73:ALA:HA | 2.39 | 0.57 |
| 42:BG:86:MET:N | 42:BG:87:PRO:HD2 | 2.20 | 0.57 |
| 43:BH:85:LYS:HE2 | 43:BH:85:LYS:O | 2.04 | 0.57 |
| 49:BQ:67:ARG:HD3 | 49:BQ:102:VAL:HG12 | 1.86 | 0.57 |
| 51:BS:30:ARG:HH22 | 51:BS:62:LYS:CG | 2.17 | 0.57 |
| 52:BT:11:GLU:CD | 52:BT:11:GLU:N | 2.55 | 0.57 |
| 55:BW:52:GLU:C | 55:BW:54:ALA:H | 2.08 | 0.57 |
| 1:AA:655:A:H2' | 1:AA:656:C:C6 | 2.39 | 0.57 |
| 1:AA:972:C:O3' | 10:AJ:57:LYS:HG2 | 2.05 | 0.57 |
| 8:AH:103:VAL:HG12 | 8:AH:108:GLY:HA3 | 1.84 | 0.57 |
| 10:AJ:16:LEU:HD11 | 10:AJ:70:ARG:CG | 2.33 | 0.57 |
| 10:AJ:94:VAL:HG12 | 10:AJ:95:GLU:N | 2.19 | 0.57 |
| 12:AL:119:LYS:O | 12:AL:120:TYR:HB2 | 2.04 | 0.57 |
| 13:AM:15:VAL:HG23 | 13:AM:34:LEU:HD11 | 1.86 | 0.57 |
| 14:AN:12:ARG:HB3 | 14:AN:14:PRO:HD2 | 1.87 | 0.57 |
| 15:AO:17:ARG:NH1 | 15:AO:17:ARG:HG3 | 2.19 | 0.57 |
| 16:AP:14:ASN:N | 16:AP:15:PRO:HD3 | 2.20 | 0.57 |
| 17:AQ:66:SER:O | 17:AQ:70:ARG:NH1 | 2.38 | 0.57 |
| 22:AV:62:C:H2' | 22:AV:63:G:C8 | 2.39 | 0.57 |
| 22:AW:18:G:H1 | 22:AW:55:U:H1' | 1.69 | 0.57 |
| 7:AG:86:GLN:HE22 | 22:AW:39:U:H5 | 1.53 | 0.57 |
| 25:AZ:5:PHE:HB2 | 25:AZ:275:LYS:HB2 | 1.87 | 0.57 |
| 25:AZ:86:ALA:O | 25:AZ:88:TYR:N | 2.35 | 0.57 |
| 27:B1:80:LEU:HB3 | 27:B1:82:LEU:CD2 | 2.35 | 0.57 |
| 30:B4:9:LEU:CD1 | 30:B4:10:VAL:H | 2.18 | 0.57 |
| 36:BA:115:C:O2' | 36:BA:116:C:H5' | 2.05 | 0.57 |
| 36:BA:259:G:H1' | 36:BA:621:A:HO2' | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:13:A:H61 | 36:BA:525:U:H3' | 1.68 | 0.57 |
| 36:BA:614:U:C2' | 36:BA:614(A):U:H5' | 2.34 | 0.57 |
| 36:BA:645:C:H3' | 36:BA:645:C:O2 | 2.04 | 0.57 |
| 36:BA:64:A:H2' | 36:BA:65:C:O4' | 2.05 | 0.57 |
| 38:BC:59:ARG:HG3 | 38:BC:164:ARG:CG | 2.35 | 0.57 |
| 39:BD:2:ALA:O | 39:BD:3:VAL:HB | 2.03 | 0.57 |
| 40:BE:111:ARG:HB3 | 50:BR:2:ARG:HH12 | 1.67 | 0.57 |
| 43:BH:102:ALA:HA | 43:BH:117:PRO:HD3 | 1.85 | 0.57 |
| 49:BQ:36:ALA:HB2 | 49:BQ:103:MET:HE3 | 1.87 | 0.57 |
| 52:BT:124:ASP:HB3 | 52:BT:125:ARG:HH12 | 1.68 | 0.57 |
| 1:AA:1202:G:C2' | 1:AA:1203:C:H5' | 2.35 | 0.57 |
| 1:AA:1240:U:H4' | 7:AG:38:LEU:HD21 | 1.87 | 0.57 |
| 1:AA:986:A:H1' | 19:AS:54:GLY:O | 2.04 | 0.57 |
| 3:AC:14:ILE:O | 3:AC:15:THR:CB | 2.53 | 0.57 |
| 9:AI:47:LEU:C | 9:AI:49:PRO:HD2 | 2.24 | 0.57 |
| 16:AP:25:ARG:NH1 | 16:AP:25:ARG:HG3 | 2.20 | 0.57 |
| 29:B3:7:LYS:O | 29:B3:54:VAL:HG13 | 2.05 | 0.57 |
| 30:B4:42:PHE:CG | 30:B4:42:PHE:O | 2.57 | 0.57 |
| 36:BA:19:C:O2' | 36:BA:20:C:H5' | 2.03 | 0.57 |
| 36:BA:2206:G:H21 | 36:BA:2207:G:H5' | 1.67 | 0.57 |
| 36:BA:2524:G:H5' | 36:BA:2524:G:H8 | 1.69 | 0.57 |
| 36:BA:2577:A:C5' | 36:BA:2578:G:H5' | 2.35 | 0.57 |
| 36:BA:2640:G:H1 | 36:BA:2774:C:H42 | 1.51 | 0.57 |
| 37:BB:98:G:O2' | 37:BB:99:G:H5' | 2.04 | 0.57 |
| 38:BC:78:ALA:HB3 | 38:BC:95:GLY:CA | 2.34 | 0.57 |
| 39:BD:224:ALA:O | 39:BD:225:ALA:HB2 | 2.03 | 0.57 |
| 41:BF:162:LEU:H | 41:BF:162:LEU:HD12 | 1.70 | 0.57 |
| 41:BF:62:ARG:HB3 | 41:BF:62:ARG:CZ | 2.35 | 0.57 |
| 49:BQ:116:GLU:O | 49:BQ:120:ILE:HG12 | 2.04 | 0.57 |
| 53:BU:57:PHE:C | 53:BU:59:ARG:N | 2.56 | 0.57 |
| 54:BV:22:VAL:O | 54:BV:23:GLU:HB2 | 2.04 | 0.57 |
| 56:BX:66:LEU:HD23 | 56:BX:67:GLY:N | 2.19 | 0.57 |
| 56:BX:8:ILE:N | 56:BX:8:ILE:HD12 | 2.20 | 0.57 |
| 57:BY:13:VAL:HG23 | 57:BY:74:PRO:HA | 1.86 | 0.57 |
| 58:BZ:17:ALA:CA | 58:BZ:20:ARG:HG2 | 2.34 | 0.57 |
| 1:AA:80:G:H3' | 1:AA:81:U:C5' | 2.35 | 0.57 |
| 7:AG:41:ARG:HG3 | 9:AI:41:VAL:HG21 | 1.86 | 0.57 |
| 10:AJ:30:SER:CA | 10:AJ:80:LYS:HD3 | 2.33 | 0.57 |
| 13:AM:98:VAL:HG12 | 13:AM:98:VAL:O | 2.05 | 0.57 |
| 16:AP:45:THR:O | 16:AP:47:ASP:N | 2.32 | 0.57 |
| 1:AA:235:C:H5' | 17:AQ:70:ARG:HG2 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:AX:16:A:H2' | 23:AX:17:U:H5' | 1.87 | 0.57 |
| 32:B6:12:GLU:HG3 | 32:B6:23:THR:CG2 | 2.35 | 0.57 |
| 36:BA:1556:C:H2' | 36:BA:1557:C:C6 | 2.39 | 0.57 |
| 36:BA:1607:C:H4' | 36:BA:1608:A:O5' | 2.05 | 0.57 |
| 36:BA:1654:A:C2 | 40:BE:113:PHE:HD2 | 2.22 | 0.57 |
| 36:BA:191:A:H2' | 36:BA:192:C:C6 | 2.40 | 0.57 |
| 36:BA:2188:C:H2' | 36:BA:2189:U:C2 | 2.40 | 0.57 |
| 36:BA:70:G:H2' | 36:BA:113:G:O2' | 2.05 | 0.57 |
| 44:BJ:25:UNK:O | 44:BJ:84:UNK:HA | 2.04 | 0.57 |
| 48:BP:121:LYS:HB2 | 48:BP:123:LEU:CD2 | 2.35 | 0.57 |
| 47:BO:64:ARG:CZ | 52:BT:70:VAL:HG21 | 2.35 | 0.57 |
| 1:AA:1146:A:C2 | 1:AA:1147:C:H1' | 2.39 | 0.57 |
| 1:AA:312:C:H2' | 1:AA:313:A:C8 | 2.40 | 0.57 |
| 1:AA:68:G:C2 | 1:AA:69:G:H1' | 2.40 | 0.57 |
| 1:AA:737:A:H2' | 1:AA:738:C:C6 | 2.40 | 0.57 |
| 2:AB:165:VAL:HG23 | 2:AB:166:ASP:N | 2.20 | 0.57 |
| 3:AC:50:ALA:HB1 | 3:AC:70:VAL:HG11 | 1.87 | 0.57 |
| 7:AG:15:ASP:HA | 7:AG:24:THR:HG22 | 1.86 | 0.57 |
| 7:AG:80:VAL:HG12 | 7:AG:81:GLY:N | 2.20 | 0.57 |
| 1:AA:963:G:H21 | 10:AJ:55:LYS:CE | 2.17 | 0.57 |
| 13:AM:80:ARG:NH2 | 19:AS:69:HIS:NE2 | 2.52 | 0.57 |
| 15:AO:82:ILE:HG12 | 15:AO:87:ILE:HB | 1.86 | 0.57 |
| 17:AQ:8:GLY:HA3 | 17:AQ:21:VAL:HG12 | 1.85 | 0.57 |
| 19:AS:47:HIS:O | 19:AS:62:ILE:CG2 | 2.52 | 0.57 |
| 25:AZ:138:VAL:O | 25:AZ:140:MET:N | 2.36 | 0.57 |
| 27:B1:11:ARG:HB3 | 27:B1:11:ARG:HH11 | 1.70 | 0.57 |
| 36:BA:1520:G:H2' | 36:BA:1523:U:H5' | 1.87 | 0.57 |
| 36:BA:1773:A:C2' | 36:BA:1774:C:H5' | 2.34 | 0.57 |
| 36:BA:197:A:C8 | 36:BA:197:A:H5' | 2.39 | 0.57 |
| 36:BA:2298:A:H2' | 36:BA:2299:G:O4' | 2.04 | 0.57 |
| 36:BA:324:A:H2' | 36:BA:325:G:O4' | 2.05 | 0.57 |
| 36:BA:852:G:O2' | 36:BA:853:G:H5' | 2.04 | 0.57 |
| 39:BD:27:THR:HG21 | 39:BD:83:GLU:HG2 | 1.86 | 0.57 |
| 57:BY:13:VAL:HG22 | 57:BY:73:ARG:O | 2.04 | 0.57 |
| 58:BZ:6:LYS:HD3 | 58:BZ:6:LYS:N | 2.20 | 0.57 |
| 1:AA:657:G:O2' | 1:AA:658:G:H5' | 2.04 | 0.57 |
| 2:AB:111:ARG:NH2 | 2:AB:114:ARG:HG2 | 2.20 | 0.57 |
| 2:AB:17:PHE:CD2 | 2:AB:17:PHE:O | 2.58 | 0.57 |
| 3:AC:141:VAL:HG11 | 3:AC:149:ALA:HB2 | 1.87 | 0.57 |
| 12:AL:55:VAL:CG2 | 12:AL:67:THR:HG23 | 2.35 | 0.57 |
| 15:AO:17:ARG:NH1 | 15:AO:77:ARG:NH1 | 2.53 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:341:GLN:HE22 | 25:AZ:390:GLU:HB2 | 1.69 | 0.57 |
| 34:B8:32:LEU:HD12 | 34:B8:36:LYS:HZ3 | 1.70 | 0.57 |
| 36:BA:2579:C:O2' | 36:BA:2580:U:H5' | 2.04 | 0.57 |
| 36:BA:686:G:H21 | 36:BA:788:A:H61 | 1.53 | 0.57 |
| 29:B3:11:SER:HB3 | 36:BA:988:A:O5' | 2.04 | 0.57 |
| 38:BC:41:VAL:CB | 38:BC:175:VAL:HB | 2.35 | 0.57 |
| 39:BD:155:LEU:HD23 | 39:BD:177:LEU:HD22 | 1.86 | 0.57 |
| 39:BD:99:ASP:OD2 | 39:BD:99:ASP:O | 2.22 | 0.57 |
| 40:BE:45:THR:O | 40:BE:46:ALA:HB2 | 2.05 | 0.57 |
| 48:BP:125:VAL:HG13 | 48:BP:125:VAL:O | 2.05 | 0.57 |
| 48:BP:38:GLN:O | 48:BP:39:LYS:HB2 | 2.05 | 0.57 |
| 36:BA:2467:C:H4' | 49:BQ:123:HIS:CD2 | 2.40 | 0.57 |
| 49:BQ:137:TYR:OH | 58:BZ:81:ARG:NE | 2.37 | 0.57 |
| 51:BS:52:SER:HB3 | 51:BS:55:ALA:HB3 | 1.86 | 0.57 |
| 52:BT:26:ASP:HB3 | 52:BT:89:VAL:O | 2.04 | 0.57 |
| 52:BT:27:THR:HG22 | 52:BT:49:VAL:HB | 1.85 | 0.57 |
| 52:BT:91:ARG:O | 52:BT:117:ASP:CB | 2.53 | 0.57 |
| 58:BZ:145:GLU:OE1 | 58:BZ:145:GLU:HA | 2.05 | 0.57 |
| 1:AA:532:A:N6 | 1:AA:1206:G:O2' | 2.37 | 0.56 |
| 1:AA:775:G:O2' | 1:AA:776:G:H5' | 2.05 | 0.56 |
| 1:AA:961:U:O2' | 1:AA:962:C:O5' | 2.23 | 0.56 |
| 2:AB:47:THR:HA | 2:AB:202:PRO:HG2 | 1.86 | 0.56 |
| 4:AD:13:ARG:O | 4:AD:16:GLY:N | 2.31 | 0.56 |
| 17:AQ:59:ILE:HG22 | 17:AQ:71:PHE:HD1 | 1.68 | 0.56 |
| 31:B5:40:LYS:HE2 | 31:B5:46:CYS:HB3 | 1.86 | 0.56 |
| 35:B9:10:ILE:O | 35:B9:11:CYS:CB | 2.52 | 0.56 |
| 36:BA:1473:G:H2' | 36:BA:1474:C:O4' | 2.04 | 0.56 |
| 36:BA:2672:G:H2' | 36:BA:2673:G:H5'' | 1.87 | 0.56 |
| 36:BA:582:G:H2' | 36:BA:583:G:C8 | 2.39 | 0.56 |
| 36:BA:760:G:H2' | 36:BA:761:A:H5' | 1.87 | 0.56 |
| 37:BB:22:U:H2' | 37:BB:23:G:H8 | 1.70 | 0.56 |
| 38:BC:74:VAL:HA | 38:BC:112:ALA:HB3 | 1.87 | 0.56 |
| 40:BE:186:GLY:O | 40:BE:187:ALA:CB | 2.52 | 0.56 |
| 40:BE:9:VAL:CG1 | 40:BE:25:VAL:HB | 2.34 | 0.56 |
| 41:BF:32:LEU:C | 41:BF:32:LEU:HD23 | 2.26 | 0.56 |
| 42:BG:16:ARG:NH1 | 42:BG:16:ARG:HG3 | 2.20 | 0.56 |
| 42:BG:5:VAL:HG12 | 42:BG:6:ALA:N | 2.18 | 0.56 |
| 46:BN:58:ASP:C | 46:BN:60:ILE:N | 2.59 | 0.56 |
| 48:BP:47:ASP:HB3 | 48:BP:49:ARG:H | 1.67 | 0.56 |
| 52:BT:48:ILE:N | 52:BT:48:ILE:HD12 | 2.20 | 0.56 |
| 58:BZ:108:PRO:HG2 | 58:BZ:111:VAL:HG23 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1126:U:OP2 | 1:AA:1281:U:O2 | 2.23 | 0.56 |
| 1:AA:190:U:H2' | 1:AA:191:G:H8 | 1.70 | 0.56 |
| 5:AE:147:ASP:HB3 | 5:AE:150:ARG:NH1 | 2.20 | 0.56 |
| 16:AP:45:THR:C | 16:AP:47:ASP:H | 2.07 | 0.56 |
| 1:AA:1503:A:N3 | 23:AX:16:A:N6 | 2.52 | 0.56 |
| 25:AZ:317:GLU:HG3 | 25:AZ:402:LYS:HB2 | 1.87 | 0.56 |
| 36:BA:1056:G:C2 | 36:BA:1102:C:H5 | 2.22 | 0.56 |
| 36:BA:1192:G:O2' | 36:BA:1193:G:H5' | 2.05 | 0.56 |
| 36:BA:1301:A:O2' | 36:BA:1302:A:C2' | 2.46 | 0.56 |
| 36:BA:1598:C:H2' | 36:BA:1599:C:H6 | 1.69 | 0.56 |
| 31:B5:10:LYS:HB2 | 36:BA:2017:U:O2 | 2.04 | 0.56 |
| 36:BA:2233:U:H2' | 36:BA:2234:G:C8 | 2.40 | 0.56 |
| 36:BA:2492:U:O2' | 36:BA:2493:U:H5' | 2.06 | 0.56 |
| 36:BA:330:A:HO2' | 36:BA:331:A:H8 | 1.51 | 0.56 |
| 36:BA:654(T):C:H2' | 36:BA:654(U):A:O4' | 2.05 | 0.56 |
| 38:BC:175:VAL:CG2 | 38:BC:189:ILE:HG12 | 2.35 | 0.56 |
| 38:BC:14:VAL:HG22 | 38:BC:28:LEU:HD11 | 1.88 | 0.56 |
| 39:BD:69:ARG:NH2 | 39:BD:128:GLY:O | 2.32 | 0.56 |
| 40:BE:111:ARG:HB3 | 50:BR:2:ARG:NH1 | 2.20 | 0.56 |
| 40:BE:114:ALA:CB | 40:BE:160:TYR:HB3 | 2.35 | 0.56 |
| 40:BE:34:VAL:HG13 | 40:BE:48:GLN:HE21 | 1.70 | 0.56 |
| 50:BR:58:GLY:HA2 | 50:BR:80:PHE:CE1 | 2.40 | 0.56 |
| 51:BS:98:VAL:HG12 | 51:BS:100:ALA:N | 2.20 | 0.56 |
| 52:BT:120:ARG:HA | 52:BT:123:GLN:HG2 | 1.87 | 0.56 |
| 52:BT:35:LYS:NZ | 52:BT:41:ARG:HD2 | 2.20 | 0.56 |
| 54:BV:28:GLU:O | 54:BV:61:VAL:HG21 | 2.06 | 0.56 |
| 1:AA:1104:G:O5' | 2:AB:111:ARG:HD2 | 2.06 | 0.56 |
| 1:AA:1151:A:O2' | 1:AA:1152:A:H8 | 1.88 | 0.56 |
| 1:AA:140:A:O2' | 1:AA:141:A:H5' | 2.05 | 0.56 |
| 5:AE:87:SER:HB3 | 5:AE:131:ILE:HD13 | 1.86 | 0.56 |
| 7:AG:26:PHE:HB2 | 7:AG:101:LEU:HD22 | 1.87 | 0.56 |
| 19:AS:16:LEU:HD12 | 19:AS:16:LEU:H | 1.69 | 0.56 |
| 25:AZ:104:LEU:HD21 | 25:AZ:120:ILE:HD11 | 1.87 | 0.56 |
| 25:AZ:228:VAL:HG21 | 25:AZ:298:VAL:HG12 | 1.87 | 0.56 |
| 25:AZ:317:GLU:O | 25:AZ:317:GLU:HG3 | 2.05 | 0.56 |
| 36:BA:1001:A:H2' | 36:BA:1002:G:O4' | 2.05 | 0.56 |
| 36:BA:1056:G:H21 | 36:BA:1104:C:N4 | 2.02 | 0.56 |
| 36:BA:2580:U:C5' | 40:BE:131:ALA:HB2 | 2.35 | 0.56 |
| 36:BA:2787:C:H2' | 36:BA:2787:C:O2 | 2.05 | 0.56 |
| 36:BA:693:C:H2' | 36:BA:694:U:C6 | 2.40 | 0.56 |
| 38:BC:116:THR:OG1 | 38:BC:119:VAL:HG22 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BD:186:HIS:CD2 | 39:BD:188:GLU:HB2 | 2.40 | 0.56 |
| 39:BD:243:GLY:O | 39:BD:244:ARG:HB3 | 2.04 | 0.56 |
| 40:BE:176:ILE:HG22 | 40:BE:178:GLU:HB3 | 1.86 | 0.56 |
| 43:BH:97:ARG:HG2 | 43:BH:98:LEU:N | 2.18 | 0.56 |
| 46:BN:28:THR:CG2 | 46:BN:29:LYS:N | 2.68 | 0.56 |
| 52:BT:82:LEU:N | 52:BT:82:LEU:HD12 | 2.17 | 0.56 |
| 54:BV:3:ALA:HB3 | 54:BV:14:VAL:HG23 | 1.85 | 0.56 |
| 54:BV:46:VAL:HG13 | 54:BV:46:VAL:O | 2.05 | 0.56 |
| 55:BW:4:LYS:HA | 55:BW:106:ILE:HG22 | 1.86 | 0.56 |
| 58:BZ:54:HIS:HB3 | 58:BZ:101:PRO:HG3 | 1.87 | 0.56 |
| 1:AA:1030:C:C2' | 1:AA:1030(A):G:H5' | 2.34 | 0.56 |
| 1:AA:272:C:H2' | 1:AA:273:A:O4' | 2.06 | 0.56 |
| 1:AA:398:C:O2' | 1:AA:399:G:H5' | 2.06 | 0.56 |
| 1:AA:737:A:H2' | 1:AA:738:C:H6 | 1.70 | 0.56 |
| 2:AB:23:ARG:O | 2:AB:23:ARG:HG3 | 2.05 | 0.56 |
| 5:AE:102:ALA:HB2 | 5:AE:120:THR:HG21 | 1.87 | 0.56 |
| 7:AG:15:ASP:HA | 7:AG:24:THR:CG2 | 2.35 | 0.56 |
| 7:AG:76:ARG:HG2 | 7:AG:76:ARG:HH11 | 1.71 | 0.56 |
| 10:AJ:32:ALA:HB3 | 10:AJ:76:ASN:HB2 | 1.85 | 0.56 |
| 11:AK:84:VAL:O | 11:AK:85:ARG:HG3 | 2.05 | 0.56 |
| 12:AL:67:THR:CG2 | 12:AL:96:VAL:HG22 | 2.36 | 0.56 |
| 15:AO:82:ILE:HD13 | 15:AO:82:ILE:C | 2.26 | 0.56 |
| 1:AA:375:U:H4' | 16:AP:17:TYR:CE2 | 2.40 | 0.56 |
| 16:AP:19:ILE:N | 16:AP:37:GLY:O | 2.32 | 0.56 |
| 19:AS:9:VAL:O | 19:AS:11:VAL:N | 2.38 | 0.56 |
| 31:B5:40:LYS:HE2 | 31:B5:46:CYS:SG | 2.44 | 0.56 |
| 34:B8:24:ALA:O | 34:B8:46:ARG:HA | 2.05 | 0.56 |
| 34:B8:35:GLN:O | 34:B8:36:LYS:HG3 | 2.05 | 0.56 |
| 35:B9:35:ARG:HH11 | 36:BA:2742:C:P | 2.28 | 0.56 |
| 35:B9:4:ARG:NH1 | 36:BA:2477:C:N3 | 2.53 | 0.56 |
| 36:BA:1301:A:HO2' | 36:BA:1302:A:P | 2.27 | 0.56 |
| 36:BA:2886:G:H2' | 36:BA:2887:U:C6 | 2.40 | 0.56 |
| 36:BA:862:G:H2' | 36:BA:863:A:O4' | 2.05 | 0.56 |
| 38:BC:75:LEU:CD1 | 38:BC:113:VAL:HA | 2.35 | 0.56 |
| 39:BD:10:THR:HG23 | 39:BD:13:ARG:HB3 | 1.87 | 0.56 |
| 40:BE:44:TYR:HD2 | 40:BE:45:THR:O | 1.87 | 0.56 |
| 42:BG:34:LEU:C | 42:BG:34:LEU:HD12 | 2.26 | 0.56 |
| 43:BH:101:ARG:O | 43:BH:117:PRO:HG3 | 2.04 | 0.56 |
| 46:BN:107:LEU:HB3 | 46:BN:108:PRO:HD2 | 1.88 | 0.56 |
| 48:BP:95:VAL:HG23 | 48:BP:125:VAL:HG23 | 1.87 | 0.56 |
| 48:BP:16:ARG:HB2 | 48:BP:16:ARG:CZ | 2.34 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:BP:16:ARG:CB | 48:BP:16:ARG:NH1 | 2.62 | 0.56 |
| 52:BT:30:VAL:CG2 | 52:BT:84:GLN:HG3 | 2.35 | 0.56 |
| 55:BW:34:ASN:O | 55:BW:37:ARG:HB3 | 2.05 | 0.56 |
| 57:BY:6:HIS:H | 57:BY:6:HIS:CD2 | 2.23 | 0.56 |
| 58:BZ:103:ARG:HG3 | 58:BZ:103:ARG:NH1 | 2.18 | 0.56 |
| 1:AA:1101:A:H4' | 1:AA:1102:A:O5' | 2.06 | 0.56 |
| 1:AA:328:C:H4' | 1:AA:329:A:H5' | 1.87 | 0.56 |
| 2:AB:8:LYS:HE2 | 2:AB:217:ARG:NH2 | 2.20 | 0.56 |
| 3:AC:134:ILE:O | 3:AC:138:VAL:HG12 | 2.05 | 0.56 |
| 5:AE:63:ARG:O | 5:AE:64:ARG:HB2 | 2.04 | 0.56 |
| 7:AG:36:LYS:O | 7:AG:39:ALA:HB3 | 2.06 | 0.56 |
| 13:AM:14:ARG:HG3 | 13:AM:44:ARG:NH1 | 2.21 | 0.56 |
| 20:AT:93:GLU:CD | 20:AT:93:GLU:C | 2.63 | 0.56 |
| 24:AY:61:C:O2' | 24:AY:62:U:H5'' | 2.05 | 0.56 |
| 25:AZ:248:LYS:HB2 | 25:AZ:248:LYS:NZ | 2.21 | 0.56 |
| 26:B0:67:VAL:HG12 | 26:B0:68:GLU:N | 2.19 | 0.56 |
| 27:B1:11:ARG:HB3 | 27:B1:12:PRO:HD2 | 1.86 | 0.56 |
| 36:BA:1056:G:H21 | 36:BA:1104:C:H42 | 1.54 | 0.56 |
| 36:BA:1138:G:H2' | 36:BA:1139:G:O4' | 2.06 | 0.56 |
| 36:BA:1140:C:OP2 | 46:BN:66:LYS:HE2 | 2.06 | 0.56 |
| 36:BA:1515:G:H2' | 36:BA:1516:C:C6 | 2.40 | 0.56 |
| 36:BA:2124:G:H22 | 38:BC:218:MET:HG2 | 1.70 | 0.56 |
| 36:BA:2369:A:H2' | 36:BA:2370:G:H8 | 1.70 | 0.56 |
| 38:BC:137:LEU:HD22 | 38:BC:138:PRO:HD2 | 1.86 | 0.56 |
| 38:BC:212:VAL:CG1 | 38:BC:224:ILE:HD11 | 2.36 | 0.56 |
| 42:BG:10:LYS:HE2 | 42:BG:14:GLU:OE2 | 2.05 | 0.56 |
| 51:BS:15:ARG:O | 51:BS:18:ILE:HG13 | 2.05 | 0.56 |
| 51:BS:97:ARG:NH2 | 51:BS:98:VAL:CA | 2.62 | 0.56 |
| 57:BY:39:VAL:HG12 | 57:BY:40:GLU:H | 1.69 | 0.56 |
| 1:AA:1234:C:H2' | 1:AA:1235:U:C6 | 2.40 | 0.56 |
| 1:AA:1305:G:C5' | 21:AU:4:GLY:CA | 2.83 | 0.56 |
| 1:AA:336:C:O2' | 1:AA:337:C:H5' | 2.05 | 0.56 |
| 2:AB:114:ARG:HD3 | 2:AB:114:ARG:O | 2.05 | 0.56 |
| 2:AB:33:TYR:O | 2:AB:34:ALA:HB2 | 2.05 | 0.56 |
| 2:AB:50:GLU:O | 2:AB:53:ARG:N | 2.38 | 0.56 |
| 2:AB:97:TRP:HZ2 | 2:AB:102:LEU:HD13 | 1.71 | 0.56 |
| 4:AD:107:ARG:NH1 | 4:AD:114:ARG:HH21 | 2.02 | 0.56 |
| 5:AE:20:GLN:HG2 | 5:AE:21:ALA:N | 2.20 | 0.56 |
| 8:AH:82:HIS:HD2 | 8:AH:138:TRP:HE1 | 1.53 | 0.56 |
| 11:AK:69:ALA:HB1 | 11:AK:103:LEU:CD2 | 2.33 | 0.56 |
| 19:AS:46:GLY:H | 19:AS:62:ILE:CG2 | 2.10 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:AT:93:GLU:O | 20:AT:95:ALA:N | 2.37 | 0.56 |
| 1:AA:1503:A:HO2' | 23:AX:16:A:H61 | 1.54 | 0.56 |
| 27:B1:53:VAL:O | 27:B1:54:ALA:HB3 | 2.06 | 0.56 |
| 31:B5:43:HIS:N | 31:B5:43:HIS:CD2 | 2.74 | 0.56 |
| 32:B6:36:LEU:HD12 | 32:B6:50:ARG:CZ | 2.36 | 0.56 |
| 35:B9:1:MET:SD | 36:BA:2477:C:H2' | 2.46 | 0.56 |
| 36:BA:1596:A:O2' | 36:BA:1597:A:H5' | 2.05 | 0.56 |
| 36:BA:1863:G:H2' | 36:BA:1864:U:O4' | 2.05 | 0.56 |
| 36:BA:1932:A:H2' | 36:BA:1933:G:O4' | 2.06 | 0.56 |
| 36:BA:2307:G:N2 | 36:BA:2308:G:H5' | 2.19 | 0.56 |
| 36:BA:608:A:H2' | 36:BA:609:A:C8 | 2.39 | 0.56 |
| 38:BC:26:ALA:HB1 | 38:BC:185:LEU:HB2 | 1.86 | 0.56 |
| 42:BG:47:LYS:HG2 | 42:BG:81:LYS:HE2 | 1.88 | 0.56 |
| 46:BN:2:LYS:NZ | 54:BV:12:TYR:HA | 2.21 | 0.56 |
| 47:BO:96:THR:O | 47:BO:97:ARG:HG2 | 2.06 | 0.56 |
| 48:BP:66:GLY:O | 48:BP:67:MET:HB2 | 2.06 | 0.56 |
| 51:BS:54:LEU:HD23 | 51:BS:59:LYS:O | 2.05 | 0.56 |
| 55:BW:72:LYS:CE | 55:BW:108:GLY:HA3 | 2.30 | 0.56 |
| 56:BX:18:TYR:HA | 56:BX:21:PHE:HE1 | 1.66 | 0.56 |
| 1:AA:1116:C:H2' | 1:AA:1117:G:C5' | 2.28 | 0.56 |
| 1:AA:56:U:H2' | 1:AA:57:G:C8 | 2.40 | 0.56 |
| 1:AA:918:A:H2' | 1:AA:919:A:H8 | 1.67 | 0.56 |
| 2:AB:165:VAL:HG23 | 2:AB:166:ASP:H | 1.69 | 0.56 |
| 8:AH:7:ALA:CB | 8:AH:85:ARG:HD3 | 2.35 | 0.56 |
| 9:AI:48:GLU:N | 9:AI:49:PRO:CD | 2.68 | 0.56 |
| 10:AJ:35:SER:OG | 10:AJ:73:ASP:HB2 | 2.05 | 0.56 |
| 7:AG:79:ARG:NH2 | 22:AW:33:U:H4' | 2.19 | 0.56 |
| 25:AZ:171:ILE:HD12 | 25:AZ:171:ILE:H | 1.69 | 0.56 |
| 27:B1:75:GLU:OE1 | 27:B1:75:GLU:HA | 2.05 | 0.56 |
| 30:B4:9:LEU:HD12 | 30:B4:10:VAL:H | 1.71 | 0.56 |
| 36:BA:1316:U:H2' | 36:BA:1317:A:C8 | 2.40 | 0.56 |
| 36:BA:1374:G:H2' | 36:BA:1375:C:C6 | 2.40 | 0.56 |
| 36:BA:1567:A:H5' | 39:BD:58:HIS:CD2 | 2.40 | 0.56 |
| 36:BA:1796:U:H2' | 36:BA:1797:C:C6 | 2.40 | 0.56 |
| 36:BA:2231:C:H2' | 36:BA:2232:U:C6 | 2.40 | 0.56 |
| 34:B8:3:LYS:HD3 | 36:BA:242:G:O5' | 2.05 | 0.56 |
| 36:BA:479:A:OP1 | 57:BY:34:LYS:NZ | 2.38 | 0.56 |
| 36:BA:761:A:C8 | 36:BA:761:A:H3' | 2.40 | 0.56 |
| 36:BA:850:C:O2' | 36:BA:851:U:H5' | 2.06 | 0.56 |
| 38:BC:41:VAL:CG1 | 38:BC:43:VAL:HG23 | 2.34 | 0.56 |
| 39:BD:70:TRP:CH2 | 39:BD:150:LYS:HA | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BF:158:THR:O | 41:BF:160:ASN:N | 2.32 | 0.56 |
| 45:BK:90:UNK:O | 45:BK:95:UNK:HA | 2.06 | 0.56 |
| 46:BN:13:TRP:O | 46:BN:135:PRO:HD2 | 2.06 | 0.56 |
| 46:BN:44:PRO:O | 46:BN:45:ASN:CB | 2.53 | 0.56 |
| 49:BQ:43:THR:OG1 | 49:BQ:46:GLN:HB2 | 2.05 | 0.56 |
| 57:BY:75:ILE:HD12 | 57:BY:79:CYS:CA | 2.25 | 0.56 |
| 58:BZ:103:ARG:HG3 | 58:BZ:103:ARG:HH11 | 1.70 | 0.56 |
| 58:BZ:18:LEU:O | 58:BZ:21:ALA:HB3 | 2.06 | 0.56 |
| 1:AA:1166:G:N2 | 1:AA:1169:A:H3' | 2.19 | 0.56 |
| 2:AB:236:TYR:HD1 | 2:AB:236:TYR:H | 1.51 | 0.56 |
| 2:AB:21:ARG:HD2 | 2:AB:39:ILE:HG12 | 1.86 | 0.56 |
| 7:AG:113:GLU:HG3 | 7:AG:119:ARG:HG2 | 1.88 | 0.56 |
| 9:AI:81:ILE:O | 9:AI:85:LEU:HG | 2.06 | 0.56 |
| 25:AZ:125:GLN:NE2 | 25:AZ:323:LEU:HD11 | 2.21 | 0.56 |
| 34:B8:4:MET:HE2 | 36:BA:592:G:N3 | 2.21 | 0.56 |
| 36:BA:1529:G:N1 | 36:BA:1541:G:N2 | 2.53 | 0.56 |
| 1:AA:1484:C:O2' | 36:BA:1961:C:H5' | 2.05 | 0.56 |
| 36:BA:2240:C:O2' | 36:BA:2241:A:H5' | 2.06 | 0.56 |
| 36:BA:1297:C:OP1 | 36:BA:2710:C:H4' | 2.05 | 0.56 |
| 36:BA:669:G:H2' | 36:BA:669:G:N3 | 2.21 | 0.56 |
| 38:BC:163:PHE:O | 38:BC:164:ARG:HB2 | 2.05 | 0.56 |
| 39:BD:9:TYR:CZ | 39:BD:13:ARG:HD3 | 2.40 | 0.56 |
| 39:BD:142:VAL:HG23 | 39:BD:192:THR:C | 2.26 | 0.56 |
| 36:BA:744:G:OP1 | 40:BE:132:HIS:HB3 | 2.05 | 0.56 |
| 40:BE:3:GLY:O | 40:BE:4:ILE:HB | 2.06 | 0.56 |
| 40:BE:1:MET:H2 | 40:BE:84:PHE:HD2 | 1.52 | 0.56 |
| 41:BF:118:ALA:HA | 41:BF:123:LEU:CB | 2.35 | 0.56 |
| 42:BG:107:LEU:HD21 | 42:BG:178:PHE:CE1 | 2.41 | 0.56 |
| 43:BH:98:LEU:HD22 | 43:BH:125:VAL:HG23 | 1.86 | 0.56 |
| 43:BH:18:GLU:HB2 | 43:BH:25:LYS:N | 2.20 | 0.56 |
| 43:BH:33:LEU:HD12 | 43:BH:75:ALA:HA | 1.87 | 0.56 |
| 45:BK:82:UNK:CB | 45:BK:98:UNK:H | 2.19 | 0.56 |
| 51:BS:40:ILE:HB | 51:BS:46:VAL:O | 2.06 | 0.56 |
| 1:AA:976:G:H5' | 1:AA:1358:U:O2' | 2.06 | 0.56 |
| 1:AA:29:G:C2' | 1:AA:30:U:H5' | 2.36 | 0.56 |
| 1:AA:513:C:H2' | 1:AA:514:C:H6 | 1.68 | 0.56 |
| 4:AD:109:GLY:O | 4:AD:161:ASN:HB3 | 2.06 | 0.56 |
| 14:AN:15:LYS:HB3 | 14:AN:16:PHE:CD2 | 2.40 | 0.56 |
| 22:AV:46:G:C3' | 22:AV:47:U:H5'' | 2.10 | 0.56 |
| 25:AZ:13:ASN:ND2 | 25:AZ:241:ARG:HG3 | 2.21 | 0.56 |
| 25:AZ:257:GLY:O | 25:AZ:302:GLN:HB3 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:338:TYR:HD2 | 25:AZ:353:VAL:HG21 | 1.70 | 0.56 |
| 25:AZ:66:ALA:O | 25:AZ:67:HIS:CG | 2.59 | 0.56 |
| 26:B0:43:THR:HG21 | 36:BA:2336:A:H61 | 1.71 | 0.56 |
| 31:B5:36:CYS:SG | 31:B5:49:CYS:SG | 3.03 | 0.56 |
| 35:B9:31:LYS:O | 35:B9:32:HIS:HD2 | 1.88 | 0.56 |
| 36:BA:2393:A:H5' | 48:BP:62:LEU:HB3 | 1.88 | 0.56 |
| 36:BA:271(F):C:O2' | 36:BA:271(G):C:H5' | 2.06 | 0.56 |
| 36:BA:301:G:OP2 | 57:BY:97:ARG:NH1 | 2.39 | 0.56 |
| 36:BA:336:C:H2' | 36:BA:337:C:H6 | 1.71 | 0.56 |
| 36:BA:875:G:H2' | 36:BA:876:C:H6 | 1.69 | 0.56 |
| 38:BC:175:VAL:HG21 | 38:BC:189:ILE:CG1 | 2.34 | 0.56 |
| 40:BE:68:ALA:C | 40:BE:70:ALA:H | 2.09 | 0.56 |
| 41:BF:103:LYS:HA | 41:BF:106:ARG:HE | 1.71 | 0.56 |
| 41:BF:7:TYR:CD2 | 41:BF:16:GLY:HA3 | 2.40 | 0.56 |
| 41:BF:185:ASP:HA | 41:BF:188:ARG:HG2 | 1.87 | 0.56 |
| 41:BF:90:PHE:O | 41:BF:91:GLY:O | 2.23 | 0.56 |
| 42:BG:33:ARG:H | 42:BG:162:THR:HB | 1.70 | 0.56 |
| 42:BG:58:GLN:O | 42:BG:62:LEU:HD13 | 2.06 | 0.56 |
| 48:BP:146:VAL:HG13 | 48:BP:147:LEU:N | 2.21 | 0.56 |
| 49:BQ:110:THR:HG23 | 49:BQ:113:GLN:HG3 | 1.88 | 0.56 |
| 49:BQ:66:ILE:HG13 | 49:BQ:66:ILE:O | 2.04 | 0.56 |
| 51:BS:61:ASN:O | 51:BS:62:LYS:CB | 2.54 | 0.56 |
| 57:BY:95:LYS:HG3 | 57:BY:101:LYS:N | 2.21 | 0.56 |
| 1:AA:1004:A:N6 | 1:AA:1035:A:C5 | 2.74 | 0.56 |
| 1:AA:1258:G:O2' | 1:AA:1259:C:H5' | 2.06 | 0.56 |
| 7:AG:52:GLU:O | 7:AG:53:LYS:C | 2.44 | 0.56 |
| 7:AG:65:ALA:CB | 7:AG:124:LEU:HD23 | 2.36 | 0.56 |
| 13:AM:19:LEU:O | 13:AM:22:ILE:HD13 | 2.06 | 0.56 |
| 27:B1:27:GLU:HG3 | 27:B1:28:GLY:N | 2.21 | 0.56 |
| 35:B9:16:VAL:HG11 | 36:BA:1032:A:H4' | 1.86 | 0.56 |
| 36:BA:1568:G:OP2 | 39:BD:63:ARG:NH2 | 2.39 | 0.56 |
| 36:BA:2133:G:H1' | 36:BA:2158:A:N6 | 2.20 | 0.56 |
| 36:BA:2893:G:H5' | 36:BA:2894:G:C5' | 2.23 | 0.56 |
| 28:B2:48:HIS:CD2 | 36:BA:96:G:H4' | 2.41 | 0.56 |
| 37:BB:15:A:H3' | 37:BB:16:G:C5' | 2.35 | 0.56 |
| 38:BC:25:ALA:O | 38:BC:29:VAL:HG13 | 2.05 | 0.56 |
| 38:BC:6:ARG:O | 38:BC:10:LEU:CD2 | 2.54 | 0.56 |
| 39:BD:35:LYS:N | 39:BD:36:PRO:CD | 2.65 | 0.56 |
| 36:BA:320:A:H2' | 41:BF:136:THR:OG1 | 2.05 | 0.56 |
| 49:BQ:79:LEU:HD23 | 49:BQ:80:GLU:N | 2.20 | 0.56 |
| 50:BR:102:GLU:O | 50:BR:103:ARG:C | 2.43 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:BU:108:GLU:O | 53:BU:112:ARG:HG2 | 2.06 | 0.56 |
| 53:BU:66:ASN:ND2 | 53:BU:76:TYR:HB2 | 2.20 | 0.56 |
| 56:BX:26:TYR:HD2 | 56:BX:92:LEU:HD12 | 1.70 | 0.56 |
| 57:BY:6:HIS:H | 57:BY:6:HIS:HD2 | 1.54 | 0.56 |
| 1:AA:1112:C:O2 | 3:AC:179:ARG:HG3 | 2.06 | 0.56 |
| 4:AD:8:VAL:HB | 4:AD:21:LEU:HD12 | 1.87 | 0.56 |
| 5:AE:11:ILE:CG2 | 5:AE:105:VAL:HG22 | 2.36 | 0.56 |
| 11:AK:108:ILE:N | 11:AK:108:ILE:HD12 | 2.20 | 0.56 |
| 16:AP:82:GLN:O | 16:AP:83:GLU:HB2 | 2.05 | 0.56 |
| 19:AS:50:ALA:HB1 | 19:AS:57:HIS:HB3 | 1.86 | 0.56 |
| 25:AZ:65:THR:HG22 | 25:AZ:82:CYS:HA | 1.87 | 0.56 |
| 27:B1:27:GLU:CG | 27:B1:28:GLY:H | 2.19 | 0.56 |
| 28:B2:7:ARG:HH11 | 28:B2:7:ARG:HG2 | 1.70 | 0.56 |
| 35:B9:13:LYS:HD2 | 35:B9:28:GLU:HB2 | 1.88 | 0.56 |
| 36:BA:1240:U:O2' | 36:BA:1241:A:H5' | 2.06 | 0.56 |
| 36:BA:1333:C:O5' | 36:BA:1333:C:H6 | 1.89 | 0.56 |
| 33:B7:7:PRO:HG3 | 36:BA:1612:C:H5' | 1.87 | 0.56 |
| 36:BA:523:C:O2' | 36:BA:524:U:H5' | 2.06 | 0.56 |
| 36:BA:7:G:HO2' | 46:BN:13:TRP:HZ2 | 1.54 | 0.56 |
| 36:BA:810:U:OP1 | 36:BA:1253:A:N7 | 2.39 | 0.56 |
| 40:BE:65:GLY:HA2 | 40:BE:70:ALA:CB | 2.36 | 0.56 |
| 43:BH:152:ARG:O | 43:BH:162:ILE:HG22 | 2.06 | 0.56 |
| 49:BQ:32:TYR:O | 49:BQ:105:GLU:HB2 | 2.05 | 0.56 |
| 51:BS:66:ALA:HA | 51:BS:69:VAL:HG12 | 1.86 | 0.56 |
| 56:BX:30:VAL:HG11 | 56:BX:39:ILE:CD1 | 2.35 | 0.56 |
| 58:BZ:67:LEU:HD12 | 58:BZ:67:LEU:N | 2.21 | 0.56 |
| 1:AA:983:A:O2' | 1:AA:1050:G:OP2 | 2.24 | 0.55 |
| 1:AA:1152:A:OP1 | 10:AJ:68:HIS:HD2 | 1.88 | 0.55 |
| 1:AA:169:C:H2' | 1:AA:170:U:H5' | 1.87 | 0.55 |
| 1:AA:197:A:H4' | 1:AA:198:G:O5' | 2.06 | 0.55 |
| 1:AA:61:G:H2' | 1:AA:62:U:O4' | 2.06 | 0.55 |
| 2:AB:193:ASP:OD2 | 2:AB:193:ASP:O | 2.23 | 0.55 |
| 2:AB:42:ILE:CD1 | 2:AB:202:PRO:HB2 | 2.36 | 0.55 |
| 9:AI:95:LYS:NZ | 9:AI:96:LEU:HD13 | 2.21 | 0.55 |
| 12:AL:86:ARG:O | 12:AL:86:ARG:HG2 | 2.05 | 0.55 |
| 13:AM:29:ARG:O | 13:AM:32:GLU:HB3 | 2.06 | 0.55 |
| 14:AN:32:SER:CB | 14:AN:41:ARG:HG2 | 2.33 | 0.55 |
| 25:AZ:46:ASP:OD1 | 25:AZ:183:HIS:HE1 | 1.89 | 0.55 |
| 26:B0:69:PHE:HB2 | 36:BA:857:C:OP1 | 2.07 | 0.55 |
| 27:B1:80:LEU:HD13 | 27:B1:82:LEU:HD21 | 1.87 | 0.55 |
| 32:B6:15:GLU:OE1 | 32:B6:18:ARG:CD | 2.54 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:B6:11:LEU:HD21 | 32:B6:51:GLU:HG2 | 1.87 | 0.55 |
| 32:B6:10:LEU:HD12 | 34:B8:34:TRP:CD1 | 2.40 | 0.55 |
| 34:B8:50:LEU:N | 34:B8:53:PRO:HD3 | 2.18 | 0.55 |
| 36:BA:1173:G:H5' | 36:BA:1174:A:O5' | 2.06 | 0.55 |
| 36:BA:1528(A):A:C8 | 36:BA:1529:G:C8 | 2.95 | 0.55 |
| 36:BA:1448:G:H1' | 36:BA:1528:A:N6 | 2.21 | 0.55 |
| 36:BA:1722:A:C2 | 36:BA:1740:G:H8 | 2.24 | 0.55 |
| 36:BA:2472:G:H3' | 36:BA:2475:C:N4 | 2.21 | 0.55 |
| 38:BC:124:GLY:O | 38:BC:128:GLY:HA3 | 2.06 | 0.55 |
| 39:BD:117:VAL:HG21 | 39:BD:128:GLY:C | 2.26 | 0.55 |
| 40:BE:146:THR:HA | 40:BE:147:PRO:C | 2.26 | 0.55 |
| 41:BF:107:LYS:O | 41:BF:110:LEU:N | 2.39 | 0.55 |
| 41:BF:170:LEU:HD13 | 41:BF:171:PRO:HD2 | 1.87 | 0.55 |
| 41:BF:155:LEU:HD12 | 41:BF:174:VAL:O | 2.06 | 0.55 |
| 46:BN:3:THR:HG22 | 46:BN:4:TYR:N | 2.17 | 0.55 |
| 48:BP:144:GLU:N | 48:BP:145:PRO:HD3 | 2.21 | 0.55 |
| 52:BT:28:VAL:HG13 | 52:BT:46:GLU:CA | 2.34 | 0.55 |
| 52:BT:27:THR:HG21 | 52:BT:49:VAL:HB | 1.88 | 0.55 |
| 52:BT:96:ARG:HH11 | 52:BT:96:ARG:HB2 | 1.70 | 0.55 |
| 57:BY:13:VAL:CG1 | 57:BY:28:LYS:HD3 | 2.36 | 0.55 |
| 1:AA:1120:G:H2' | 1:AA:1121:U:C6 | 2.39 | 0.55 |
| 1:AA:454:C:H5'' | 1:AA:455:C:C5 | 2.41 | 0.55 |
| 1:AA:909:A:OP1 | 12:AL:21:LYS:HD3 | 2.06 | 0.55 |
| 4:AD:103:ASN:O | 4:AD:106:TYR:HB3 | 2.07 | 0.55 |
| 11:AK:59:TYR:CE1 | 11:AK:63:LEU:HD21 | 2.41 | 0.55 |
| 25:AZ:321:TYR:HD1 | 25:AZ:367:ASN:HD22 | 1.54 | 0.55 |
| 29:B3:23:LEU:CD2 | 29:B3:50:VAL:HG11 | 2.36 | 0.55 |
| 32:B6:19:ARG:CG | 32:B6:20:ASN:N | 2.69 | 0.55 |
| 36:BA:1106:G:H2' | 36:BA:1107:G:O4' | 2.05 | 0.55 |
| 36:BA:1010:A:H1' | 36:BA:1153:C:C1' | 2.34 | 0.55 |
| 36:BA:1349:A:N6 | 36:BA:1598:C:N4 | 2.54 | 0.55 |
| 36:BA:2133:G:H1' | 36:BA:2158:A:H61 | 1.72 | 0.55 |
| 36:BA:2195:C:O2' | 36:BA:2196:C:H5' | 2.06 | 0.55 |
| 36:BA:2295:C:H2' | 36:BA:2296:U:H6 | 1.72 | 0.55 |
| 36:BA:2839:G:H2' | 36:BA:2840:C:C6 | 2.41 | 0.55 |
| 36:BA:77:C:H2' | 36:BA:78:A:C8 | 2.42 | 0.55 |
| 40:BE:4:ILE:HG23 | 40:BE:4:ILE:O | 2.06 | 0.55 |
| 41:BF:202:PHE:CE2 | 41:BF:206:ILE:HG13 | 2.41 | 0.55 |
| 42:BG:171:ALA:HA | 42:BG:174:GLU:HB3 | 1.87 | 0.55 |
| 53:BU:24:TYR:CB | 53:BU:29:SER:HB3 | 2.16 | 0.55 |
| 53:BU:34:LYS:HE2 | 53:BU:34:LYS:HA | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:310:A:P | 57:BY:18:GLY:HA2 | 2.47 | 0.55 |
| 57:BY:2:ARG:CD | 57:BY:3:VAL:HG23 | 2.37 | 0.55 |
| 1:AA:1429:C:H2' | 1:AA:1430:C:H6 | 1.71 | 0.55 |
| 2:AB:60:ASP:CB | 2:AB:64:ARG:HH21 | 2.18 | 0.55 |
| 12:AL:8:ASN:ND2 | 17:AQ:34:LYS:HE2 | 2.21 | 0.55 |
| 13:AM:23:TYR:HB3 | 13:AM:67:GLU:HB3 | 1.87 | 0.55 |
| 16:AP:21:VAL:CG1 | 16:AP:34:GLU:HB3 | 2.36 | 0.55 |
| 18:AR:36:ASN:HB2 | 18:AR:39:VAL:HG23 | 1.89 | 0.55 |
| 19:AS:28:LYS:HE2 | 19:AS:29:ARG:CZ | 2.36 | 0.55 |
| 19:AS:41:VAL:HG23 | 19:AS:44:MET:HG2 | 1.88 | 0.55 |
| 19:AS:62:ILE:HD12 | 19:AS:66:MET:HG3 | 1.87 | 0.55 |
| 1:AA:1305:G:C5' | 21:AU:4:GLY:C | 2.75 | 0.55 |
| 26:B0:41:ARG:O | 26:B0:42:GLY:C | 2.44 | 0.55 |
| 27:B1:4:VAL:HG23 | 27:B1:11:ARG:HG2 | 1.89 | 0.55 |
| 36:BA:2126:A:H1' | 36:BA:2127:G:C8 | 2.41 | 0.55 |
| 36:BA:43:A:O2' | 36:BA:44:G:H5' | 2.06 | 0.55 |
| 38:BC:10:LEU:N | 38:BC:10:LEU:HD22 | 2.21 | 0.55 |
| 38:BC:164:ARG:C | 38:BC:171:ILE:HD12 | 2.25 | 0.55 |
| 38:BC:51:PRO:HG2 | 38:BC:52:ARG:H | 1.72 | 0.55 |
| 39:BD:242:ARG:HD2 | 39:BD:242:ARG:N | 2.21 | 0.55 |
| 42:BG:37:VAL:HG21 | 42:BG:103:LEU:HD12 | 1.88 | 0.55 |
| 46:BN:35:ARG:NH2 | 46:BN:42:TRP:HH2 | 2.04 | 0.55 |
| 48:BP:24:GLY:O | 48:BP:25:SER:HB3 | 2.06 | 0.55 |
| 51:BS:15:ARG:NH1 | 51:BS:18:ILE:HD11 | 2.19 | 0.55 |
| 1:AA:1019:C:O2' | 1:AA:1020:U:H5' | 2.05 | 0.55 |
| 1:AA:189(J):G:O2' | 1:AA:189(K):U:H5' | 2.06 | 0.55 |
| 1:AA:368:U:P | 25:AZ:291:ARG:HH11 | 2.29 | 0.55 |
| 1:AA:714:G:H2' | 1:AA:715:A:C8 | 2.41 | 0.55 |
| 2:AB:111:ARG:O | 2:AB:145:LEU:HD11 | 2.07 | 0.55 |
| 2:AB:8:LYS:O | 2:AB:10:LEU:N | 2.40 | 0.55 |
| 3:AC:130:VAL:HG12 | 3:AC:134:ILE:HD11 | 1.87 | 0.55 |
| 15:AO:32:LEU:HD12 | 15:AO:63:ARG:HB2 | 1.87 | 0.55 |
| 19:AS:49:ILE:O | 19:AS:60:VAL:HG13 | 2.06 | 0.55 |
| 20:AT:100:ILE:C | 20:AT:102:GLY:H | 2.10 | 0.55 |
| 24:AY:68:C:H2' | 24:AY:69:C:C6 | 2.41 | 0.55 |
| 25:AZ:133:VAL:HG12 | 25:AZ:134:PHE:N | 2.22 | 0.55 |
| 25:AZ:298:VAL:HA | 25:AZ:302:GLN:OE1 | 2.06 | 0.55 |
| 26:B0:40:GLN:HE22 | 26:B0:43:THR:HA | 1.72 | 0.55 |
| 30:B4:9:LEU:O | 30:B4:10:VAL:HB | 2.07 | 0.55 |
| 31:B5:2:ALA:HA | 36:BA:2015:A:C1' | 2.30 | 0.55 |
| 31:B5:48:GLU:O | 31:B5:49:CYS:CB | 2.54 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:BA:1064:C:C3' | 36:BA:1065:U:H5'' | 2.37 | 0.55 |
| 36:BA:1188:U:H4' | 54:BV:79:VAL:CG1 | 2.37 | 0.55 |
| 36:BA:1429:G:H2' | 36:BA:1430:C:C6 | 2.40 | 0.55 |
| 31:B5:2:ALA:CA | 36:BA:2015:A:H1' | 2.30 | 0.55 |
| 36:BA:2469:A:N3 | 36:BA:2469:A:H5' | 2.22 | 0.55 |
| 36:BA:628:G:O2' | 36:BA:629:G:H5'' | 2.05 | 0.55 |
| 36:BA:671:C:H2' | 36:BA:672:C:C6 | 2.42 | 0.55 |
| 36:BA:723:G:H2' | 36:BA:724:U:H6 | 1.66 | 0.55 |
| 39:BD:9:TYR:C | 39:BD:10:THR:HG22 | 2.27 | 0.55 |
| 40:BE:108:SER:O | 40:BE:162:ALA:HA | 2.07 | 0.55 |
| 41:BF:9:ILE:HG12 | 41:BF:14:PRO:CA | 2.30 | 0.55 |
| 46:BN:22:THR:OG1 | 46:BN:25:ARG:HB2 | 2.06 | 0.55 |
| 55:BW:21:VAL:C | 55:BW:23:LEU:H | 2.08 | 0.55 |
| 1:AA:1234:C:H2' | 1:AA:1235:U:H6 | 1.71 | 0.55 |
| 1:AA:1443:G:N3 | 1:AA:1443:G:H2' | 2.21 | 0.55 |
| 1:AA:1498:U:C4' | 1:AA:1519:A:H2 | 2.19 | 0.55 |
| 1:AA:189(I):G:H2' | 1:AA:189(J):G:C8 | 2.42 | 0.55 |
| 1:AA:370:C:O2' | 1:AA:371:G:H5' | 2.06 | 0.55 |
| 1:AA:735:C:H2' | 1:AA:736:C:H6 | 1.70 | 0.55 |
| 3:AC:153:VAL:O | 3:AC:154:SER:CB | 2.54 | 0.55 |
| 3:AC:60:ALA:HB3 | 3:AC:63:ASN:ND2 | 2.22 | 0.55 |
| 4:AD:61:LYS:CE | 4:AD:62:GLN:NE2 | 2.68 | 0.55 |
| 5:AE:41:VAL:HG13 | 5:AE:113:ALA:HA | 1.89 | 0.55 |
| 19:AS:19:VAL:O | 19:AS:23:ASN:HB2 | 2.06 | 0.55 |
| 19:AS:43:GLU:C | 19:AS:45:VAL:N | 2.57 | 0.55 |
| 25:AZ:341:GLN:N | 25:AZ:341:GLN:NE2 | 2.53 | 0.55 |
| 34:B8:14:VAL:HG21 | 34:B8:22:VAL:HG12 | 1.89 | 0.55 |
| 36:BA:1551:C:H2' | 36:BA:1552:G:O4' | 2.07 | 0.55 |
| 36:BA:1831:G:H2' | 36:BA:1832:C:C6 | 2.42 | 0.55 |
| 36:BA:2078:C:H2' | 36:BA:2079:U:C6 | 2.42 | 0.55 |
| 36:BA:2791:C:H41 | 36:BA:2801(A):A:H62 | 1.53 | 0.55 |
| 36:BA:64:A:C2 | 56:BX:66:LEU:HD13 | 2.42 | 0.55 |
| 36:BA:71:A:H5'' | 36:BA:73:A:C8 | 2.41 | 0.55 |
| 36:BA:880:G:H1 | 36:BA:897:C:H42 | 1.55 | 0.55 |
| 37:BB:56:G:H4' | 37:BB:57:A:O5' | 2.06 | 0.55 |
| 39:BD:72:LYS:HD2 | 39:BD:103:ARG:HH11 | 1.71 | 0.55 |
| 41:BF:126:VAL:HG21 | 41:BF:129:PHE:CZ | 2.42 | 0.55 |
| 43:BH:139:GLN:O | 43:BH:143:GLN:HB2 | 2.06 | 0.55 |
| 48:BP:24:GLY:CA | 48:BP:33:ARG:NH1 | 2.67 | 0.55 |
| 53:BU:9:VAL:O | 53:BU:13:LYS:HG2 | 2.05 | 0.55 |
| 53:BU:38:THR:O | 53:BU:41:ALA:HB3 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:BV:38:LEU:C | 54:BV:39:LEU:HD13 | 2.27 | 0.55 |
| 54:BV:39:LEU:N | 54:BV:39:LEU:HD22 | 2.22 | 0.55 |
| 3:AC:131:ARG:HH11 | 3:AC:166:GLU:HG3 | 1.72 | 0.55 |
| 8:AH:89:PRO:HA | 8:AH:92:ARG:HH11 | 1.71 | 0.55 |
| 11:AK:17:GLY:O | 11:AK:80:VAL:HA | 2.06 | 0.55 |
| 12:AL:47:LYS:CB | 12:AL:48:PRO:CD | 2.74 | 0.55 |
| 16:AP:67:THR:HG22 | 16:AP:68:ASP:N | 2.21 | 0.55 |
| 26:B0:36:ILE:HA | 26:B0:60:PHE:HA | 1.88 | 0.55 |
| 32:B6:19:ARG:O | 32:B6:20:ASN:O | 2.25 | 0.55 |
| 36:BA:1349:A:N6 | 36:BA:1598:C:H42 | 2.05 | 0.55 |
| 36:BA:2024:G:H2' | 36:BA:2025:C:C6 | 2.42 | 0.55 |
| 36:BA:2185:C:H2' | 36:BA:2186:G:C5' | 2.34 | 0.55 |
| 36:BA:341:G:O2' | 36:BA:342:G:H5' | 2.06 | 0.55 |
| 36:BA:598:G:H2' | 36:BA:599:G:O4' | 2.07 | 0.55 |
| 38:BC:132:GLY:N | 38:BC:133:PRO:CD | 2.69 | 0.55 |
| 42:BG:110:ALA:HB2 | 42:BG:140:ILE:HD13 | 1.89 | 0.55 |
| 44:BJ:23:UNK:HA | 44:BJ:118:UNK:CB | 2.36 | 0.55 |
| 46:BN:108:PRO:HG2 | 46:BN:113:GLY:HA3 | 1.88 | 0.55 |
| 46:BN:94:HIS:HA | 46:BN:96:GLU:OE1 | 2.07 | 0.55 |
| 49:BQ:109:VAL:HG13 | 49:BQ:113:GLN:OE1 | 2.06 | 0.55 |
| 51:BS:106:ARG:O | 51:BS:106:ARG:HD2 | 2.07 | 0.55 |
| 51:BS:66:ALA:CB | 51:BS:99:LYS:HD3 | 2.37 | 0.55 |
| 52:BT:46:GLU:O | 52:BT:65:LYS:HD2 | 2.07 | 0.55 |
| 58:BZ:30:ASN:O | 58:BZ:32:HIS:N | 2.40 | 0.55 |
| 1:AA:1270:C:H5' | 1:AA:1270:C:H6 | 1.72 | 0.55 |
| 1:AA:1525:G:O2' | 1:AA:1526:G:H5' | 2.07 | 0.55 |
| 1:AA:269:C:H2' | 1:AA:270:A:H8 | 1.71 | 0.55 |
| 1:AA:575:G:H4' | 1:AA:576:G:C5' | 2.37 | 0.55 |
| 12:AL:24:VAL:CG1 | 12:AL:24:VAL:O | 2.54 | 0.55 |
| 19:AS:41:VAL:CG2 | 19:AS:44:MET:HG2 | 2.36 | 0.55 |
| 22:AV:4:C:H2' | 22:AV:5:G:C5' | 2.33 | 0.55 |
| 25:AZ:145:GLU:O | 25:AZ:145:GLU:CG | 2.54 | 0.55 |
| 25:AZ:161:TYR:O | 25:AZ:162:GLU:HB2 | 2.07 | 0.55 |
| 32:B6:5:VAL:O | 32:B6:6:ARG:HB2 | 2.07 | 0.55 |
| 36:BA:1858:G:O2' | 36:BA:1884:A:N6 | 2.39 | 0.55 |
| 36:BA:2363:C:O2' | 36:BA:2364:C:H5' | 2.06 | 0.55 |
| 36:BA:2717:G:O2' | 52:BT:96:ARG:HD3 | 2.07 | 0.55 |
| 36:BA:2854:G:H2' | 36:BA:2855:C:H6 | 1.71 | 0.55 |
| 36:BA:610:G:N2 | 36:BA:619:G:H1' | 2.22 | 0.55 |
| 36:BA:61:G:H1 | 36:BA:94:C:N4 | 1.97 | 0.55 |
| 37:BB:114:C:H2' | 37:BB:115:G:H8 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BD:218:ARG:HG3 | 39:BD:218:ARG:HH11 | 1.71 | 0.55 |
| 39:BD:35:LYS:CB | 39:BD:63:ARG:HA | 2.36 | 0.55 |
| 40:BE:197:ILE:HD11 | 40:BE:199:ARG:NH2 | 2.22 | 0.55 |
| 41:BF:137:LYS:HA | 41:BF:140:LEU:HB3 | 1.87 | 0.55 |
| 42:BG:107:LEU:HD22 | 42:BG:177:GLY:O | 2.05 | 0.55 |
| 42:BG:16:ARG:HD3 | 42:BG:31:VAL:HG21 | 1.87 | 0.55 |
| 46:BN:28:THR:CG2 | 46:BN:29:LYS:H | 2.18 | 0.55 |
| 49:BQ:32:TYR:CE2 | 49:BQ:111:GLU:HG3 | 2.40 | 0.55 |
| 49:BQ:70:PRO:HA | 49:BQ:94:VAL:O | 2.07 | 0.55 |
| 50:BR:11:ASN:O | 50:BR:12:ARG:CB | 2.55 | 0.55 |
| 51:BS:65:VAL:O | 51:BS:69:VAL:HG12 | 2.06 | 0.55 |
| 53:BU:85:LYS:CD | 53:BU:117:GLN:HE22 | 2.20 | 0.55 |
| 36:BA:337:C:OP1 | 57:BY:6:HIS:O | 2.25 | 0.55 |
| 1:AA:1402:C:H2' | 1:AA:1403:C:O4' | 2.07 | 0.55 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.41 | 0.55 |
| 1:AA:979:C:C3' | 1:AA:980:C:C5' | 2.81 | 0.55 |
| 5:AE:110:LEU:HD13 | 5:AE:118:ILE:HD13 | 1.88 | 0.55 |
| 8:AH:103:VAL:HB | 8:AH:109:ILE:H | 1.71 | 0.55 |
| 11:AK:111:ASP:OD2 | 11:AK:111:ASP:O | 2.24 | 0.55 |
| 15:AO:29:VAL:CG1 | 15:AO:67:LEU:HD21 | 2.36 | 0.55 |
| 25:AZ:188:THR:HG22 | 25:AZ:188:THR:O | 2.07 | 0.55 |
| 24:AY:1:A:C5' | 25:AZ:90:LYS:NZ | 2.58 | 0.55 |
| 32:B6:15:GLU:CD | 32:B6:18:ARG:NH2 | 2.60 | 0.55 |
| 36:BA:996:A:H61 | 36:BA:1159:U:H3 | 1.55 | 0.55 |
| 36:BA:2197:U:H1' | 36:BA:2198:A:C8 | 2.42 | 0.55 |
| 36:BA:272(D):G:H1 | 36:BA:364:C:H42 | 1.52 | 0.55 |
| 36:BA:654(M):C:H2' | 36:BA:654(N):G:N7 | 2.21 | 0.55 |
| 36:BA:894:C:C2' | 36:BA:895:U:H5' | 2.37 | 0.55 |
| 38:BC:215:THR:CB | 38:BC:221:SER:HA | 2.36 | 0.55 |
| 40:BE:81:ILE:O | 40:BE:81:ILE:HG22 | 2.07 | 0.55 |
| 42:BG:103:LEU:HD21 | 42:BG:178:PHE:HZ | 1.70 | 0.55 |
| 42:BG:36:LYS:HD3 | 42:BG:38:VAL:HG23 | 1.89 | 0.55 |
| 43:BH:98:LEU:HD12 | 43:BH:102:ALA:O | 2.06 | 0.55 |
| 52:BT:28:VAL:HG22 | 52:BT:46:GLU:C | 2.27 | 0.55 |
| 52:BT:48:ILE:C | 52:BT:63:VAL:HG13 | 2.27 | 0.55 |
| 1:AA:1228:C:OP1 | 13:AM:108:ARG:NH2 | 2.35 | 0.55 |
| 1:AA:122:G:H8 | 1:AA:122:G:O5' | 1.90 | 0.55 |
| 1:AA:1308:U:H2' | 1:AA:1309:G:C8 | 2.42 | 0.55 |
| 1:AA:1327:C:H5'' | 21:AU:20:LYS:HD3 | 1.89 | 0.55 |
| 1:AA:1369:C:H2' | 1:AA:1370:G:C8 | 2.42 | 0.55 |
| 1:AA:158:G:H2' | 1:AA:159:G:C8 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:266:G:H5' | 1:AA:268:C:H41 | 1.71 | 0.55 |
| 6:AF:74:ASP:HB3 | 6:AF:77:ARG:HH21 | 1.70 | 0.55 |
| 7:AG:75:VAL:HG12 | 7:AG:88:PRO:CB | 2.31 | 0.55 |
| 9:AI:40:LEU:O | 9:AI:42:ARG:N | 2.38 | 0.55 |
| 1:AA:1329:A:P | 13:AM:28:ALA:HB3 | 2.46 | 0.55 |
| 17:AQ:60:ILE:HG23 | 17:AQ:62:SER:OG | 2.07 | 0.55 |
| 19:AS:40:ILE:HG22 | 19:AS:67:VAL:HA | 1.89 | 0.55 |
| 28:B2:47:ASN:ND2 | 36:BA:94(A):G:N3 | 2.55 | 0.55 |
| 35:B9:19:ARG:C | 35:B9:21:GLY:H | 2.10 | 0.55 |
| 36:BA:2839:G:H1' | 50:BR:93:GLY:H | 1.72 | 0.55 |
| 36:BA:803:U:O2' | 36:BA:804:A:H5' | 2.06 | 0.55 |
| 38:BC:99:ILE:HG23 | 38:BC:102:LYS:HD2 | 1.89 | 0.55 |
| 38:BC:171:ILE:HG12 | 38:BC:196:LEU:HD21 | 1.88 | 0.55 |
| 39:BD:60:ARG:HG3 | 39:BD:86:PRO:CB | 2.34 | 0.55 |
| 41:BF:195:ASP:HB3 | 41:BF:198:ALA:HB3 | 1.89 | 0.55 |
| 36:BA:674:G:C1' | 41:BF:74:ARG:HD3 | 2.36 | 0.55 |
| 46:BN:48:MET:H | 46:BN:48:MET:HE3 | 1.71 | 0.55 |
| 48:BP:114:ILE:CG2 | 48:BP:130:PHE:CD1 | 2.89 | 0.55 |
| 49:BQ:76:LYS:CB | 49:BQ:91:GLU:HG3 | 2.29 | 0.55 |
| 50:BR:21:TYR:OH | 50:BR:43:GLU:HG2 | 2.07 | 0.55 |
| 50:BR:82:GLU:O | 50:BR:86:ARG:HG3 | 2.07 | 0.55 |
| 55:BW:17:VAL:C | 55:BW:19:LEU:N | 2.58 | 0.55 |
| 56:BX:12:VAL:CG2 | 56:BX:13:LEU:N | 2.69 | 0.55 |
| 1:AA:338:A:O2' | 1:AA:339:C:H5' | 2.07 | 0.55 |
| 1:AA:426:G:H2' | 1:AA:427:U:C6 | 2.42 | 0.55 |
| 7:AG:111:ARG:HD2 | 7:AG:123:GLU:HB2 | 1.88 | 0.55 |
| 1:AA:1291:G:H4' | 9:AI:39:GLY:HA3 | 1.89 | 0.55 |
| 20:AT:47:GLY:O | 20:AT:49:ALA:N | 2.33 | 0.55 |
| 30:B4:7:PRO:O | 30:B4:8:LYS:CB | 2.55 | 0.55 |
| 36:BA:110:G:O2' | 36:BA:111:A:H5' | 2.07 | 0.55 |
| 36:BA:1341:U:OP1 | 36:BA:1397:U:N3 | 2.36 | 0.55 |
| 36:BA:2008:C:H2' | 36:BA:2009:G:H8 | 1.71 | 0.55 |
| 36:BA:2881:C:C2 | 36:BA:2882:A:C8 | 2.94 | 0.55 |
| 36:BA:968:G:O2' | 36:BA:969:U:H5' | 2.07 | 0.55 |
| 37:BB:15:A:H1' | 37:BB:110:G:C5 | 2.42 | 0.55 |
| 39:BD:267:SER:C | 39:BD:269:PHE:H | 2.10 | 0.55 |
| 36:BA:1568:G:P | 39:BD:63:ARG:HH22 | 2.29 | 0.55 |
| 40:BE:200:GLU:N | 40:BE:200:GLU:OE2 | 2.40 | 0.55 |
| 36:BA:2632:A:C2 | 40:BE:61:ARG:HD2 | 2.42 | 0.55 |
| 43:BH:143:GLN:NE2 | 43:BH:143:GLN:HA | 2.19 | 0.55 |
| 48:BP:92:GLU:HG3 | 48:BP:121:LYS:NZ | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:BQ:109:VAL:HG12 | 49:BQ:113:GLN:HB2 | 1.89 | 0.55 |
| 54:BV:61:VAL:HG23 | 54:BV:61:VAL:O | 2.05 | 0.55 |
| 1:AA:346:G:HO2' | 1:AA:347:G:H8 | 1.53 | 0.54 |
| 1:AA:414:A:H2' | 1:AA:415:A:O4' | 2.07 | 0.54 |
| 3:AC:6:HIS:CD2 | 3:AC:8:ILE:HB | 2.43 | 0.54 |
| 5:AE:80:ILE:HG21 | 5:AE:142:LEU:HD23 | 1.89 | 0.54 |
| 11:AK:50:TYR:OH | 11:AK:59:TYR:HE2 | 1.90 | 0.54 |
| 11:AK:87:THR:HG22 | 11:AK:88:GLY:N | 2.23 | 0.54 |
| 15:AO:82:ILE:HG23 | 15:AO:83:GLU:N | 2.22 | 0.54 |
| 29:B3:35:ARG:HG2 | 29:B3:36:VAL:N | 2.22 | 0.54 |
| 32:B6:33:LYS:O | 32:B6:34:LEU:HB2 | 2.07 | 0.54 |
| 36:BA:2174:C:H5' | 38:BC:3:HIS:NE2 | 2.21 | 0.54 |
| 36:BA:2892:A:N7 | 36:BA:2893:G:N3 | 2.55 | 0.54 |
| 36:BA:813:U:H2' | 36:BA:814:C:C6 | 2.41 | 0.54 |
| 36:BA:968:G:H2' | 36:BA:969:U:C6 | 2.42 | 0.54 |
| 38:BC:186:ALA:HB1 | 38:BC:190:ARG:CZ | 2.36 | 0.54 |
| 39:BD:131:LEU:HB2 | 39:BD:136:ILE:CD1 | 2.37 | 0.54 |
| 39:BD:9:TYR:CD2 | 39:BD:10:THR:HG22 | 2.42 | 0.54 |
| 42:BG:28:VAL:O | 42:BG:28:VAL:HG12 | 2.07 | 0.54 |
| 42:BG:60:LEU:O | 42:BG:63:ILE:HG12 | 2.06 | 0.54 |
| 48:BP:146:VAL:O | 48:BP:148:LEU:HG | 2.07 | 0.54 |
| 50:BR:63:ARG:HG3 | 50:BR:80:PHE:CE2 | 2.40 | 0.54 |
| 51:BS:106:ARG:HB3 | 51:BS:106:ARG:HH11 | 1.73 | 0.54 |
| 51:BS:25:ARG:NH2 | 51:BS:40:ILE:HD11 | 2.21 | 0.54 |
| 54:BV:40:LEU:HA | 54:BV:45:THR:HB | 1.89 | 0.54 |
| 1:AA:1216:G:OP1 | 14:AN:2:ALA:CB | 2.56 | 0.54 |
| 1:AA:319:G:O2' | 1:AA:320:C:H5' | 2.07 | 0.54 |
| 1:AA:344:A:O2' | 1:AA:345:C:OP1 | 2.24 | 0.54 |
| 1:AA:534:U:C6 | 1:AA:534:U:H5' | 2.41 | 0.54 |
| 3:AC:153:VAL:O | 3:AC:154:SER:HB3 | 2.07 | 0.54 |
| 7:AG:27:ILE:HD13 | 7:AG:40:ALA:HA | 1.88 | 0.54 |
| 17:AQ:91:ARG:HH11 | 17:AQ:91:ARG:CB | 2.20 | 0.54 |
| 19:AS:40:ILE:HD13 | 19:AS:62:ILE:CD1 | 2.38 | 0.54 |
| 20:AT:16:HIS:O | 20:AT:19:SER:HB3 | 2.07 | 0.54 |
| 20:AT:41:ILE:HG22 | 20:AT:91:LEU:CD1 | 2.38 | 0.54 |
| 22:AV:65:G:H2' | 22:AV:66:U:C6 | 2.42 | 0.54 |
| 25:AZ:222:LEU:HD23 | 25:AZ:243:GLU:HG2 | 1.88 | 0.54 |
| 26:B0:26:TYR:CD1 | 26:B0:26:TYR:N | 2.74 | 0.54 |
| 27:B1:17:SER:O | 27:B1:37:ILE:HA | 2.07 | 0.54 |
| 28:B2:28:LYS:O | 28:B2:53:LEU:HD21 | 2.07 | 0.54 |
| 30:B4:25:TYR:O | 30:B4:26:SER:HB3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:B7:8:ASN:ND2 | 33:B7:10:ARG:N | 2.55 | 0.54 |
| 36:BA:1053:C:H2' | 36:BA:1054:A:C8 | 2.39 | 0.54 |
| 36:BA:1543:C:C3' | 36:BA:1544:A:H5'' | 2.34 | 0.54 |
| 36:BA:1605:C:O4' | 36:BA:1610:A:C6 | 2.60 | 0.54 |
| 36:BA:2020:A:OP1 | 53:BU:27:LEU:HD13 | 2.07 | 0.54 |
| 36:BA:2672:G:C2' | 36:BA:2673:G:H5'' | 2.37 | 0.54 |
| 36:BA:315:G:H2' | 36:BA:316:C:C6 | 2.42 | 0.54 |
| 36:BA:426:C:O2' | 36:BA:427:U:H5' | 2.07 | 0.54 |
| 36:BA:587:C:H4' | 36:BA:588:U:OP2 | 2.06 | 0.54 |
| 36:BA:761:A:O5' | 36:BA:761:A:C8 | 2.60 | 0.54 |
| 36:BA:94:C:H2' | 36:BA:94:C:O2 | 2.07 | 0.54 |
| 38:BC:100:ILE:HD12 | 38:BC:126:LYS:HE2 | 1.88 | 0.54 |
| 46:BN:23:LEU:HB3 | 46:BN:60:ILE:HG21 | 1.87 | 0.54 |
| 49:BQ:48:GLU:HA | 49:BQ:51:ARG:HB3 | 1.88 | 0.54 |
| 49:BQ:87:LYS:O | 49:BQ:88:GLY:O | 2.24 | 0.54 |
| 51:BS:35:ILE:HD11 | 51:BS:99:LYS:HE3 | 1.89 | 0.54 |
| 52:BT:28:VAL:HG22 | 52:BT:47:GLY:H | 1.69 | 0.54 |
| 53:BU:13:LYS:NZ | 53:BU:16:LYS:HZ1 | 2.04 | 0.54 |
| 57:BY:6:HIS:N | 57:BY:6:HIS:CD2 | 2.72 | 0.54 |
| 1:AA:1030(C):G:O2' | 1:AA:1030(D):A:H5' | 2.07 | 0.54 |
| 1:AA:1202:G:C2 | 14:AN:42:ILE:HG21 | 2.43 | 0.54 |
| 1:AA:1236:A:H4' | 1:AA:1304:G:H4' | 1.90 | 0.54 |
| 1:AA:261:U:O2 | 1:AA:263:A:C8 | 2.61 | 0.54 |
| 1:AA:398:C:O5' | 1:AA:398:C:H6 | 1.90 | 0.54 |
| 17:AQ:58:GLU:OE1 | 17:AQ:75:ARG:NE | 2.41 | 0.54 |
| 18:AR:36:ASN:C | 18:AR:38:GLU:H | 2.11 | 0.54 |
| 20:AT:37:SER:O | 20:AT:41:ILE:HG12 | 2.08 | 0.54 |
| 24:AY:75:C:C6 | 25:AZ:230:THR:O | 2.60 | 0.54 |
| 27:B1:65:SER:O | 27:B1:66:HIS:ND1 | 2.40 | 0.54 |
| 28:B2:9:GLN:O | 28:B2:13:ALA:HB2 | 2.06 | 0.54 |
| 31:B5:47:PRO:C | 31:B5:49:CYS:H | 2.10 | 0.54 |
| 35:B9:1:MET:HA | 35:B9:4:ARG:CZ | 2.37 | 0.54 |
| 36:BA:1164:G:O2' | 36:BA:1165:U:H5' | 2.07 | 0.54 |
| 36:BA:323:G:HO2' | 36:BA:1205:U:H3 | 1.55 | 0.54 |
| 36:BA:1400:G:H2' | 36:BA:1401:G:H8 | 1.72 | 0.54 |
| 36:BA:1528(A):A:H8 | 36:BA:1529:G:C8 | 2.24 | 0.54 |
| 36:BA:1682:G:H2' | 36:BA:1683:C:C6 | 2.42 | 0.54 |
| 36:BA:2787:C:C2 | 40:BE:61:ARG:HD3 | 2.42 | 0.54 |
| 37:BB:87:G:H5'' | 37:BB:88:C:OP2 | 2.08 | 0.54 |
| 38:BC:175:VAL:HG11 | 38:BC:189:ILE:HG13 | 1.89 | 0.54 |
| 39:BD:63:ARG:O | 39:BD:65:ILE:HD13 | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:1997:G:OP1 | 40:BE:123:ALA:HB1 | 2.07 | 0.54 |
| 40:BE:61:ARG:HG2 | 40:BE:62:PRO:HD3 | 1.89 | 0.54 |
| 43:BH:118:PRO:HG2 | 43:BH:121:ILE:HD12 | 1.89 | 0.54 |
| 49:BQ:26:TYR:CE1 | 49:BQ:28:ALA:HB2 | 2.42 | 0.54 |
| 51:BS:49:VAL:O | 51:BS:50:SER:HB3 | 2.07 | 0.54 |
| 52:BT:62:THR:HG22 | 52:BT:75:ILE:HG23 | 1.90 | 0.54 |
| 52:BT:29:ARG:HE | 52:BT:86:ILE:CG2 | 2.20 | 0.54 |
| 58:BZ:108:PRO:HG2 | 58:BZ:111:VAL:CG2 | 2.38 | 0.54 |
| 3:AC:10:PHE:CE2 | 3:AC:178:LEU:HD13 | 2.42 | 0.54 |
| 7:AG:80:VAL:HG12 | 7:AG:81:GLY:H | 1.71 | 0.54 |
| 10:AJ:40:LEU:HD23 | 10:AJ:69:ASN:O | 2.06 | 0.54 |
| 1:AA:1196:U:H5'' | 23:AX:26:A:N1 | 2.22 | 0.54 |
| 25:AZ:342:PHE:HB2 | 25:AZ:344:PHE:CE1 | 2.42 | 0.54 |
| 32:B6:35:GLU:HA | 32:B6:35:GLU:OE1 | 2.07 | 0.54 |
| 32:B6:53:LYS:CD | 32:B6:54:ILE:H | 2.17 | 0.54 |
| 36:BA:2538:C:H2' | 36:BA:2539:C:C6 | 2.42 | 0.54 |
| 36:BA:545:C:H2' | 36:BA:547:A:C8 | 2.42 | 0.54 |
| 36:BA:761:A:H8 | 36:BA:761:A:O5' | 1.91 | 0.54 |
| 36:BA:78:A:H2' | 36:BA:79:G:H8 | 1.72 | 0.54 |
| 38:BC:114:VAL:HG21 | 38:BC:149:ILE:HD11 | 1.90 | 0.54 |
| 39:BD:183:ARG:HH11 | 39:BD:183:ARG:HG2 | 1.72 | 0.54 |
| 41:BF:160:ASN:HD21 | 41:BF:162:LEU:CD1 | 2.14 | 0.54 |
| 46:BN:39:ARG:C | 46:BN:41:ASP:H | 2.09 | 0.54 |
| 52:BT:33:LYS:NZ | 52:BT:43:GLN:HG2 | 2.22 | 0.54 |
| 36:BA:995:C:O4' | 53:BU:57:PHE:HD1 | 1.90 | 0.54 |
| 54:BV:45:THR:O | 54:BV:46:VAL:HG12 | 2.07 | 0.54 |
| 36:BA:483:A:H1' | 57:BY:60:PHE:CZ | 2.42 | 0.54 |
| 1:AA:1118:C:OP1 | 9:AI:104:ARG:NH1 | 2.41 | 0.54 |
| 1:AA:1323:G:H2' | 1:AA:1324:A:C8 | 2.43 | 0.54 |
| 1:AA:860:A:H2' | 1:AA:861:G:O4' | 2.08 | 0.54 |
| 2:AB:97:TRP:CZ2 | 2:AB:173:ALA:HA | 2.42 | 0.54 |
| 1:AA:939:G:C5' | 7:AG:102:ARG:NH2 | 2.67 | 0.54 |
| 7:AG:72:ARG:HA | 7:AG:96:GLN:NE2 | 2.20 | 0.54 |
| 11:AK:37:GLY:C | 11:AK:38:ASN:HD22 | 2.11 | 0.54 |
| 14:AN:55:GLY:O | 14:AN:56:VAL:O | 2.25 | 0.54 |
| 13:AM:87:TYR:HE1 | 19:AS:81:ARG:NH2 | 2.05 | 0.54 |
| 25:AZ:138:VAL:HG23 | 25:AZ:173:GLY:O | 2.06 | 0.54 |
| 29:B3:19:GLN:HE22 | 29:B3:52:HIS:HE1 | 1.55 | 0.54 |
| 35:B9:10:ILE:HD12 | 35:B9:10:ILE:H | 1.73 | 0.54 |
| 36:BA:1067:A:C3' | 36:BA:1068:G:H5'' | 2.34 | 0.54 |
| 29:B3:31:LEU:O | 36:BA:1158:C:H4' | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:BA:1257:C:H2' | 36:BA:1258:C:C6 | 2.43 | 0.54 |
| 36:BA:1308:A:H2' | 36:BA:1309:G:O4' | 2.07 | 0.54 |
| 36:BA:2649:U:H2' | 36:BA:2650:U:C6 | 2.42 | 0.54 |
| 36:BA:2688:U:H3' | 36:BA:2688:U:O2 | 2.07 | 0.54 |
| 36:BA:2845:G:O2' | 36:BA:2846:G:H5' | 2.07 | 0.54 |
| 36:BA:653:A:N3 | 36:BA:653:A:H2' | 2.21 | 0.54 |
| 36:BA:1654:A:C2 | 40:BE:113:PHE:CD2 | 2.96 | 0.54 |
| 40:BE:64:LYS:O | 40:BE:64:LYS:HG2 | 2.07 | 0.54 |
| 42:BG:42:GLY:CA | 42:BG:90:LEU:H | 2.20 | 0.54 |
| 46:BN:44:PRO:O | 46:BN:45:ASN:HB3 | 2.06 | 0.54 |
| 48:BP:115:LEU:N | 48:BP:115:LEU:HD23 | 2.22 | 0.54 |
| 51:BS:30:ARG:HH22 | 51:BS:62:LYS:CD | 2.21 | 0.54 |
| 54:BV:62:LEU:HD21 | 54:BV:95:LEU:HB2 | 1.89 | 0.54 |
| 58:BZ:105:VAL:O | 58:BZ:141:VAL:HG23 | 2.07 | 0.54 |
| 37:BB:75:G:H2' | 58:BZ:85:HIS:CE1 | 2.42 | 0.54 |
| 1:AA:1153:C:O2' | 1:AA:1154:G:P | 2.65 | 0.54 |
| 1:AA:135:C:H2' | 1:AA:136:C:H5' | 1.89 | 0.54 |
| 1:AA:192:U:H2' | 1:AA:193:C:C6 | 2.34 | 0.54 |
| 1:AA:632:A:C2 | 1:AA:633:G:H1' | 2.43 | 0.54 |
| 2:AB:122:PHE:HA | 2:AB:139:LYS:HZ1 | 1.72 | 0.54 |
| 2:AB:51:LEU:HD23 | 2:AB:201:ILE:HD12 | 1.88 | 0.54 |
| 19:AS:29:ARG:HD2 | 19:AS:29:ARG:N | 2.22 | 0.54 |
| 36:BA:1086:A:H3' | 36:BA:1086:A:N3 | 2.23 | 0.54 |
| 36:BA:1270:C:H5'' | 36:BA:1271:G:O5' | 2.08 | 0.54 |
| 36:BA:1794:U:H2' | 36:BA:1795:C:H6 | 1.68 | 0.54 |
| 36:BA:2061:G:H5'' | 36:BA:2503:A:C2 | 2.42 | 0.54 |
| 36:BA:2173:A:O3' | 38:BC:218:MET:HE1 | 2.08 | 0.54 |
| 36:BA:2305:A:H5'' | 42:BG:134:GLY:HA3 | 1.89 | 0.54 |
| 36:BA:2735:G:H2' | 36:BA:2736:G:H8 | 1.72 | 0.54 |
| 36:BA:298:G:C8 | 36:BA:298:G:OP2 | 2.61 | 0.54 |
| 36:BA:614(A):U:C4' | 36:BA:614(B):G:H5'' | 2.36 | 0.54 |
| 36:BA:884:C:C2' | 36:BA:885:C:H5' | 2.31 | 0.54 |
| 37:BB:70:C:O2' | 37:BB:71:C:H5' | 2.08 | 0.54 |
| 38:BC:50:ASP:OD2 | 38:BC:53:ARG:HG3 | 2.08 | 0.54 |
| 36:BA:1844:C:H5' | 39:BD:256:GLY:O | 2.07 | 0.54 |
| 41:BF:2:LYS:HG3 | 41:BF:25:PRO:HG2 | 1.88 | 0.54 |
| 47:BO:64:ARG:NH2 | 47:BO:100:GLY:HA3 | 2.22 | 0.54 |
| 41:BF:34:TRP:CE3 | 48:BP:12:ALA:HA | 2.43 | 0.54 |
| 53:BU:8:VAL:O | 53:BU:12:ARG:HG3 | 2.07 | 0.54 |
| 55:BW:10:VAL:HG23 | 55:BW:101:SER:O | 2.08 | 0.54 |
| 1:AA:1040:U:H2' | 1:AA:1041:A:C8 | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:1126:U:P | 1:AA:1281:U:O2 | 2.65 | 0.54 |
| 1:AA:160:A:H1' | 1:AA:344:A:N7 | 2.23 | 0.54 |
| 1:AA:647:C:O2' | 1:AA:648:A:H5' | 2.08 | 0.54 |
| 2:AB:93:VAL:HG21 | 2:AB:97:TRP:HD1 | 1.72 | 0.54 |
| 11:AK:82:VAL:CG1 | 11:AK:108:ILE:HG23 | 2.38 | 0.54 |
| 14:AN:19:ARG:O | 14:AN:20:ALA:O | 2.25 | 0.54 |
| 18:AR:84:LYS:N | 18:AR:84:LYS:NZ | 2.55 | 0.54 |
| 25:AZ:277:LEU:HD12 | 25:AZ:279:GLU:N | 2.21 | 0.54 |
| 36:BA:1666:G:H8 | 36:BA:1666:G:H5' | 1.71 | 0.54 |
| 36:BA:181:A:H5' | 36:BA:181:A:H8 | 1.72 | 0.54 |
| 36:BA:2580:U:C5' | 40:BE:131:ALA:N | 2.71 | 0.54 |
| 36:BA:407:G:H2' | 36:BA:408:G:H8 | 1.73 | 0.54 |
| 36:BA:654(L):G:H5'' | 36:BA:654(L):G:N3 | 2.22 | 0.54 |
| 28:B2:61:LEU:HD12 | 36:BA:72:U:C6 | 2.42 | 0.54 |
| 36:BA:733:G:O6 | 36:BA:761:A:C8 | 2.60 | 0.54 |
| 38:BC:78:ALA:HB3 | 38:BC:95:GLY:H | 1.73 | 0.54 |
| 40:BE:52:LEU:CD1 | 52:BT:1:MET:HG2 | 2.37 | 0.54 |
| 42:BG:51:ARG:HD3 | 42:BG:53:LEU:CD2 | 2.35 | 0.54 |
| 54:BV:47:VAL:HG23 | 54:BV:47:VAL:O | 2.07 | 0.54 |
| 54:BV:82:ARG:N | 54:BV:82:ARG:HD2 | 2.22 | 0.54 |
| 1:AA:1328:C:O2' | 1:AA:1329:A:H5' | 2.08 | 0.54 |
| 2:AB:122:PHE:HA | 2:AB:139:LYS:HZ2 | 1.72 | 0.54 |
| 2:AB:194:PRO:O | 2:AB:197:VAL:N | 2.39 | 0.54 |
| 4:AD:61:LYS:HD2 | 4:AD:207:TYR:OH | 2.08 | 0.54 |
| 4:AD:3:ARG:HG2 | 4:AD:3:ARG:HH21 | 1.71 | 0.54 |
| 7:AG:111:ARG:HB3 | 7:AG:113:GLU:HG2 | 1.89 | 0.54 |
| 8:AH:44:PHE:HE2 | 8:AH:109:ILE:HG21 | 1.72 | 0.54 |
| 1:AA:1152:A:H5'' | 10:AJ:13:HIS:HD2 | 1.71 | 0.54 |
| 12:AL:41:ARG:NH2 | 12:AL:57:LYS:NZ | 2.52 | 0.54 |
| 13:AM:7:VAL:CG2 | 42:BG:115:ARG:HA | 2.38 | 0.54 |
| 17:AQ:67:LYS:CA | 17:AQ:70:ARG:HH12 | 2.16 | 0.54 |
| 24:AY:17:H2U:OP1 | 24:AY:18:G:H4' | 2.08 | 0.54 |
| 25:AZ:13:ASN:O | 25:AZ:100:ASP:N | 2.39 | 0.54 |
| 25:AZ:158:LEU:O | 25:AZ:163:PHE:HB2 | 2.08 | 0.54 |
| 25:AZ:138:VAL:HG21 | 25:AZ:173:GLY:H | 1.72 | 0.54 |
| 25:AZ:42:VAL:HG23 | 25:AZ:70:TYR:HA | 1.89 | 0.54 |
| 32:B6:17:LYS:HB3 | 32:B6:18:ARG:NH1 | 2.23 | 0.54 |
| 34:B8:29:LYS:HG2 | 34:B8:44:LYS:HG2 | 1.90 | 0.54 |
| 36:BA:1779:U:C5 | 36:BA:1784:A:N7 | 2.68 | 0.54 |
| 36:BA:2529:G:OP2 | 36:BA:2530:A:H5'' | 2.08 | 0.54 |
| 36:BA:2792:G:O2' | 36:BA:2793:G:H5' | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BA:2864:G:H2' | 36:BA:2865:U:C6 | 2.43 | 0.54 |
| 40:BE:114:ALA:HB3 | 40:BE:160:TYR:HB3 | 1.90 | 0.54 |
| 40:BE:1:MET:HB3 | 40:BE:200:GLU:CD | 2.27 | 0.54 |
| 40:BE:30:PRO:O | 40:BE:32:PRO:HD3 | 2.08 | 0.54 |
| 41:BF:9:ILE:CG1 | 41:BF:14:PRO:HA | 2.30 | 0.54 |
| 43:BH:105:LEU:CD2 | 43:BH:105:LEU:H | 2.21 | 0.54 |
| 46:BN:67:LEU:HB3 | 46:BN:88:GLU:CG | 2.37 | 0.54 |
| 48:BP:24:GLY:N | 48:BP:33:ARG:CZ | 2.71 | 0.54 |
| 50:BR:3:HIS:O | 50:BR:5:LYS:N | 2.40 | 0.54 |
| 51:BS:34:HIS:CE1 | 51:BS:54:LEU:HB3 | 2.42 | 0.54 |
| 52:BT:12:SER:O | 52:BT:13:ARG:NH2 | 2.41 | 0.54 |
| 52:BT:29:ARG:HE | 52:BT:86:ILE:HG23 | 1.72 | 0.54 |
| 49:BQ:134:ARG:CZ | 58:BZ:122:ARG:NE | 2.71 | 0.54 |
| 1:AA:1023:G:C2' | 1:AA:1024:G:H5' | 2.36 | 0.54 |
| 1:AA:1503:A:C2 | 1:AA:1507:A:OP2 | 2.61 | 0.54 |
| 1:AA:255:G:H1' | 17:AQ:16:GLN:NE2 | 2.23 | 0.54 |
| 1:AA:444:C:O2' | 1:AA:445:G:H5' | 2.08 | 0.54 |
| 1:AA:513:C:H2' | 1:AA:514:C:C6 | 2.43 | 0.54 |
| 2:AB:21:ARG:HB3 | 2:AB:39:ILE:HA | 1.90 | 0.54 |
| 7:AG:141:VAL:O | 7:AG:144:MET:HB2 | 2.08 | 0.54 |
| 9:AI:121:ARG:HG2 | 9:AI:121:ARG:NH1 | 2.23 | 0.54 |
| 9:AI:9:ARG:CG | 9:AI:14:VAL:HG22 | 2.35 | 0.54 |
| 9:AI:28:VAL:HA | 9:AI:63:ILE:O | 2.08 | 0.54 |
| 10:AJ:90:LEU:N | 10:AJ:91:PRO:HD3 | 2.22 | 0.54 |
| 14:AN:4:LYS:O | 14:AN:7:ILE:HG12 | 2.08 | 0.54 |
| 24:AY:72:U:H2' | 24:AY:73:G:C5' | 2.37 | 0.54 |
| 25:AZ:356:PRO:HD3 | 25:AZ:370:PHE:HA | 1.90 | 0.54 |
| 26:B0:45:PHE:HE2 | 26:B0:77:ARG:HH21 | 1.55 | 0.54 |
| 27:B1:80:LEU:HB3 | 27:B1:82:LEU:HD23 | 1.89 | 0.54 |
| 28:B2:47:ASN:O | 28:B2:48:HIS:C | 2.46 | 0.54 |
| 34:B8:34:TRP:O | 34:B8:35:GLN:HB2 | 2.08 | 0.54 |
| 34:B8:50:LEU:N | 34:B8:53:PRO:CD | 2.71 | 0.54 |
| 36:BA:1385:G:HO2' | 36:BA:1396:U:H6 | 1.53 | 0.54 |
| 36:BA:142(A):C:O2' | 36:BA:143:G:H5' | 2.08 | 0.54 |
| 36:BA:1842:G:H2' | 36:BA:1843:C:C6 | 2.43 | 0.54 |
| 22:AW:19:G:N2 | 36:BA:2169:A:H4' | 2.23 | 0.54 |
| 26:B0:36:ILE:HG12 | 36:BA:2354:G:O2' | 2.08 | 0.54 |
| 36:BA:2790:A:N3 | 36:BA:2790:A:H2' | 2.22 | 0.54 |
| 36:BA:332:A:O2' | 36:BA:333:G:O5' | 2.26 | 0.54 |
| 36:BA:634:C:H2' | 36:BA:635:C:C6 | 2.43 | 0.54 |
| 37:BB:55:U:H2' | 37:BB:56:G:C8 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BB:73:A:H2' | 37:BB:74:U:H5' | 1.90 | 0.54 |
| 38:BC:49:ILE:HG21 | 38:BC:208:PHE:HE1 | 1.73 | 0.54 |
| 39:BD:72:LYS:HB3 | 39:BD:72:LYS:HZ3 | 1.72 | 0.54 |
| 41:BF:113:ALA:HB2 | 41:BF:183:VAL:HG12 | 1.90 | 0.54 |
| 46:BN:76:SER:HB3 | 46:BN:81:GLY:O | 2.07 | 0.54 |
| 36:BA:943:U:OP2 | 48:BP:38:GLN:HG2 | 2.08 | 0.54 |
| 48:BP:38:GLN:HG3 | 48:BP:39:LYS:N | 2.23 | 0.54 |
| 48:BP:58:THR:C | 48:BP:61:ARG:HE | 2.11 | 0.54 |
| 50:BR:4:LEU:HD12 | 50:BR:7:GLY:HA3 | 1.90 | 0.54 |
| 52:BT:8:LYS:HA | 52:BT:11:GLU:OE1 | 2.07 | 0.54 |
| 53:BU:36:ARG:HH11 | 53:BU:36:ARG:HB2 | 1.73 | 0.54 |
| 53:BU:3:ARG:NH1 | 53:BU:5:LYS:HB3 | 2.22 | 0.54 |
| 57:BY:7:VAL:HG21 | 57:BY:8:LYS:HZ2 | 1.73 | 0.54 |
| 1:AA:355:C:N4 | 1:AA:356:A:N6 | 2.56 | 0.54 |
| 2:AB:19:HIS:NE2 | 2:AB:206:ASP:HB2 | 2.22 | 0.54 |
| 2:AB:42:ILE:HG12 | 2:AB:43:ASP:N | 2.23 | 0.54 |
| 1:AA:973:G:H1' | 10:AJ:55:LYS:NZ | 2.22 | 0.54 |
| 1:AA:750:G:N3 | 15:AO:23:GLY:HA3 | 2.23 | 0.54 |
| 22:AW:57:G:H2' | 22:AW:58:A:C4' | 2.38 | 0.54 |
| 25:AZ:355:LEU:HD11 | 25:AZ:362:VAL:HG23 | 1.90 | 0.54 |
| 29:B3:4:LEU:HG | 29:B3:39:ASP:HB2 | 1.89 | 0.54 |
| 34:B8:5:LYS:HE2 | 36:BA:254:G:N7 | 2.23 | 0.54 |
| 36:BA:1092:C:H42 | 36:BA:1100:C:N4 | 2.05 | 0.54 |
| 36:BA:2073:C:O2' | 36:BA:2074:U:H5' | 2.08 | 0.54 |
| 36:BA:2236:C:H2' | 36:BA:2237:G:O4' | 2.08 | 0.54 |
| 36:BA:2394:C:O2' | 36:BA:2395:C:H5' | 2.08 | 0.54 |
| 36:BA:536:A:H2' | 36:BA:537:C:C6 | 2.43 | 0.54 |
| 26:B0:26:TYR:CE2 | 36:BA:857:C:H1' | 2.43 | 0.54 |
| 38:BC:137:LEU:HD22 | 38:BC:138:PRO:CD | 2.37 | 0.54 |
| 38:BC:21:THR:OG1 | 38:BC:24:GLU:HB2 | 2.08 | 0.54 |
| 39:BD:44:ASN:CB | 39:BD:49:ILE:HA | 2.37 | 0.54 |
| 40:BE:2:LYS:HB3 | 40:BE:95:ILE:CG2 | 2.38 | 0.54 |
| 42:BG:115:ARG:HH22 | 42:BG:136:ARG:CB | 2.03 | 0.54 |
| 43:BH:85:LYS:HD2 | 43:BH:133:VAL:HB | 1.90 | 0.54 |
| 46:BN:62:VAL:O | 46:BN:63:THR:O | 2.26 | 0.54 |
| 53:BU:52:ARG:HH11 | 53:BU:52:ARG:CB | 2.21 | 0.54 |
| 1:AA:1305:G:H5' | 21:AU:4:GLY:CA | 2.34 | 0.53 |
| 1:AA:1503:A:HO2' | 23:AX:16:A:N6 | 2.06 | 0.53 |
| 1:AA:180:U:C2' | 1:AA:181:G:H5' | 2.39 | 0.53 |
| 1:AA:189(H):G:O2' | 1:AA:189(I):G:H8 | 1.91 | 0.53 |
| 3:AC:164:ARG:HH21 | 3:AC:166:GLU:HB2 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:AH:103:VAL:CG2 | 8:AH:110:ALA:HB2 | 2.38 | 0.53 |
| 8:AH:104:ARG:CZ | 8:AH:138:TRP:CZ2 | 2.91 | 0.53 |
| 14:AN:29:ARG:NH1 | 14:AN:29:ARG:HG2 | 2.19 | 0.53 |
| 14:AN:57:ARG:HG3 | 14:AN:58:LYS:N | 2.22 | 0.53 |
| 15:AO:23:GLY:O | 15:AO:24:SER:HB3 | 2.08 | 0.53 |
| 16:AP:53:VAL:O | 16:AP:54:GLU:C | 2.46 | 0.53 |
| 19:AS:49:ILE:N | 19:AS:49:ILE:HD12 | 2.16 | 0.53 |
| 22:AW:12:U:H3 | 22:AW:23:A:H61 | 1.56 | 0.53 |
| 22:AW:19:G:C2 | 36:BA:2169:A:H4' | 2.42 | 0.53 |
| 24:AY:75:C:H41 | 25:AZ:232:THR:HG1 | 1.55 | 0.53 |
| 28:B2:19:VAL:CG1 | 28:B2:23:LYS:HE3 | 2.37 | 0.53 |
| 34:B8:29:LYS:HD3 | 34:B8:44:LYS:CB | 2.38 | 0.53 |
| 36:BA:1141:U:H2' | 46:BN:63:THR:HG22 | 1.90 | 0.53 |
| 36:BA:1577:C:H2' | 36:BA:1578:U:C1' | 2.37 | 0.53 |
| 36:BA:1946:U:H2' | 36:BA:1947:C:C6 | 2.43 | 0.53 |
| 36:BA:1267:U:C5 | 36:BA:2012:G:C2 | 2.96 | 0.53 |
| 37:BB:15:A:H3' | 37:BB:16:G:H5' | 1.89 | 0.53 |
| 39:BD:261:LYS:CE | 39:BD:263:ARG:NH2 | 2.70 | 0.53 |
| 42:BG:111:LEU:CD2 | 42:BG:179:PRO:HG2 | 2.38 | 0.53 |
| 50:BR:65:LEU:O | 50:BR:68:ARG:HB2 | 2.08 | 0.53 |
| 52:BT:91:ARG:HG2 | 52:BT:116:ALA:HA | 1.89 | 0.53 |
| 55:BW:29:LEU:HG | 55:BW:33:ARG:CD | 2.29 | 0.53 |
| 57:BY:2:ARG:C | 57:BY:4:LYS:H | 2.11 | 0.53 |
| 58:BZ:8:TYR:HD2 | 58:BZ:38:TYR:HH | 1.56 | 0.53 |
| 1:AA:177:C:H2' | 1:AA:178:C:H6 | 1.72 | 0.53 |
| 1:AA:381:C:H2' | 1:AA:382:A:O4' | 2.08 | 0.53 |
| 1:AA:865:A:H2' | 1:AA:866:C:C6 | 2.42 | 0.53 |
| 2:AB:145:LEU:O | 2:AB:149:LEU:HB2 | 2.08 | 0.53 |
| 12:AL:45:PRO:HG3 | 12:AL:53:ARG:HD3 | 1.90 | 0.53 |
| 17:AQ:52:LYS:N | 17:AQ:52:LYS:HD2 | 2.19 | 0.53 |
| 27:B1:75:GLU:O | 27:B1:78:LYS:HG2 | 2.08 | 0.53 |
| 31:B5:49:CYS:O | 31:B5:56:LYS:HD2 | 2.08 | 0.53 |
| 35:B9:30:PRO:HG2 | 36:BA:2528:U:OP1 | 2.07 | 0.53 |
| 36:BA:2065:C:H2' | 36:BA:2066:C:C6 | 2.42 | 0.53 |
| 36:BA:2640:G:H2' | 36:BA:2641:G:C5' | 2.33 | 0.53 |
| 36:BA:814:C:H2' | 36:BA:815:C:H6 | 1.72 | 0.53 |
| 13:AM:93:ARG:CG | 36:BA:888:C:OP1 | 2.55 | 0.53 |
| 38:BC:15:ASP:N | 38:BC:20:TYR:OH | 2.42 | 0.53 |
| 39:BD:247:ALA:CA | 39:BD:254:THR:HG22 | 2.38 | 0.53 |
| 41:BF:17:ARG:NH1 | 41:BF:17:ARG:HG3 | 2.21 | 0.53 |
| 41:BF:43:LYS:HB2 | 41:BF:98:SER:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:BG:126:ASP:O | 42:BG:128:ARG:N | 2.38 | 0.53 |
| 36:BA:1275:A:C4 | 50:BR:16:HIS:ND1 | 2.77 | 0.53 |
| 36:BA:2012:G:H4' | 55:BW:96:ILE:CD1 | 2.36 | 0.53 |
| 58:BZ:140:ASP:O | 58:BZ:141:VAL:CG2 | 2.57 | 0.53 |
| 1:AA:1158:C:O2' | 1:AA:1159:U:H4' | 2.09 | 0.53 |
| 2:AB:178:ARG:NH2 | 8:AH:68:ARG:HH22 | 2.07 | 0.53 |
| 4:AD:9:CYS:SG | 4:AD:31:CYS:O | 2.67 | 0.53 |
| 5:AE:33:VAL:HG21 | 5:AE:109:ILE:HG12 | 1.89 | 0.53 |
| 22:AW:53:G:O2' | 22:AW:54:U:H5' | 2.09 | 0.53 |
| 25:AZ:197:ASP:C | 25:AZ:198:LYS:HE2 | 2.28 | 0.53 |
| 26:B0:14:ARG:HD2 | 36:BA:2279:G:O6 | 2.08 | 0.53 |
| 32:B6:45:LYS:H | 32:B6:45:LYS:CD | 1.99 | 0.53 |
| 34:B8:49:VAL:HG12 | 34:B8:50:LEU:H | 1.73 | 0.53 |
| 36:BA:2223:G:H2' | 36:BA:2224:G:H5' | 1.90 | 0.53 |
| 36:BA:2460:U:O2' | 36:BA:2461:C:H5' | 2.08 | 0.53 |
| 36:BA:2819:G:H2' | 36:BA:2821:A:N7 | 2.23 | 0.53 |
| 36:BA:605:C:C2' | 36:BA:606:U:H5' | 2.37 | 0.53 |
| 36:BA:863:A:H2' | 36:BA:864:G:C8 | 2.44 | 0.53 |
| 38:BC:191:ALA:HA | 38:BC:194:ARG:CD | 2.37 | 0.53 |
| 40:BE:78:LEU:C | 40:BE:79:ARG:HD2 | 2.29 | 0.53 |
| 41:BF:40:GLN:HE22 | 41:BF:184:TYR:HB3 | 1.74 | 0.53 |
| 42:BG:138:GLN:HG3 | 42:BG:139:LEU:N | 2.23 | 0.53 |
| 42:BG:178:PHE:HB3 | 42:BG:180:PHE:CE1 | 2.43 | 0.53 |
| 43:BH:12:PRO:HB2 | 43:BH:15:VAL:CG1 | 2.38 | 0.53 |
| 52:BT:106:SER:C | 52:BT:107:ASP:OD1 | 2.46 | 0.53 |
| 52:BT:80:SER:CB | 52:BT:81:PRO:CD | 2.81 | 0.53 |
| 56:BX:12:VAL:HG12 | 56:BX:27:THR:C | 2.28 | 0.53 |
| 58:BZ:76:LEU:O | 58:BZ:82:ARG:O | 2.26 | 0.53 |
| 1:AA:628:G:O2' | 1:AA:629:G:H5' | 2.08 | 0.53 |
| 1:AA:837:G:N1 | 1:AA:850:U:O2 | 2.42 | 0.53 |
| 7:AG:54:THR:HG22 | 7:AG:125:MET:CE | 2.38 | 0.53 |
| 8:AH:125:ARG:HG3 | 8:AH:125:ARG:NH1 | 2.23 | 0.53 |
| 19:AS:29:ARG:HB3 | 19:AS:48:THR:HB | 1.89 | 0.53 |
| 24:AY:73:G:H2' | 24:AY:74:C:H5' | 1.90 | 0.53 |
| 26:B0:27:GLU:CB | 26:B0:68:GLU:HA | 2.27 | 0.53 |
| 28:B2:64:LEU:O | 28:B2:68:ARG:HB2 | 2.09 | 0.53 |
| 31:B5:55:ARG:HD3 | 31:B5:56:LYS:H | 1.74 | 0.53 |
| 32:B6:19:ARG:HG3 | 32:B6:20:ASN:N | 2.09 | 0.53 |
| 33:B7:9:ARG:HG3 | 33:B7:9:ARG:NH1 | 2.24 | 0.53 |
| 36:BA:105:C:O2' | 57:BY:2:ARG:HB2 | 2.08 | 0.53 |
| 36:BA:271(M):G:C2' | 36:BA:271(N):U:H5'' | 2.34 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:2753:A:O2' | 36:BA:2754:U:H5' | 2.08 | 0.53 |
| 37:BB:81:G:H2' | 37:BB:82:G:H5' | 1.91 | 0.53 |
| 38:BC:100:ILE:HG21 | 38:BC:126:LYS:HE3 | 1.90 | 0.53 |
| 41:BF:168:ARG:HB2 | 41:BF:175:THR:HG21 | 1.91 | 0.53 |
| 41:BF:95:ARG:CG | 41:BF:95:ARG:O | 2.57 | 0.53 |
| 52:BT:61:PHE:HD2 | 52:BT:61:PHE:H | 1.55 | 0.53 |
| 1:AA:475:G:O2' | 1:AA:476:G:H5' | 2.08 | 0.53 |
| 1:AA:300:A:H1' | 1:AA:565:U:O2 | 2.09 | 0.53 |
| 1:AA:967:C:H4' | 9:AI:125:TYR:CE2 | 2.36 | 0.53 |
| 4:AD:107:ARG:NH1 | 4:AD:114:ARG:NH2 | 2.56 | 0.53 |
| 4:AD:151:LYS:HG2 | 4:AD:151:LYS:O | 2.07 | 0.53 |
| 7:AG:48:LYS:O | 7:AG:51:GLN:HB2 | 2.08 | 0.53 |
| 1:AA:778:G:H21 | 11:AK:120:ARG:HD2 | 1.73 | 0.53 |
| 14:AN:13:THR:O | 14:AN:14:PRO:O | 2.26 | 0.53 |
| 19:AS:11:VAL:CA | 19:AS:38:SER:HB2 | 2.31 | 0.53 |
| 24:AY:74:C:O2 | 25:AZ:295:ARG:NH2 | 2.40 | 0.53 |
| 35:B9:22:ARG:HB2 | 35:B9:24:TYR:HE1 | 1.74 | 0.53 |
| 36:BA:1022:G:N7 | 46:BN:66:LYS:HE3 | 2.24 | 0.53 |
| 36:BA:1292:U:H6 | 36:BA:1292:U:H5' | 1.73 | 0.53 |
| 36:BA:2092:U:H5 | 36:BA:2226:C:OP2 | 1.92 | 0.53 |
| 36:BA:2408:U:H2' | 36:BA:2409:G:H8 | 1.72 | 0.53 |
| 36:BA:304:G:H2' | 36:BA:305:U:C6 | 2.43 | 0.53 |
| 36:BA:27:G:H22 | 36:BA:512:G:H2' | 1.72 | 0.53 |
| 36:BA:568:U:H2' | 36:BA:570:G:OP2 | 2.09 | 0.53 |
| 37:BB:42:C:O2' | 37:BB:43:C:P | 2.67 | 0.53 |
| 39:BD:26:LYS:O | 39:BD:27:THR:CB | 2.56 | 0.53 |
| 40:BE:13:ARG:O | 52:BT:57:PHE:HE1 | 1.91 | 0.53 |
| 43:BH:35:VAL:HG11 | 43:BH:71:LEU:O | 2.09 | 0.53 |
| 46:BN:93:THR:HG23 | 46:BN:93:THR:O | 2.08 | 0.53 |
| 48:BP:120:ALA:HB3 | 48:BP:137:LYS:O | 2.08 | 0.53 |
| 48:BP:138:LEU:HD21 | 48:BP:143:GLY:O | 2.09 | 0.53 |
| 56:BX:27:THR:HA | 56:BX:79:ALA:O | 2.08 | 0.53 |
| 2:AB:152:PHE:O | 2:AB:153:ARG:CB | 2.55 | 0.53 |
| 6:AF:48:LEU:HD13 | 6:AF:52:ILE:CG1 | 2.39 | 0.53 |
| 12:AL:88:GLY:H | 12:AL:98:TYR:HA | 1.73 | 0.53 |
| 13:AM:49:THR:O | 13:AM:53:VAL:HG23 | 2.07 | 0.53 |
| 19:AS:64:GLU:O | 19:AS:67:VAL:HG23 | 2.08 | 0.53 |
| 20:AT:26:ASN:N | 20:AT:26:ASN:HD22 | 2.05 | 0.53 |
| 25:AZ:194:GLU:O | 25:AZ:198:LYS:HE3 | 2.08 | 0.53 |
| 25:AZ:55:GLU:O | 25:AZ:56:GLU:C | 2.45 | 0.53 |
| 27:B1:43:TYR:N | 27:B1:43:TYR:HD2 | 2.05 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:BA:145:G:H2' | 36:BA:146:G:O4' | 2.08 | 0.53 |
| 36:BA:1509(B):A:C2' | 36:BA:1510:G:H5' | 2.39 | 0.53 |
| 36:BA:654(R):C:H2' | 36:BA:654(S):G:C8 | 2.44 | 0.53 |
| 37:BB:86:G:H2' | 37:BB:87:G:H8 | 1.73 | 0.53 |
| 43:BH:66:GLY:CA | 43:BH:69:ARG:HB3 | 2.35 | 0.53 |
| 48:BP:62:LEU:O | 48:BP:62:LEU:HG | 2.07 | 0.53 |
| 49:BQ:56:ARG:HG3 | 49:BQ:56:ARG:HH11 | 1.74 | 0.53 |
| 1:AA:1053:G:H4' | 1:AA:1054:C:C5' | 2.14 | 0.53 |
| 1:AA:1342:C:O2' | 1:AA:1343:G:H5' | 2.08 | 0.53 |
| 1:AA:1452:C:H5' | 1:AA:1456:G:N2 | 2.24 | 0.53 |
| 1:AA:284:G:H2' | 1:AA:285:G:H8 | 1.74 | 0.53 |
| 1:AA:310:G:H2' | 1:AA:311:C:H6 | 1.74 | 0.53 |
| 1:AA:429:U:C1' | 1:AA:430:A:H5'' | 2.38 | 0.53 |
| 1:AA:990:C:H2' | 1:AA:991:U:C6 | 2.43 | 0.53 |
| 3:AC:55:VAL:HG12 | 3:AC:55:VAL:O | 2.08 | 0.53 |
| 9:AI:28:VAL:HG22 | 9:AI:63:ILE:HB | 1.91 | 0.53 |
| 9:AI:77:ILE:O | 9:AI:81:ILE:HG12 | 2.09 | 0.53 |
| 9:AI:99:LEU:N | 9:AI:99:LEU:HD22 | 2.24 | 0.53 |
| 1:AA:1124:G:H5' | 10:AJ:35:SER:HB2 | 1.91 | 0.53 |
| 18:AR:84:LYS:HZ3 | 18:AR:84:LYS:N | 2.06 | 0.53 |
| 25:AZ:34:VAL:HG11 | 25:AZ:199:ILE:HG21 | 1.89 | 0.53 |
| 25:AZ:352:VAL:HG12 | 25:AZ:353:VAL:N | 2.24 | 0.53 |
| 25:AZ:389:ARG:O | 25:AZ:390:GLU:CB | 2.56 | 0.53 |
| 27:B1:50:ARG:HG2 | 27:B1:59:THR:HG22 | 1.91 | 0.53 |
| 27:B1:83:GLU:OE1 | 27:B1:83:GLU:N | 2.42 | 0.53 |
| 30:B4:8:LYS:O | 30:B4:9:LEU:CB | 2.56 | 0.53 |
| 36:BA:1292:U:H2' | 36:BA:1293:C:C6 | 2.44 | 0.53 |
| 36:BA:1970:A:H5'' | 36:BA:1971:A:OP1 | 2.08 | 0.53 |
| 36:BA:610:G:H2' | 36:BA:611:C:C6 | 2.44 | 0.53 |
| 38:BC:107:TRP:NE1 | 38:BC:110:PHE:CE2 | 2.73 | 0.53 |
| 39:BD:268:ARG:N | 39:BD:270:ILE:HD11 | 2.23 | 0.53 |
| 40:BE:15:PHE:HE1 | 40:BE:20:ALA:HB2 | 1.73 | 0.53 |
| 40:BE:179:GLU:O | 40:BE:180:ASN:HB2 | 2.09 | 0.53 |
| 41:BF:195:ASP:HB3 | 41:BF:198:ALA:CB | 2.38 | 0.53 |
| 42:BG:42:GLY:HA2 | 42:BG:90:LEU:N | 2.24 | 0.53 |
| 42:BG:68:PRO:HA | 42:BG:92:VAL:HB | 1.91 | 0.53 |
| 48:BP:24:GLY:HA3 | 48:BP:33:ARG:CZ | 2.38 | 0.53 |
| 51:BS:30:ARG:NH2 | 51:BS:62:LYS:HD3 | 2.24 | 0.53 |
| 52:BT:38:ASN:ND2 | 52:BT:38:ASN:O | 2.36 | 0.53 |
| 52:BT:54:ARG:HA | 52:BT:59:THR:CB | 2.38 | 0.53 |
| 36:BA:2875:C:H4' | 52:BT:5:ALA:CB | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BX:10:ALA:HB1 | 56:BX:11:PRO:CD | 2.36 | 0.53 |
| 57:BY:12:THR:CG2 | 57:BY:75:ILE:HG21 | 2.39 | 0.53 |
| 58:BZ:144:LEU:CD1 | 58:BZ:150:LEU:HD22 | 2.36 | 0.53 |
| 1:AA:1128:C:N4 | 1:AA:1139:G:H2' | 2.24 | 0.53 |
| 1:AA:137:C:H42 | 1:AA:226:G:H1 | 1.55 | 0.53 |
| 3:AC:96:GLY:O | 3:AC:97:LYS:HG2 | 2.09 | 0.53 |
| 4:AD:70:ILE:CG2 | 4:AD:71:SER:N | 2.71 | 0.53 |
| 8:AH:28:ALA:H | 8:AH:58:TYR:HA | 1.73 | 0.53 |
| 11:AK:52:GLY:N | 11:AK:55:LYS:HE3 | 2.24 | 0.53 |
| 19:AS:49:ILE:O | 19:AS:60:VAL:CG1 | 2.57 | 0.53 |
| 20:AT:50:GLU:HG3 | 20:AT:100:ILE:HG12 | 1.90 | 0.53 |
| 25:AZ:208:GLU:O | 25:AZ:210:ILE:N | 2.41 | 0.53 |
| 30:B4:30:GLU:C | 30:B4:31:ILE:HD12 | 2.29 | 0.53 |
| 36:BA:1025:G:N3 | 36:BA:1135:C:H1' | 2.24 | 0.53 |
| 36:BA:1491:G:O4' | 39:BD:99:ASP:OD2 | 2.27 | 0.53 |
| 36:BA:648:G:C4' | 36:BA:2351:G:H5'' | 2.38 | 0.53 |
| 36:BA:2839:G:C5' | 50:BR:46:GLY:HA2 | 2.39 | 0.53 |
| 36:BA:672:C:O3' | 41:BF:81:PRO:HG3 | 2.08 | 0.53 |
| 37:BB:7:G:H4' | 51:BS:29:PHE:HD1 | 1.73 | 0.53 |
| 38:BC:7:TYR:OH | 38:BC:11:LEU:HD21 | 2.08 | 0.53 |
| 39:BD:141:VAL:HG23 | 39:BD:141:VAL:O | 2.08 | 0.53 |
| 39:BD:76:PRO:HG2 | 39:BD:98:VAL:CG2 | 2.38 | 0.53 |
| 40:BE:77:ILE:CG2 | 40:BE:78:LEU:N | 2.66 | 0.53 |
| 41:BF:107:LYS:C | 41:BF:109:GLY:N | 2.62 | 0.53 |
| 41:BF:83:PHE:O | 41:BF:84:VAL:O | 2.26 | 0.53 |
| 47:BO:61:VAL:HG12 | 47:BO:87:ILE:HD11 | 1.91 | 0.53 |
| 49:BQ:141:GLN:HB2 | 58:BZ:99:TYR:CD2 | 2.44 | 0.53 |
| 51:BS:25:ARG:HG2 | 51:BS:25:ARG:NH1 | 2.24 | 0.53 |
| 53:BU:36:ARG:HB2 | 53:BU:36:ARG:NH1 | 2.23 | 0.53 |
| 36:BA:1188:U:H4' | 54:BV:79:VAL:HG13 | 1.91 | 0.53 |
| 55:BW:12:ILE:HD12 | 55:BW:42:ARG:NH1 | 2.23 | 0.53 |
| 1:AA:56:U:H2' | 1:AA:57:G:H8 | 1.74 | 0.53 |
| 2:AB:46:LYS:O | 2:AB:49:GLU:N | 2.42 | 0.53 |
| 11:AK:57:THR:HG22 | 11:AK:60:ALA:CB | 2.39 | 0.53 |
| 12:AL:53:ARG:HB3 | 12:AL:93:LEU:HD11 | 1.90 | 0.53 |
| 19:AS:13:ASP:O | 19:AS:15:LEU:N | 2.42 | 0.53 |
| 22:AW:31:A:N1 | 22:AW:39:U:O4 | 2.42 | 0.53 |
| 36:BA:2027:G:O2' | 36:BA:2028:U:H5' | 2.09 | 0.53 |
| 36:BA:2153:G:H2' | 36:BA:2154:G:O4' | 2.08 | 0.53 |
| 36:BA:2478:A:H2' | 36:BA:2479:G:H5' | 1.91 | 0.53 |
| 36:BA:2796:U:O2' | 36:BA:2799:C:H5' | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:543:C:N4 | 36:BA:549:G:H1 | 2.01 | 0.53 |
| 37:BB:106:G:H2' | 37:BB:107:G:C8 | 2.39 | 0.53 |
| 38:BC:107:TRP:HZ3 | 38:BC:131:LEU:HD21 | 1.69 | 0.53 |
| 38:BC:28:LEU:O | 38:BC:32:LEU:HG | 2.09 | 0.53 |
| 39:BD:73:VAL:HG13 | 39:BD:120:GLY:CA | 2.39 | 0.53 |
| 43:BH:76:VAL:C | 43:BH:78:GLY:N | 2.62 | 0.53 |
| 46:BN:103:VAL:O | 46:BN:106:MET:N | 2.42 | 0.53 |
| 46:BN:87:LEU:HD13 | 46:BN:87:LEU:C | 2.30 | 0.53 |
| 34:B8:25:MET:SD | 48:BP:64:LYS:HD3 | 2.49 | 0.53 |
| 52:BT:29:ARG:CB | 52:BT:85:LYS:HA | 2.38 | 0.53 |
| 55:BW:60:ASN:OD1 | 55:BW:60:ASN:O | 2.25 | 0.53 |
| 57:BY:86:ARG:C | 57:BY:88:LYS:HZ2 | 2.11 | 0.53 |
| 58:BZ:70:LEU:HD23 | 58:BZ:70:LEU:N | 2.24 | 0.53 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.43 | 0.53 |
| 1:AA:1269:A:C2 | 1:AA:1325:C:O2 | 2.62 | 0.53 |
| 1:AA:457:C:C2 | 1:AA:458:C:H5 | 2.27 | 0.53 |
| 2:AB:46:LYS:O | 2:AB:47:THR:C | 2.48 | 0.53 |
| 2:AB:51:LEU:O | 2:AB:55:PHE:CD2 | 2.60 | 0.53 |
| 4:AD:17:VAL:HG11 | 4:AD:197:PRO:HB2 | 1.91 | 0.53 |
| 10:AJ:6:ILE:HA | 10:AJ:97:GLU:O | 2.09 | 0.53 |
| 10:AJ:65:LEU:CD1 | 14:AN:56:VAL:H | 2.18 | 0.53 |
| 1:AA:128:G:H5' | 17:AQ:2:PRO:O | 2.09 | 0.53 |
| 17:AQ:60:ILE:HB | 17:AQ:74:LEU:HD23 | 1.89 | 0.53 |
| 19:AS:4:SER:O | 19:AS:5:LEU:O | 2.26 | 0.53 |
| 22:AV:61:C:H2' | 22:AV:62:C:C5' | 2.38 | 0.53 |
| 25:AZ:356:PRO:CD | 25:AZ:370:PHE:HA | 2.39 | 0.53 |
| 27:B1:43:TYR:CD2 | 27:B1:43:TYR:N | 2.75 | 0.53 |
| 36:BA:2124:G:H3' | 36:BA:2125:G:C8 | 2.44 | 0.53 |
| 36:BA:2287:A:H2 | 36:BA:2346:A:C2 | 2.25 | 0.53 |
| 36:BA:2317:C:H2' | 36:BA:2318:G:C5' | 2.36 | 0.53 |
| 36:BA:2621:A:P | 40:BE:119:ARG:HH22 | 2.32 | 0.53 |
| 36:BA:2631:G:H22 | 40:BE:61:ARG:NH1 | 2.06 | 0.53 |
| 36:BA:2820:A:O2' | 40:BE:191:PRO:HG3 | 2.09 | 0.53 |
| 39:BD:2:ALA:O | 39:BD:3:VAL:CB | 2.57 | 0.53 |
| 40:BE:97:LYS:O | 40:BE:100:GLU:HG3 | 2.09 | 0.53 |
| 46:BN:101:HIS:O | 46:BN:103:VAL:N | 2.42 | 0.53 |
| 48:BP:21:ARG:HH11 | 48:BP:29:LYS:HG2 | 1.73 | 0.53 |
| 49:BQ:133:ARG:NH1 | 49:BQ:133:ARG:HB2 | 2.21 | 0.53 |
| 36:BA:519:U:H5'' | 55:BW:25:ARG:HH22 | 1.74 | 0.53 |
| 58:BZ:8:TYR:HB2 | 58:BZ:38:TYR:CZ | 2.44 | 0.53 |
| 1:AA:1105:A:O2' | 1:AA:1106:G:H5' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:84:U:C2' | 1:AA:88:A:H5' | 2.39 | 0.52 |
| 1:AA:995:C:O2' | 1:AA:996:A:P | 2.66 | 0.52 |
| 5:AE:82:VAL:HG21 | 5:AE:138:ALA:HA | 1.91 | 0.52 |
| 8:AH:108:GLY:C | 8:AH:109:ILE:HG22 | 2.29 | 0.52 |
| 9:AI:57:GLY:O | 9:AI:58:ARG:HB3 | 2.09 | 0.52 |
| 16:AP:58:TYR:CD1 | 16:AP:58:TYR:C | 2.82 | 0.52 |
| 19:AS:78:ARG:HB2 | 19:AS:81:ARG:NH1 | 2.25 | 0.52 |
| 25:AZ:140:MET:O | 25:AZ:141:VAL:O | 2.26 | 0.52 |
| 29:B3:13:ILE:HG22 | 29:B3:13:ILE:O | 2.09 | 0.52 |
| 29:B3:26:LEU:CB | 29:B3:28:LEU:HD21 | 2.37 | 0.52 |
| 36:BA:1047:G:N2 | 36:BA:1110:G:H2' | 2.24 | 0.52 |
| 36:BA:1556:C:H2' | 36:BA:1557:C:H6 | 1.74 | 0.52 |
| 36:BA:528:A:H2 | 36:BA:2043:C:C5' | 2.21 | 0.52 |
| 36:BA:2186:G:C2 | 36:BA:2187:G:C6 | 2.97 | 0.52 |
| 36:BA:2392:A:H2 | 36:BA:2424:C:H42 | 1.57 | 0.52 |
| 31:B5:7:PRO:HA | 36:BA:2615:U:C6 | 2.44 | 0.52 |
| 36:BA:319:C:O2' | 36:BA:320:A:H5' | 2.10 | 0.52 |
| 36:BA:706:A:H2' | 36:BA:707:G:O4' | 2.08 | 0.52 |
| 36:BA:762:U:H4' | 36:BA:763:G:O5' | 2.08 | 0.52 |
| 38:BC:53:ARG:HD3 | 38:BC:56:GLN:NE2 | 2.24 | 0.52 |
| 39:BD:209:ALA:O | 39:BD:212:SER:HB2 | 2.10 | 0.52 |
| 41:BF:40:GLN:NE2 | 41:BF:184:TYR:HB3 | 2.24 | 0.52 |
| 51:BS:77:ALA:C | 51:BS:79:ALA:H | 2.12 | 0.52 |
| 52:BT:105:LEU:HD22 | 52:BT:109:GLU:OE1 | 2.10 | 0.52 |
| 58:BZ:141:VAL:HA | 58:BZ:144:LEU:HD23 | 1.91 | 0.52 |
| 58:BZ:30:ASN:HA | 58:BZ:89:PHE:HE2 | 1.73 | 0.52 |
| 1:AA:613:C:H2' | 1:AA:614:A:C8 | 2.43 | 0.52 |
| 2:AB:7:VAL:HG13 | 2:AB:11:LEU:HD12 | 1.91 | 0.52 |
| 2:AB:61:LEU:HD23 | 2:AB:68:ILE:HD11 | 1.91 | 0.52 |
| 2:AB:75:LYS:C | 2:AB:75:LYS:HD3 | 2.30 | 0.52 |
| 5:AE:20:GLN:HE22 | 5:AE:25:ARG:HH21 | 1.57 | 0.52 |
| 7:AG:18:TYR:C | 7:AG:20:ASP:H | 2.13 | 0.52 |
| 9:AI:53:VAL:HG11 | 9:AI:92:TYR:CE2 | 2.44 | 0.52 |
| 14:AN:4:LYS:HD3 | 14:AN:7:ILE:HD11 | 1.91 | 0.52 |
| 15:AO:59:MET:O | 15:AO:62:GLN:HB3 | 2.09 | 0.52 |
| 1:AA:191:G:N3 | 20:AT:105:SER:HB3 | 2.24 | 0.52 |
| 25:AZ:385:ARG:HA | 25:AZ:399:VAL:HG12 | 1.92 | 0.52 |
| 25:AZ:36:ALA:HA | 25:AZ:42:VAL:HG11 | 1.89 | 0.52 |
| 26:B0:5:LYS:NZ | 26:B0:5:LYS:HB3 | 2.25 | 0.52 |
| 31:B5:34:PRO:O | 31:B5:35:GLU:HG2 | 2.08 | 0.52 |
| 36:BA:1353:A:H4' | 39:BD:38:LYS:CE | 2.38 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:BA:1529:G:C2 | 36:BA:1541:G:N2 | 2.77 | 0.52 |
| 36:BA:1827:C:C2' | 36:BA:1828:G:H5' | 2.39 | 0.52 |
| 36:BA:1971:A:C4 | 39:BD:241:PRO:HD3 | 2.44 | 0.52 |
| 36:BA:2296:U:O2 | 36:BA:2333:A:N3 | 2.42 | 0.52 |
| 36:BA:2872:G:C2 | 36:BA:2873:A:N6 | 2.76 | 0.52 |
| 22:AW:56:C:OP2 | 38:BC:137:LEU:HB3 | 2.09 | 0.52 |
| 38:BC:74:VAL:CG2 | 38:BC:157:LYS:HG2 | 2.39 | 0.52 |
| 39:BD:35:LYS:HA | 39:BD:63:ARG:HA | 1.91 | 0.52 |
| 40:BE:51:PHE:O | 40:BE:52:LEU:C | 2.47 | 0.52 |
| 41:BF:8:GLN:O | 41:BF:10:PRO:HD3 | 2.09 | 0.52 |
| 43:BH:107:VAL:O | 43:BH:107:VAL:HG23 | 2.10 | 0.52 |
| 49:BQ:35:VAL:HG23 | 49:BQ:101:ARG:O | 2.09 | 0.52 |
| 37:BB:7:G:H4' | 51:BS:29:PHE:CD1 | 2.44 | 0.52 |
| 53:BU:56:ASP:O | 53:BU:60:LEU:HG | 2.09 | 0.52 |
| 53:BU:65:ILE:HD11 | 53:BU:96:ALA:HB3 | 1.90 | 0.52 |
| 1:AA:1444:C:H2' | 1:AA:1445:C:C6 | 2.44 | 0.52 |
| 1:AA:1503:A:O2' | 23:AX:16:A:N6 | 2.41 | 0.52 |
| 1:AA:642:A:H2' | 1:AA:643:C:H6 | 1.73 | 0.52 |
| 1:AA:665:A:N3 | 1:AA:732:C:H2' | 2.24 | 0.52 |
| 4:AD:30:LYS:C | 4:AD:32:ALA:N | 2.62 | 0.52 |
| 6:AF:48:LEU:HD13 | 6:AF:52:ILE:HD12 | 1.92 | 0.52 |
| 7:AG:80:VAL:C | 7:AG:82:GLY:H | 2.12 | 0.52 |
| 1:AA:36:C:H5' | 12:AL:121:GLY:O | 2.09 | 0.52 |
| 12:AL:28:LYS:O | 12:AL:29:GLY:C | 2.47 | 0.52 |
| 16:AP:75:ARG:O | 16:AP:78:GLY:N | 2.33 | 0.52 |
| 19:AS:17:GLU:O | 19:AS:17:GLU:HG2 | 2.08 | 0.52 |
| 20:AT:26:ASN:H | 20:AT:26:ASN:ND2 | 2.08 | 0.52 |
| 27:B1:18:ILE:HG12 | 27:B1:37:ILE:HG22 | 1.91 | 0.52 |
| 28:B2:25:VAL:C | 28:B2:27:GLU:N | 2.62 | 0.52 |
| 35:B9:35:ARG:O | 35:B9:36:GLN:O | 2.27 | 0.52 |
| 36:BA:1131:G:C8 | 36:BA:2025:C:H4' | 2.44 | 0.52 |
| 36:BA:1313:U:H3' | 36:BA:1313:U:O2 | 2.09 | 0.52 |
| 36:BA:1316:U:O2' | 36:BA:1317:A:H5' | 2.09 | 0.52 |
| 36:BA:1509(B):A:H2' | 36:BA:1510:G:H5' | 1.92 | 0.52 |
| 36:BA:2147:G:H2' | 36:BA:2148:G:C5' | 2.40 | 0.52 |
| 36:BA:2119:A:C6 | 36:BA:2170:A:C6 | 2.98 | 0.52 |
| 36:BA:445:C:O2' | 36:BA:446:G:H5' | 2.10 | 0.52 |
| 31:B5:3:LYS:HB2 | 36:BA:747:U:H5 | 1.71 | 0.52 |
| 28:B2:47:ASN:HD22 | 36:BA:94(A):G:H21 | 1.55 | 0.52 |
| 37:BB:78:A:H2' | 37:BB:79:C:O4' | 2.09 | 0.52 |
| 38:BC:100:ILE:HD13 | 38:BC:126:LYS:CB | 2.38 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BC:46:LYS:HG3 | 38:BC:210:ARG:HB2 | 1.91 | 0.52 |
| 38:BC:49:ILE:HD12 | 38:BC:49:ILE:C | 2.29 | 0.52 |
| 36:BA:1658:C:OP1 | 40:BE:132:HIS:O | 2.27 | 0.52 |
| 42:BG:6:ALA:HB3 | 42:BG:104:GLU:OE2 | 2.10 | 0.52 |
| 43:BH:126:PRO:HB2 | 43:BH:130:ARG:NH2 | 2.25 | 0.52 |
| 43:BH:12:PRO:HB2 | 43:BH:15:VAL:HG13 | 1.91 | 0.52 |
| 43:BH:85:LYS:HE2 | 43:BH:85:LYS:C | 2.29 | 0.52 |
| 46:BN:74:ARG:HH21 | 46:BN:83:LYS:HD3 | 1.74 | 0.52 |
| 46:BN:96:GLU:CD | 46:BN:96:GLU:H | 2.12 | 0.52 |
| 49:BQ:140:ALA:O | 49:BQ:141:GLN:HG2 | 2.09 | 0.52 |
| 40:BE:52:LEU:HD11 | 52:BT:1:MET:HG2 | 1.91 | 0.52 |
| 56:BX:14:SER:OG | 56:BX:17:ALA:HB2 | 2.09 | 0.52 |
| 58:BZ:126:VAL:HA | 58:BZ:163:LEU:HA | 1.91 | 0.52 |
| 1:AA:1306:A:N6 | 1:AA:1331:G:H1' | 2.24 | 0.52 |
| 1:AA:386:C:C2' | 1:AA:387:U:H5' | 2.39 | 0.52 |
| 1:AA:502:G:O2' | 1:AA:503:C:H5' | 2.10 | 0.52 |
| 1:AA:511:C:HO2' | 1:AA:512:U:H6 | 1.56 | 0.52 |
| 1:AA:676:A:H1' | 11:AK:115:PRO:HB3 | 1.91 | 0.52 |
| 4:AD:2:GLY:O | 4:AD:3:ARG:C | 2.47 | 0.52 |
| 10:AJ:15:THR:O | 10:AJ:19:SER:HB3 | 2.09 | 0.52 |
| 11:AK:57:THR:HG23 | 11:AK:59:TYR:H | 1.75 | 0.52 |
| 17:AQ:5:VAL:HG13 | 17:AQ:59:ILE:O | 2.10 | 0.52 |
| 19:AS:51:VAL:O | 19:AS:58:VAL:HG22 | 2.09 | 0.52 |
| 25:AZ:56:GLU:CG | 25:AZ:63:ILE:H | 2.22 | 0.52 |
| 31:B5:40:LYS:NZ | 31:B5:46:CYS:N | 2.42 | 0.52 |
| 36:BA:10:G:N2 | 36:BA:2895:U:H3 | 2.08 | 0.52 |
| 36:BA:145:G:H3' | 36:BA:146:G:H5'' | 1.92 | 0.52 |
| 36:BA:1902:C:H5' | 39:BD:246:PRO:HD3 | 1.91 | 0.52 |
| 36:BA:563:G:C4 | 36:BA:2018:G:C2 | 2.98 | 0.52 |
| 36:BA:2317:C:O2' | 36:BA:2318:G:H5' | 2.09 | 0.52 |
| 35:B9:30:PRO:CB | 36:BA:2527:C:H5' | 2.28 | 0.52 |
| 36:BA:2572:A:C5 | 40:BE:144:ARG:HD3 | 2.44 | 0.52 |
| 36:BA:494:G:O2' | 55:BW:5:ALA:O | 2.27 | 0.52 |
| 36:BA:519:U:H2' | 36:BA:520:G:C8 | 2.43 | 0.52 |
| 36:BA:583:G:OP2 | 53:BU:10:ARG:NH1 | 2.42 | 0.52 |
| 39:BD:75:ILE:HD13 | 39:BD:75:ILE:H | 1.75 | 0.52 |
| 40:BE:183:LEU:HD12 | 40:BE:183:LEU:N | 2.24 | 0.52 |
| 40:BE:197:ILE:HD11 | 40:BE:199:ARG:HH22 | 1.74 | 0.52 |
| 40:BE:49:LEU:O | 40:BE:78:LEU:CB | 2.58 | 0.52 |
| 40:BE:70:ALA:O | 40:BE:72:VAL:N | 2.35 | 0.52 |
| 44:BJ:24:UNK:HA | 44:BJ:86:UNK:HA | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:BN:55:VAL:CG2 | 46:BN:126:PRO:HA | 2.40 | 0.52 |
| 48:BP:101:VAL:CG2 | 48:BP:102:ARG:N | 2.72 | 0.52 |
| 48:BP:30:THR:CG2 | 48:BP:31:ALA:N | 2.72 | 0.52 |
| 48:BP:95:VAL:O | 48:BP:125:VAL:HA | 2.09 | 0.52 |
| 58:BZ:28:MET:SD | 58:BZ:35:ARG:O | 2.68 | 0.52 |
| 1:AA:265:G:H2' | 1:AA:267:C:H5 | 1.74 | 0.52 |
| 1:AA:502:G:OP1 | 12:AL:118:SER:CB | 2.58 | 0.52 |
| 1:AA:589:C:O2' | 1:AA:590:C:H5' | 2.10 | 0.52 |
| 2:AB:163:PHE:HA | 2:AB:185:ILE:O | 2.09 | 0.52 |
| 2:AB:19:HIS:ND1 | 2:AB:204:ASN:OD1 | 2.43 | 0.52 |
| 3:AC:35:GLU:OE2 | 3:AC:59:ARG:NH1 | 2.31 | 0.52 |
| 4:AD:58:LEU:HD23 | 4:AD:206:PHE:CE1 | 2.45 | 0.52 |
| 6:AF:63:TYR:O | 6:AF:64:GLN:HB2 | 2.10 | 0.52 |
| 22:AW:43:C:H6 | 22:AW:43:C:OP2 | 1.91 | 0.52 |
| 25:AZ:67:HIS:CE1 | 25:AZ:80:VAL:HG22 | 2.44 | 0.52 |
| 25:AZ:7:ARG:O | 25:AZ:7:ARG:HG3 | 2.09 | 0.52 |
| 27:B1:48:LYS:HE3 | 27:B1:59:THR:HB | 1.90 | 0.52 |
| 28:B2:10:LEU:O | 28:B2:13:ALA:HB3 | 2.10 | 0.52 |
| 30:B4:5:ILE:O | 30:B4:5:ILE:CG1 | 2.56 | 0.52 |
| 31:B5:46:CYS:SG | 31:B5:48:GLU:HB2 | 2.48 | 0.52 |
| 32:B6:14:THR:HG23 | 32:B6:16:CYS:H | 1.75 | 0.52 |
| 36:BA:2008:C:H2' | 36:BA:2009:G:C8 | 2.44 | 0.52 |
| 36:BA:528:A:H2 | 36:BA:2043:C:H5' | 1.75 | 0.52 |
| 27:B1:40:ARG:HH12 | 36:BA:2232:U:P | 2.32 | 0.52 |
| 36:BA:2392:A:H1' | 48:BP:60:MET:HB3 | 1.92 | 0.52 |
| 36:BA:2469:A:C5 | 36:BA:2470:G:H1' | 2.45 | 0.52 |
| 36:BA:2810:A:N3 | 40:BE:61:ARG:NH2 | 2.56 | 0.52 |
| 36:BA:314:A:H2' | 36:BA:315:G:C8 | 2.44 | 0.52 |
| 36:BA:440:G:H2' | 36:BA:441:U:H6 | 1.75 | 0.52 |
| 36:BA:680:G:H2' | 36:BA:681:G:H8 | 1.72 | 0.52 |
| 39:BD:232:PRO:HD2 | 39:BD:249:PRO:HA | 1.90 | 0.52 |
| 40:BE:199:ARG:HH11 | 40:BE:199:ARG:CB | 2.22 | 0.52 |
| 43:BH:67:LEU:HG | 43:BH:71:LEU:HD12 | 1.89 | 0.52 |
| 49:BQ:21:THR:CG2 | 49:BQ:101:ARG:HD2 | 2.40 | 0.52 |
| 51:BS:35:ILE:HG23 | 51:BS:35:ILE:O | 2.10 | 0.52 |
| 52:BT:83:ILE:O | 52:BT:84:GLN:O | 2.27 | 0.52 |
| 53:BU:52:ARG:HG2 | 53:BU:55:ARG:HH12 | 1.75 | 0.52 |
| 55:BW:1:MET:HE1 | 55:BW:62:HIS:CD2 | 2.45 | 0.52 |
| 55:BW:70:TYR:HE2 | 55:BW:72:LYS:HE2 | 1.74 | 0.52 |
| 58:BZ:139:VAL:O | 58:BZ:140:ASP:HB3 | 2.10 | 0.52 |
| 58:BZ:74:VAL:O | 58:BZ:75:ASN:C | 2.47 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:BQ:140:ALA:HA | 58:BZ:99:TYR:CD1 | 2.44 | 0.52 |
| 1:AA:1258:G:H2' | 1:AA:1259:C:C6 | 2.44 | 0.52 |
| 1:AA:167:G:O2' | 1:AA:168:G:H5' | 2.10 | 0.52 |
| 1:AA:858:G:C8 | 1:AA:858:G:C5' | 2.88 | 0.52 |
| 2:AB:59:GLU:HB2 | 2:AB:221:LEU:HD11 | 1.91 | 0.52 |
| 3:AC:23:TYR:CD2 | 3:AC:24:ALA:N | 2.77 | 0.52 |
| 7:AG:20:ASP:HB3 | 7:AG:23:VAL:CG2 | 2.40 | 0.52 |
| 12:AL:42:THR:O | 12:AL:42:THR:HG23 | 2.09 | 0.52 |
| 16:AP:22:THR:HA | 16:AP:33:ILE:HG12 | 1.91 | 0.52 |
| 16:AP:45:THR:HG22 | 16:AP:47:ASP:N | 2.24 | 0.52 |
| 17:AQ:26:GLN:O | 17:AQ:27:PHE:CB | 2.57 | 0.52 |
| 22:AW:43:C:H2' | 22:AW:44:G:H1' | 1.90 | 0.52 |
| 25:AZ:120:ILE:HG22 | 25:AZ:161:TYR:HD1 | 1.74 | 0.52 |
| 25:AZ:330:ARG:HG2 | 25:AZ:330:ARG:HH11 | 1.75 | 0.52 |
| 29:B3:31:LEU:HD23 | 29:B3:32:GLN:H | 1.72 | 0.52 |
| 34:B8:33:ASN:HA | 34:B8:36:LYS:HD3 | 1.91 | 0.52 |
| 36:BA:2479:G:OP1 | 36:BA:2537:U:H1' | 2.09 | 0.52 |
| 36:BA:2749:A:H4' | 43:BH:62:LYS:HG2 | 1.91 | 0.52 |
| 36:BA:2839:G:H2' | 36:BA:2840:C:H6 | 1.74 | 0.52 |
| 37:BB:106:G:H5'' | 58:BZ:31:ARG:HB3 | 1.92 | 0.52 |
| 38:BC:104:LEU:HD22 | 38:BC:127:LEU:HD21 | 1.90 | 0.52 |
| 38:BC:30:LYS:CD | 38:BC:185:LEU:HD11 | 2.40 | 0.52 |
| 40:BE:68:ALA:O | 40:BE:70:ALA:N | 2.41 | 0.52 |
| 46:BN:65:LYS:CB | 46:BN:65:LYS:NZ | 2.73 | 0.52 |
| 47:BO:64:ARG:NH1 | 47:BO:83:ALA:HB2 | 2.25 | 0.52 |
| 48:BP:146:VAL:CG2 | 48:BP:147:LEU:H | 2.08 | 0.52 |
| 48:BP:16:ARG:HH11 | 48:BP:16:ARG:C | 2.12 | 0.52 |
| 50:BR:48:VAL:HG13 | 50:BR:49:ASP:N | 2.25 | 0.52 |
| 54:BV:39:LEU:CD1 | 54:BV:51:VAL:HA | 2.40 | 0.52 |
| 54:BV:28:GLU:O | 54:BV:61:VAL:CG2 | 2.58 | 0.52 |
| 1:AA:189(C):C:O2' | 1:AA:189(D):C:H5' | 2.09 | 0.52 |
| 1:AA:1060:C:C4 | 3:AC:2:GLY:HA3 | 2.44 | 0.52 |
| 3:AC:3:ASN:O | 3:AC:4:LYS:CB | 2.57 | 0.52 |
| 3:AC:22:TRP:CD1 | 3:AC:59:ARG:HG3 | 2.44 | 0.52 |
| 5:AE:64:ARG:HH11 | 5:AE:64:ARG:HG3 | 1.75 | 0.52 |
| 10:AJ:6:ILE:CG1 | 10:AJ:72:VAL:HB | 2.37 | 0.52 |
| 13:AM:69:GLU:HA | 13:AM:69:GLU:OE1 | 2.09 | 0.52 |
| 14:AN:29:ARG:CG | 14:AN:29:ARG:HH11 | 2.14 | 0.52 |
| 16:AP:58:TYR:O | 16:AP:62:VAL:HG22 | 2.10 | 0.52 |
| 18:AR:30:ASP:OD1 | 18:AR:32:ARG:HB3 | 2.09 | 0.52 |
| 19:AS:78:ARG:N | 19:AS:81:ARG:NH1 | 2.54 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AW:7:A:C4 | 22:AW:49:C:H5 | 2.27 | 0.52 |
| 25:AZ:124:ARG:HD2 | 25:AZ:163:PHE:CE2 | 2.44 | 0.52 |
| 31:B5:33:CYS:SG | 31:B5:49:CYS:SG | 3.05 | 0.52 |
| 34:B8:60:LEU:C | 34:B8:63:PRO:HD2 | 2.30 | 0.52 |
| 36:BA:1064:C:H3' | 36:BA:1065:U:C5' | 2.40 | 0.52 |
| 36:BA:1234:U:H2' | 36:BA:1235:G:O4' | 2.10 | 0.52 |
| 36:BA:1798:U:H5' | 39:BD:259:THR:CG2 | 2.37 | 0.52 |
| 36:BA:2822:G:H2' | 36:BA:2823:A:H5'' | 1.92 | 0.52 |
| 38:BC:103:ILE:HG22 | 38:BC:103:ILE:O | 2.10 | 0.52 |
| 38:BC:163:PHE:HD1 | 38:BC:171:ILE:HD11 | 1.75 | 0.52 |
| 39:BD:32:SER:O | 39:BD:36:PRO:HD3 | 2.10 | 0.52 |
| 39:BD:77:ALA:HB1 | 39:BD:95:LEU:HD13 | 1.91 | 0.52 |
| 41:BF:29:ASN:HB3 | 41:BF:112:MET:SD | 2.50 | 0.52 |
| 41:BF:129:PHE:C | 41:BF:131:GLY:H | 2.13 | 0.52 |
| 43:BH:52:VAL:HG12 | 43:BH:65:HIS:ND1 | 2.24 | 0.52 |
| 46:BN:134:ARG:N | 46:BN:135:PRO:HD3 | 2.23 | 0.52 |
| 47:BO:87:ILE:HG22 | 47:BO:88:ASN:O | 2.10 | 0.52 |
| 48:BP:16:ARG:O | 48:BP:18:ARG:N | 2.43 | 0.52 |
| 51:BS:66:ALA:O | 51:BS:67:ARG:C | 2.48 | 0.52 |
| 57:BY:69:ALA:O | 57:BY:72:VAL:HG22 | 2.09 | 0.52 |
| 58:BZ:134:PRO:HG2 | 58:BZ:161:VAL:HG21 | 1.92 | 0.52 |
| 58:BZ:6:LYS:HG3 | 58:BZ:60:GLU:HB2 | 1.91 | 0.52 |
| 1:AA:1119:C:O2' | 1:AA:1120:G:H5' | 2.10 | 0.52 |
| 1:AA:1444:C:H2' | 1:AA:1445:C:H6 | 1.75 | 0.52 |
| 1:AA:223:U:H2' | 1:AA:224:C:C6 | 2.45 | 0.52 |
| 1:AA:814:A:H2' | 1:AA:816:A:H5'' | 1.92 | 0.52 |
| 2:AB:35:GLU:HG2 | 2:AB:35:GLU:O | 2.10 | 0.52 |
| 8:AH:28:ALA:HB3 | 8:AH:57:PRO:HB2 | 1.90 | 0.52 |
| 22:AW:1:G:H2' | 22:AW:1:G:N3 | 2.25 | 0.52 |
| 25:AZ:99:MET:HE2 | 25:AZ:102:ALA:CB | 2.38 | 0.52 |
| 25:AZ:311:THR:CG2 | 25:AZ:312:PRO:HD2 | 2.38 | 0.52 |
| 25:AZ:125:GLN:HE22 | 25:AZ:323:LEU:HD11 | 1.74 | 0.52 |
| 32:B6:16:CYS:SG | 32:B6:48:VAL:CG2 | 2.98 | 0.52 |
| 34:B8:13:ARG:HD3 | 48:BP:61:ARG:HD2 | 1.90 | 0.52 |
| 35:B9:10:ILE:HG12 | 36:BA:2477:C:C5 | 2.44 | 0.52 |
| 36:BA:1050:A:H2' | 36:BA:1050:A:N3 | 2.25 | 0.52 |
| 36:BA:1076:C:H2' | 36:BA:1077:A:C8 | 2.44 | 0.52 |
| 36:BA:1902:C:C2' | 36:BA:1903:G:O5' | 2.58 | 0.52 |
| 36:BA:2126:A:O2' | 36:BA:2127:G:H8 | 1.93 | 0.52 |
| 36:BA:2385:C:O2' | 36:BA:2386:C:H5' | 2.10 | 0.52 |
| 36:BA:2692:C:H2' | 36:BA:2693:A:C8 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:BB:37:C:H2' | 37:BB:38:C:O4' | 2.09 | 0.52 |
| 37:BB:95:C:O2' | 37:BB:96:U:H5' | 2.10 | 0.52 |
| 36:BA:469:G:OP1 | 41:BF:78:ILE:HD11 | 2.10 | 0.52 |
| 43:BH:156:ALA:C | 43:BH:158:HIS:N | 2.63 | 0.52 |
| 43:BH:12:PRO:N | 43:BH:48:GLY:HA2 | 2.24 | 0.52 |
| 43:BH:50:VAL:HG12 | 43:BH:51:ARG:H | 1.73 | 0.52 |
| 45:BK:30:UNK:O | 45:BK:31:UNK:CB | 2.58 | 0.52 |
| 46:BN:72:TYR:HE1 | 46:BN:87:LEU:HD23 | 1.73 | 0.52 |
| 57:BY:14:LEU:O | 57:BY:72:VAL:HA | 2.09 | 0.52 |
| 1:AA:105:G:H2' | 1:AA:106:C:C6 | 2.44 | 0.52 |
| 1:AA:22:G:H4' | 1:AA:885:G:C8 | 2.45 | 0.52 |
| 1:AA:96:U:H2' | 1:AA:97:G:C8 | 2.45 | 0.52 |
| 2:AB:8:LYS:C | 2:AB:10:LEU:H | 2.13 | 0.52 |
| 2:AB:8:LYS:O | 2:AB:11:LEU:N | 2.43 | 0.52 |
| 7:AG:26:PHE:O | 7:AG:30:ILE:HG12 | 2.10 | 0.52 |
| 13:AM:108:ARG:N | 13:AM:108:ARG:HD2 | 2.24 | 0.52 |
| 13:AM:36:LYS:HE2 | 13:AM:59:TYR:CZ | 2.44 | 0.52 |
| 21:AU:12:LYS:HB3 | 21:AU:22:ARG:HD2 | 1.91 | 0.52 |
| 25:AZ:11:HIS:CD2 | 25:AZ:12:VAL:N | 2.77 | 0.52 |
| 25:AZ:148:ASP:HA | 25:AZ:172:ARG:NH2 | 2.20 | 0.52 |
| 25:AZ:318:ALA:HA | 25:AZ:401:THR:H | 1.75 | 0.52 |
| 25:AZ:355:LEU:HD11 | 25:AZ:362:VAL:CG2 | 2.40 | 0.52 |
| 30:B4:31:ILE:CG2 | 30:B4:33:VAL:HG23 | 2.40 | 0.52 |
| 36:BA:1026:U:C6 | 36:BA:1026:U:OP2 | 2.63 | 0.52 |
| 36:BA:1153:C:H2' | 36:BA:1153:C:O2 | 2.09 | 0.52 |
| 36:BA:1845:G:O2' | 36:BA:1846:G:H5' | 2.10 | 0.52 |
| 36:BA:2287:A:N6 | 36:BA:2344:U:N3 | 2.50 | 0.52 |
| 36:BA:2289:G:O5' | 36:BA:2289:G:H8 | 1.92 | 0.52 |
| 36:BA:1955:U:O4 | 36:BA:2554:U:H5 | 1.93 | 0.52 |
| 37:BB:70:C:H2' | 37:BB:71:C:H6 | 1.75 | 0.52 |
| 38:BC:104:LEU:O | 38:BC:105:ASP:CB | 2.57 | 0.52 |
| 38:BC:6:ARG:NH1 | 38:BC:34:THR:O | 2.43 | 0.52 |
| 39:BD:142:VAL:HG21 | 39:BD:191:ALA:HB1 | 1.91 | 0.52 |
| 39:BD:26:LYS:O | 39:BD:27:THR:HB | 2.09 | 0.52 |
| 40:BE:120:TRP:CD2 | 40:BE:155:LYS:HB3 | 2.44 | 0.52 |
| 40:BE:134:ILE:HA | 40:BE:137:HIS:CD2 | 2.45 | 0.52 |
| 40:BE:82:ARG:HG3 | 40:BE:83:ASP:H | 1.75 | 0.52 |
| 42:BG:67:LYS:CD | 42:BG:67:LYS:N | 2.63 | 0.52 |
| 46:BN:22:THR:HA | 46:BN:61:ARG:HB2 | 1.91 | 0.52 |
| 52:BT:33:LYS:HE2 | 52:BT:43:GLN:NE2 | 2.24 | 0.52 |
| 57:BY:14:LEU:HG | 57:BY:15:VAL:N | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1050:G:O2' | 1:AA:1051:C:H6 | 1.93 | 0.52 |
| 1:AA:1118:C:O2' | 1:AA:1119:C:H5' | 2.11 | 0.52 |
| 1:AA:1243:C:H2' | 1:AA:1244:C:C6 | 2.45 | 0.52 |
| 1:AA:234:C:H2' | 1:AA:235:C:C6 | 2.45 | 0.52 |
| 1:AA:725:G:O2' | 1:AA:726:C:H5' | 2.10 | 0.52 |
| 5:AE:122:GLU:OE2 | 5:AE:131:ILE:HG21 | 2.10 | 0.52 |
| 7:AG:120:ILE:O | 7:AG:124:LEU:HB2 | 2.09 | 0.52 |
| 16:AP:48:TRP:O | 16:AP:49:LEU:HB2 | 2.10 | 0.52 |
| 17:AQ:47:PRO:HG2 | 17:AQ:48:GLU:H | 1.75 | 0.52 |
| 17:AQ:77:VAL:O | 17:AQ:78:GLU:HB3 | 2.10 | 0.52 |
| 19:AS:31:ILE:HG22 | 19:AS:48:THR:O | 2.10 | 0.52 |
| 20:AT:41:ILE:HG22 | 20:AT:91:LEU:HD12 | 1.91 | 0.52 |
| 20:AT:51:GLU:O | 20:AT:55:ILE:HG12 | 2.10 | 0.52 |
| 20:AT:74:LYS:CG | 20:AT:75:ASN:H | 2.21 | 0.52 |
| 25:AZ:114:PRO:HA | 25:AZ:117:ARG:HH12 | 1.75 | 0.52 |
| 25:AZ:272:MET:O | 25:AZ:275:LYS:HG2 | 2.10 | 0.52 |
| 32:B6:53:LYS:HD3 | 32:B6:54:ILE:N | 2.19 | 0.52 |
| 36:BA:1038:C:C3' | 36:BA:1039:G:H5'' | 2.40 | 0.52 |
| 36:BA:1210:A:H5'' | 36:BA:1212:G:O4' | 2.10 | 0.52 |
| 36:BA:1251:C:P | 53:BU:10:ARG:HG3 | 2.50 | 0.52 |
| 36:BA:176:G:O2' | 36:BA:177:G:H5' | 2.10 | 0.52 |
| 36:BA:1790:C:H5'' | 36:BA:1791:A:OP1 | 2.10 | 0.52 |
| 36:BA:2162:G:O2' | 36:BA:2163:C:H5' | 2.10 | 0.52 |
| 36:BA:2563:U:H4' | 47:BO:28:SER:HA | 1.92 | 0.52 |
| 36:BA:332:A:H4' | 36:BA:333:G:OP1 | 2.09 | 0.52 |
| 36:BA:850:C:H2' | 36:BA:851:U:C6 | 2.45 | 0.52 |
| 38:BC:123:VAL:HG13 | 38:BC:124:GLY:N | 2.24 | 0.52 |
| 38:BC:59:ARG:HH11 | 38:BC:141:LYS:NZ | 2.08 | 0.52 |
| 38:BC:62:VAL:O | 38:BC:160:ARG:HG2 | 2.10 | 0.52 |
| 39:BD:270:ILE:N | 39:BD:270:ILE:HD12 | 2.15 | 0.52 |
| 41:BF:160:ASN:ND2 | 41:BF:162:LEU:HB2 | 2.25 | 0.52 |
| 41:BF:16:GLY:O | 41:BF:17:ARG:HG3 | 2.11 | 0.52 |
| 41:BF:84:VAL:O | 41:BF:85:GLY:C | 2.48 | 0.52 |
| 44:BJ:72:UNK:O | 44:BJ:73:UNK:CB | 2.58 | 0.52 |
| 44:BJ:79:UNK:O | 44:BJ:80:UNK:CB | 2.57 | 0.52 |
| 48:BP:46:LYS:HB3 | 48:BP:52:GLU:HG2 | 1.92 | 0.52 |
| 51:BS:74:ALA:HB1 | 51:BS:103:GLU:HG2 | 1.91 | 0.52 |
| 53:BU:47:TYR:HE2 | 54:BV:74:LYS:HZ2 | 1.58 | 0.52 |
| 56:BX:31:HIS:HB3 | 56:BX:34:ALA:HB2 | 1.91 | 0.52 |
| 56:BX:30:VAL:HG11 | 56:BX:39:ILE:HD12 | 1.91 | 0.52 |
| 58:BZ:76:LEU:O | 58:BZ:84:GLU:HG3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:37:ARG:NH2 | 8:AH:41:ARG:HH22 | 2.08 | 0.51 |
| 10:AJ:40:LEU:HB2 | 10:AJ:41:PRO:HD2 | 1.92 | 0.51 |
| 11:AK:126:ARG:O | 11:AK:128:ALA:N | 2.43 | 0.51 |
| 11:AK:71:LYS:O | 11:AK:74:ALA:HB3 | 2.10 | 0.51 |
| 19:AS:31:ILE:HG23 | 19:AS:31:ILE:O | 2.10 | 0.51 |
| 25:AZ:212:THR:N | 25:AZ:213:PRO:CD | 2.72 | 0.51 |
| 25:AZ:221:PHE:CE2 | 25:AZ:247:VAL:HG11 | 2.44 | 0.51 |
| 25:AZ:317:GLU:O | 25:AZ:401:THR:HG22 | 2.09 | 0.51 |
| 28:B2:50:ILE:N | 28:B2:50:ILE:HD12 | 2.24 | 0.51 |
| 32:B6:20:ASN:O | 32:B6:21:TYR:CG | 2.62 | 0.51 |
| 34:B8:21:LYS:HD3 | 34:B8:48:PHE:CE2 | 2.45 | 0.51 |
| 36:BA:1576:U:H2' | 36:BA:1577:C:C6 | 2.45 | 0.51 |
| 36:BA:1810:A:H2' | 36:BA:1811:G:O4' | 2.09 | 0.51 |
| 36:BA:1947:C:O2' | 36:BA:1948:G:H5'' | 2.10 | 0.51 |
| 36:BA:593:G:H2' | 36:BA:594:U:O4' | 2.11 | 0.51 |
| 38:BC:6:ARG:NH1 | 38:BC:6:ARG:O | 2.42 | 0.51 |
| 38:BC:8:ARG:O | 38:BC:12:GLU:HG2 | 2.11 | 0.51 |
| 39:BD:16:MET:HE1 | 39:BD:208:LYS:HD3 | 1.92 | 0.51 |
| 39:BD:267:SER:CA | 39:BD:270:ILE:HD11 | 2.39 | 0.51 |
| 40:BE:15:PHE:CE1 | 40:BE:20:ALA:HB2 | 2.45 | 0.51 |
| 41:BF:28:ILE:O | 41:BF:28:ILE:HG12 | 2.10 | 0.51 |
| 44:BJ:74:UNK:C | 44:BJ:76:UNK:H | 2.23 | 0.51 |
| 36:BA:1666:G:O3' | 47:BO:6:THR:HG23 | 2.10 | 0.51 |
| 48:BP:101:VAL:HG23 | 48:BP:102:ARG:N | 2.25 | 0.51 |
| 36:BA:631:A:H4' | 48:BP:65:ARG:HD3 | 1.92 | 0.51 |
| 50:BR:53:HIS:ND1 | 50:BR:53:HIS:O | 2.43 | 0.51 |
| 54:BV:36:PRO:HA | 54:BV:56:SER:HB2 | 1.92 | 0.51 |
| 56:BX:64:LYS:HZ3 | 56:BX:73:ARG:HH21 | 1.54 | 0.51 |
| 57:BY:14:LEU:HB3 | 57:BY:73:ARG:HB2 | 1.91 | 0.51 |
| 57:BY:31:LEU:CB | 57:BY:32:PRO:CA | 2.88 | 0.51 |
| 58:BZ:103:ARG:HD2 | 58:BZ:136:PHE:CB | 2.38 | 0.51 |
| 58:BZ:140:ASP:O | 58:BZ:141:VAL:HG23 | 2.10 | 0.51 |
| 49:BQ:63:LYS:HD2 | 58:BZ:175:VAL:HG21 | 1.92 | 0.51 |
| 58:BZ:8:TYR:HB2 | 58:BZ:38:TYR:CE2 | 2.44 | 0.51 |
| 1:AA:1143:G:H2' | 1:AA:1144:G:H8 | 1.73 | 0.51 |
| 1:AA:1219:U:C2 | 1:AA:1220:G:C8 | 2.99 | 0.51 |
| 1:AA:347:G:H21 | 1:AA:348:G:H1' | 1.75 | 0.51 |
| 1:AA:453:A:O2' | 1:AA:454:C:H5'' | 2.09 | 0.51 |
| 2:AB:116:GLU:C | 2:AB:118:LEU:N | 2.64 | 0.51 |
| 5:AE:110:LEU:O | 5:AE:113:ALA:HB3 | 2.09 | 0.51 |
| 5:AE:80:ILE:HA | 8:AH:104:ARG:NH2 | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:12:ASN:N | 13:AM:12:ASN:HD22 | 1.90 | 0.51 |
| 13:AM:79:LYS:O | 13:AM:82:MET:HB3 | 2.11 | 0.51 |
| 16:AP:21:VAL:HG11 | 16:AP:34:GLU:HB3 | 1.91 | 0.51 |
| 18:AR:37:VAL:HG11 | 18:AR:78:LEU:HB3 | 1.92 | 0.51 |
| 19:AS:28:LYS:HE2 | 19:AS:29:ARG:NH1 | 2.25 | 0.51 |
| 19:AS:63:THR:OG1 | 19:AS:64:GLU:N | 2.43 | 0.51 |
| 22:AW:59:U:C2' | 22:AW:60:U:H5' | 2.38 | 0.51 |
| 25:AZ:136:ASN:O | 25:AZ:137:LYS:HB2 | 2.11 | 0.51 |
| 25:AZ:253:VAL:HA | 25:AZ:307:PRO:HD3 | 1.93 | 0.51 |
| 26:B0:16:SER:HB2 | 36:BA:2262:U:C5 | 2.45 | 0.51 |
| 36:BA:1148:A:N3 | 36:BA:1148:A:H2' | 2.25 | 0.51 |
| 36:BA:117:G:C6 | 36:BA:119:A:C6 | 2.97 | 0.51 |
| 36:BA:1316:U:H2' | 36:BA:1317:A:H8 | 1.72 | 0.51 |
| 36:BA:188:G:H2' | 36:BA:189:G:H5' | 1.92 | 0.51 |
| 36:BA:1769:G:O2' | 36:BA:1958:C:OP1 | 2.22 | 0.51 |
| 36:BA:2181:G:H2' | 36:BA:2182:G:H8 | 1.75 | 0.51 |
| 36:BA:252:G:H2' | 36:BA:253:C:H6 | 1.76 | 0.51 |
| 36:BA:272(B):G:O2' | 36:BA:272(C):G:H5' | 2.10 | 0.51 |
| 36:BA:2892:A:H62 | 36:BA:2893:G:H21 | 1.57 | 0.51 |
| 36:BA:784:A:C6 | 39:BD:229:VAL:HG11 | 2.45 | 0.51 |
| 36:BA:812:C:C2 | 36:BA:813:U:C5 | 2.98 | 0.51 |
| 37:BB:82:G:O2' | 37:BB:83:G:H5' | 2.10 | 0.51 |
| 37:BB:86:G:O2' | 37:BB:87:G:H5' | 2.10 | 0.51 |
| 38:BC:141:LYS:HB2 | 38:BC:141:LYS:HZ2 | 1.73 | 0.51 |
| 38:BC:30:LYS:HE2 | 38:BC:178:ALA:O | 2.10 | 0.51 |
| 36:BA:1902:C:H1' | 39:BD:244:ARG:HG3 | 1.90 | 0.51 |
| 39:BD:21:PHE:O | 39:BD:24:ILE:HG23 | 2.11 | 0.51 |
| 40:BE:49:LEU:HD11 | 40:BE:91:VAL:HG21 | 1.92 | 0.51 |
| 42:BG:47:LYS:HZ1 | 42:BG:81:LYS:HB2 | 1.75 | 0.51 |
| 43:BH:98:LEU:HD22 | 43:BH:125:VAL:CG2 | 2.39 | 0.51 |
| 43:BH:40:GLU:O | 43:BH:41:MET:CB | 2.58 | 0.51 |
| 46:BN:62:VAL:HG22 | 46:BN:66:LYS:HB2 | 1.90 | 0.51 |
| 48:BP:105:LEU:N | 48:BP:105:LEU:HD12 | 2.25 | 0.51 |
| 49:BQ:54:MET:CE | 49:BQ:64:ILE:HD13 | 2.40 | 0.51 |
| 51:BS:46:VAL:HG12 | 51:BS:47:THR:H | 1.75 | 0.51 |
| 51:BS:97:ARG:C | 51:BS:97:ARG:NE | 2.64 | 0.51 |
| 52:BT:28:VAL:O | 52:BT:29:ARG:CD | 2.58 | 0.51 |
| 52:BT:92:GLY:O | 52:BT:93:ARG:C | 2.48 | 0.51 |
| 53:BU:57:PHE:C | 53:BU:59:ARG:H | 2.13 | 0.51 |
| 54:BV:34:GLU:O | 54:BV:36:PRO:HD2 | 2.10 | 0.51 |
| 56:BX:18:TYR:HA | 56:BX:21:PHE:CD1 | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1001(A):G:O2' | 1:AA:1002:G:H5' | 2.11 | 0.51 |
| 1:AA:1222:G:O2' | 1:AA:1223:C:H5' | 2.10 | 0.51 |
| 1:AA:1465:C:H2' | 1:AA:1466:C:O4' | 2.10 | 0.51 |
| 1:AA:221:C:H2' | 1:AA:222:U:H6 | 1.75 | 0.51 |
| 1:AA:390:C:H2' | 1:AA:391:G:C8 | 2.45 | 0.51 |
| 1:AA:60:A:H4' | 1:AA:61:G:O5' | 2.09 | 0.51 |
| 2:AB:62:ALA:HB2 | 2:AB:222:ILE:HG23 | 1.92 | 0.51 |
| 4:AD:126:ILE:CG2 | 4:AD:127:THR:N | 2.73 | 0.51 |
| 10:AJ:7:LYS:HG2 | 10:AJ:71:LEU:HD13 | 1.93 | 0.51 |
| 13:AM:9:ILE:N | 13:AM:9:ILE:HD12 | 2.26 | 0.51 |
| 15:AO:82:ILE:HD11 | 15:AO:87:ILE:C | 2.31 | 0.51 |
| 25:AZ:265:THR:HG22 | 25:AZ:266:VAL:H | 1.74 | 0.51 |
| 27:B1:23:LYS:HD2 | 27:B1:28:GLY:HA3 | 1.92 | 0.51 |
| 30:B4:36:CYS:HB2 | 42:BG:108:ASN:O | 2.11 | 0.51 |
| 32:B6:13:CYS:O | 32:B6:21:TYR:HA | 2.10 | 0.51 |
| 36:BA:1666:G:H2' | 36:BA:1667:G:C5' | 2.38 | 0.51 |
| 36:BA:2742:C:O2' | 36:BA:2743:C:H5' | 2.11 | 0.51 |
| 36:BA:671:C:H2' | 36:BA:672:C:H6 | 1.75 | 0.51 |
| 36:BA:830:G:H1' | 36:BA:2448:A:N1 | 2.24 | 0.51 |
| 39:BD:254:THR:O | 39:BD:254:THR:OG1 | 2.24 | 0.51 |
| 42:BG:10:LYS:O | 42:BG:15:VAL:HG23 | 2.11 | 0.51 |
| 43:BH:88:LEU:HD22 | 43:BH:88:LEU:N | 2.25 | 0.51 |
| 45:BK:62:UNK:O | 45:BK:63:UNK:C | 2.57 | 0.51 |
| 46:BN:54:VAL:HB | 46:BN:122:VAL:HG22 | 1.92 | 0.51 |
| 51:BS:54:LEU:C | 51:BS:56:LEU:N | 2.62 | 0.51 |
| 53:BU:5:LYS:HG3 | 53:BU:7:GLY:H | 1.75 | 0.51 |
| 36:BA:1187:G:H5" | 54:BV:81:TYR:CZ | 2.45 | 0.51 |
| 57:BY:81:LYS:NZ | 57:BY:99:CYS:HB2 | 2.25 | 0.51 |
| 1:AA:1176:A:H2' | 1:AA:1177:G:C8 | 2.45 | 0.51 |
| 1:AA:35:G:H2' | 1:AA:36:C:C6 | 2.45 | 0.51 |
| 2:AB:68:ILE:O | 2:AB:90:MET:HE2 | 2.10 | 0.51 |
| 3:AC:130:VAL:HG21 | 3:AC:157:ILE:HG23 | 1.92 | 0.51 |
| 4:AD:108:LEU:CD1 | 4:AD:174:LEU:HD13 | 2.40 | 0.51 |
| 6:AF:24:GLU:O | 6:AF:27:GLN:HB2 | 2.10 | 0.51 |
| 7:AG:80:VAL:O | 7:AG:82:GLY:N | 2.41 | 0.51 |
| 7:AG:87:VAL:HG13 | 7:AG:151:TYR:O | 2.11 | 0.51 |
| 10:AJ:30:SER:HB2 | 10:AJ:80:LYS:HZ3 | 1.74 | 0.51 |
| 15:AO:74:ASP:CG | 15:AO:77:ARG:HG2 | 2.30 | 0.51 |
| 18:AR:25:THR:O | 18:AR:26:LEU:HG | 2.09 | 0.51 |
| 19:AS:16:LEU:O | 19:AS:18:LYS:N | 2.44 | 0.51 |
| 25:AZ:16:THR:HB | 25:AZ:79:HIS:HE2 | 1.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B1:50:ARG:HD3 | 27:B1:57:GLU:OE1 | 2.10 | 0.51 |
| 28:B2:2:LYS:O | 28:B2:6:VAL:HG23 | 2.10 | 0.51 |
| 32:B6:19:ARG:NH1 | 32:B6:43:CYS:SG | 2.83 | 0.51 |
| 36:BA:105:C:H2' | 36:BA:106:C:C6 | 2.43 | 0.51 |
| 36:BA:1528:A:N1 | 36:BA:1542:A:H2 | 2.08 | 0.51 |
| 36:BA:1541:G:H1' | 36:BA:1542:A:C4 | 2.45 | 0.51 |
| 36:BA:1884:A:C3' | 36:BA:1885:A:H5'' | 2.41 | 0.51 |
| 36:BA:2143:C:O2' | 36:BA:2144:U:H5' | 2.10 | 0.51 |
| 36:BA:2262:U:H2' | 36:BA:2263:C:H6 | 1.75 | 0.51 |
| 36:BA:863:A:O2' | 36:BA:864:G:H5' | 2.11 | 0.51 |
| 38:BC:183:GLU:HB2 | 38:BC:184:LYS:NZ | 2.25 | 0.51 |
| 36:BA:784:A:H5'' | 39:BD:227:ASN:OD1 | 2.10 | 0.51 |
| 41:BF:2:LYS:HG3 | 41:BF:25:PRO:CG | 2.40 | 0.51 |
| 43:BH:136:ILE:HD12 | 43:BH:136:ILE:N | 2.24 | 0.51 |
| 43:BH:68:THR:C | 43:BH:70:THR:N | 2.62 | 0.51 |
| 48:BP:107:LYS:C | 48:BP:109:GLY:N | 2.62 | 0.51 |
| 49:BQ:10:ARG:HB2 | 49:BQ:10:ARG:NH1 | 2.25 | 0.51 |
| 52:BT:16:ARG:H | 52:BT:79:HIS:CD2 | 2.29 | 0.51 |
| 52:BT:28:VAL:O | 52:BT:28:VAL:HG12 | 2.10 | 0.51 |
| 54:BV:47:VAL:O | 54:BV:49:THR:N | 2.44 | 0.51 |
| 1:AA:1032:G:H2' | 1:AA:1033:G:C8 | 2.46 | 0.51 |
| 1:AA:1265:G:C2 | 1:AA:1271:G:C2 | 2.98 | 0.51 |
| 1:AA:382:A:H2' | 1:AA:383:A:C8 | 2.46 | 0.51 |
| 1:AA:865:A:H5' | 1:AA:1078:U:O4 | 2.10 | 0.51 |
| 2:AB:162:ILE:CG2 | 2:AB:184:VAL:HG22 | 2.41 | 0.51 |
| 1:AA:1117:G:O3' | 9:AI:104:ARG:NH1 | 2.43 | 0.51 |
| 1:AA:954:G:O3' | 13:AM:120:LYS:HD2 | 2.11 | 0.51 |
| 13:AM:34:LEU:HD13 | 13:AM:41:PRO:HA | 1.91 | 0.51 |
| 1:AA:235:C:H1' | 17:AQ:61:GLU:OE1 | 2.11 | 0.51 |
| 22:AV:73:A:H5' | 22:AV:73:A:N3 | 2.26 | 0.51 |
| 34:B8:61:LEU:C | 34:B8:63:PRO:HD2 | 2.31 | 0.51 |
| 36:BA:1257:C:H2' | 36:BA:1258:C:H6 | 1.76 | 0.51 |
| 36:BA:145:G:C2' | 36:BA:146:G:H5'' | 2.40 | 0.51 |
| 38:BC:147:PHE:C | 38:BC:149:ILE:H | 2.14 | 0.51 |
| 42:BG:114:ILE:HG23 | 42:BG:114:ILE:O | 2.10 | 0.51 |
| 43:BH:15:VAL:HG23 | 43:BH:16:SER:N | 2.26 | 0.51 |
| 47:BO:115:VAL:CG1 | 47:BO:121:VAL:HG21 | 2.39 | 0.51 |
| 48:BP:16:ARG:O | 48:BP:16:ARG:NH1 | 2.44 | 0.51 |
| 48:BP:95:VAL:O | 48:BP:95:VAL:HG23 | 2.10 | 0.51 |
| 49:BQ:32:TYR:OH | 49:BQ:111:GLU:HB2 | 2.10 | 0.51 |
| 49:BQ:43:THR:O | 49:BQ:46:GLN:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:BR:93:GLY:C | 50:BR:94:TYR:HD2 | 2.13 | 0.51 |
| 52:BT:46:GLU:OE2 | 52:BT:88:ILE:HG13 | 2.10 | 0.51 |
| 53:BU:79:PHE:CE1 | 53:BU:83:LEU:HD21 | 2.45 | 0.51 |
| 55:BW:52:GLU:O | 55:BW:54:ALA:N | 2.35 | 0.51 |
| 56:BX:54:VAL:CG2 | 56:BX:81:VAL:HG12 | 2.40 | 0.51 |
| 58:BZ:127:LYS:NZ | 58:BZ:127:LYS:HB3 | 2.25 | 0.51 |
| 1:AA:1320:C:H2' | 1:AA:1321:C:O4' | 2.10 | 0.51 |
| 1:AA:175:C:O2' | 1:AA:176:C:H5' | 2.11 | 0.51 |
| 1:AA:180:U:H2' | 1:AA:181:G:H5' | 1.92 | 0.51 |
| 1:AA:254:G:N2 | 17:AQ:16:GLN:HE22 | 2.06 | 0.51 |
| 1:AA:502:G:OP1 | 12:AL:118:SER:HB2 | 2.11 | 0.51 |
| 9:AI:93:ARG:C | 9:AI:95:LYS:N | 2.64 | 0.51 |
| 13:AM:119:GLY:O | 13:AM:120:LYS:CB | 2.58 | 0.51 |
| 13:AM:58:GLU:O | 13:AM:62:ASN:HB2 | 2.10 | 0.51 |
| 18:AR:53:ARG:C | 18:AR:55:ARG:N | 2.63 | 0.51 |
| 19:AS:19:VAL:CG1 | 19:AS:44:MET:HG3 | 2.40 | 0.51 |
| 24:AY:24:A:H2' | 24:AY:25:C:C6 | 2.46 | 0.51 |
| 24:AY:37:MIA:H121 | 24:AY:38:A:N1 | 2.26 | 0.51 |
| 26:B0:45:PHE:HE2 | 26:B0:77:ARG:NH2 | 2.08 | 0.51 |
| 31:B5:47:PRO:O | 31:B5:49:CYS:N | 2.34 | 0.51 |
| 32:B6:8:LYS:O | 32:B6:9:LEU:HB3 | 2.11 | 0.51 |
| 36:BA:1221:C:H2' | 36:BA:1221(A):C:C6 | 2.44 | 0.51 |
| 36:BA:1766:U:H2' | 36:BA:1767:C:C6 | 2.46 | 0.51 |
| 36:BA:2020:A:O2' | 36:BA:2021:C:H5' | 2.10 | 0.51 |
| 36:BA:2688:U:H1' | 36:BA:2721:A:H61 | 1.73 | 0.51 |
| 36:BA:2829:C:H2' | 36:BA:2830:G:O4' | 2.10 | 0.51 |
| 36:BA:511:U:H5'' | 36:BA:512:G:OP2 | 2.09 | 0.51 |
| 40:BE:65:GLY:O | 40:BE:66:HIS:C | 2.47 | 0.51 |
| 36:BA:1278:A:H5'' | 50:BR:36:THR:HG22 | 1.93 | 0.51 |
| 36:BA:1654:A:OP2 | 50:BR:3:HIS:HD2 | 1.94 | 0.51 |
| 52:BT:28:VAL:HG22 | 52:BT:46:GLU:CA | 2.41 | 0.51 |
| 53:BU:83:LEU:CD1 | 53:BU:83:LEU:H | 2.24 | 0.51 |
| 53:BU:85:LYS:C | 53:BU:87:GLY:N | 2.64 | 0.51 |
| 54:BV:40:LEU:HD22 | 54:BV:40:LEU:N | 2.26 | 0.51 |
| 56:BX:18:TYR:HD1 | 56:BX:21:PHE:HE1 | 1.59 | 0.51 |
| 56:BX:36:LYS:HE2 | 56:BX:54:VAL:O | 2.10 | 0.51 |
| 57:BY:10:GLY:CA | 57:BY:27:VAL:HG13 | 2.41 | 0.51 |
| 57:BY:86:ARG:CD | 57:BY:88:LYS:HG3 | 2.40 | 0.51 |
| 1:AA:1216:G:H2' | 1:AA:1217:C:H6 | 1.75 | 0.51 |
| 1:AA:1309:G:OP1 | 13:AM:92:HIS:HE1 | 1.92 | 0.51 |
| 1:AA:417:C:O2' | 1:AA:418:C:H5' | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AL:27:LEU:O | 12:AL:28:LYS:C | 2.49 | 0.51 |
| 16:AP:3:LYS:O | 16:AP:21:VAL:HA | 2.11 | 0.51 |
| 22:AV:18:G:H2' | 22:AV:57:G:N2 | 2.25 | 0.51 |
| 25:AZ:171:ILE:N | 25:AZ:171:ILE:HD12 | 2.26 | 0.51 |
| 32:B6:41:PRO:HG3 | 32:B6:49:HIS:CE1 | 2.45 | 0.51 |
| 35:B9:13:LYS:HD2 | 35:B9:28:GLU:CB | 2.41 | 0.51 |
| 36:BA:1625:C:C2' | 36:BA:1626:G:H5' | 2.41 | 0.51 |
| 36:BA:1801:G:OP2 | 39:BD:154:LYS:HE3 | 2.10 | 0.51 |
| 36:BA:963:U:H2' | 36:BA:964:C:C6 | 2.46 | 0.51 |
| 37:BB:73:A:C2' | 37:BB:74:U:H5' | 2.41 | 0.51 |
| 39:BD:73:VAL:HG13 | 39:BD:120:GLY:HA3 | 1.92 | 0.51 |
| 36:BA:2580:U:H5' | 40:BE:131:ALA:HB2 | 1.93 | 0.51 |
| 40:BE:24:THR:HB | 40:BE:184:VAL:CG2 | 2.40 | 0.51 |
| 51:BS:54:LEU:CD2 | 51:BS:58:LEU:O | 2.59 | 0.51 |
| 52:BT:106:SER:O | 52:BT:107:ASP:CB | 2.58 | 0.51 |
| 54:BV:47:VAL:CG1 | 54:BV:52:VAL:HB | 2.25 | 0.51 |
| 56:BX:55:ASN:HB2 | 56:BX:80:ILE:HG12 | 1.91 | 0.51 |
| 58:BZ:98:MET:O | 58:BZ:126:VAL:HG22 | 2.11 | 0.51 |
| 1:AA:1128:C:O2' | 1:AA:1130:A:N7 | 2.42 | 0.51 |
| 1:AA:176:C:H2' | 1:AA:177:C:C5 | 2.46 | 0.51 |
| 1:AA:622:A:C8 | 1:AA:623:C:C6 | 2.99 | 0.51 |
| 1:AA:80:G:H3' | 1:AA:81:U:H5' | 1.92 | 0.51 |
| 2:AB:32:ILE:HD11 | 2:AB:40:HIS:CB | 2.40 | 0.51 |
| 13:AM:94:ARG:HH22 | 36:BA:887:A:H5' | 1.76 | 0.51 |
| 22:AV:57:G:O2' | 22:AV:58:A:H5' | 2.10 | 0.51 |
| 25:AZ:334:PHE:CE2 | 25:AZ:353:VAL:HG11 | 2.45 | 0.51 |
| 27:B1:67:ILE:N | 27:B1:68:PRO:CD | 2.74 | 0.51 |
| 32:B6:22:ALA:O | 32:B6:23:THR:HG23 | 2.09 | 0.51 |
| 35:B9:1:MET:HB2 | 35:B9:34:GLN:OE1 | 2.11 | 0.51 |
| 35:B9:7:VAL:HG13 | 35:B9:34:GLN:CG | 2.39 | 0.51 |
| 36:BA:1131:G:H8 | 36:BA:2025:C:H4' | 1.75 | 0.51 |
| 36:BA:1744:C:C2' | 36:BA:1745:C:H5' | 2.41 | 0.51 |
| 36:BA:2483:C:H2' | 36:BA:2483:C:O2 | 2.10 | 0.51 |
| 36:BA:2735:G:H2' | 36:BA:2736:G:C8 | 2.46 | 0.51 |
| 36:BA:2789:C:H1' | 36:BA:2892:A:C2 | 2.45 | 0.51 |
| 36:BA:470:A:OP1 | 41:BF:59:TYR:CE2 | 2.63 | 0.51 |
| 36:BA:485:C:N3 | 36:BA:496:G:C2 | 2.79 | 0.51 |
| 38:BC:76:ALA:HB2 | 38:BC:153:ILE:HD11 | 1.92 | 0.51 |
| 36:BA:2512:C:H4' | 40:BE:122:PHE:CE2 | 2.45 | 0.51 |
| 42:BG:57:ALA:HA | 42:BG:90:LEU:HD21 | 1.93 | 0.51 |
| 42:BG:96:ARG:HA | 42:BG:99:MET:HE2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:BP:24:GLY:CA | 48:BP:33:ARG:CZ | 2.89 | 0.51 |
| 56:BX:9:LEU:HD23 | 56:BX:9:LEU:N | 2.25 | 0.51 |
| 57:BY:94:LYS:O | 57:BY:101:LYS:HA | 2.11 | 0.51 |
| 1:AA:1347:G:N2 | 1:AA:1373:G:H2' | 2.25 | 0.51 |
| 1:AA:1351:U:H5' | 7:AG:33:ASP:OD1 | 2.10 | 0.51 |
| 1:AA:502:G:H2' | 1:AA:503:C:O4' | 2.11 | 0.51 |
| 4:AD:47:ARG:HD3 | 4:AD:49:ARG:NH2 | 2.23 | 0.51 |
| 8:AH:11:THR:HA | 8:AH:14:ARG:HH12 | 1.76 | 0.51 |
| 9:AI:11:LYS:O | 9:AI:13:ALA:N | 2.44 | 0.51 |
| 11:AK:117:ASN:N | 11:AK:117:ASN:HD22 | 2.07 | 0.51 |
| 32:B6:27:LYS:O | 32:B6:27:LYS:HG3 | 2.11 | 0.51 |
| 35:B9:10:ILE:HG12 | 36:BA:2477:C:H5 | 1.76 | 0.51 |
| 36:BA:1149:G:H2' | 36:BA:1150:C:C6 | 2.46 | 0.51 |
| 36:BA:229:A:H3' | 36:BA:230:U:C5' | 2.33 | 0.51 |
| 36:BA:270:A:H2' | 36:BA:271:A:H5' | 1.92 | 0.51 |
| 36:BA:89:G:H3' | 36:BA:90:U:C5' | 2.41 | 0.51 |
| 37:BB:111:G:O2' | 37:BB:112:U:H5' | 2.10 | 0.51 |
| 39:BD:69:ARG:HD2 | 39:BD:119:ALA:HB2 | 1.93 | 0.51 |
| 42:BG:88:ILE:CG2 | 42:BG:89:GLY:N | 2.73 | 0.51 |
| 48:BP:113:LYS:HA | 48:BP:129:ALA:O | 2.10 | 0.51 |
| 48:BP:29:LYS:HD2 | 48:BP:29:LYS:N | 2.26 | 0.51 |
| 51:BS:12:PHE:H | 51:BS:12:PHE:HD2 | 1.59 | 0.51 |
| 53:BU:109:LEU:O | 53:BU:113:ALA:N | 2.43 | 0.51 |
| 57:BY:31:LEU:CB | 57:BY:32:PRO:HA | 2.35 | 0.51 |
| 1:AA:1002:G:H2' | 1:AA:1003:G:H8 | 1.74 | 0.51 |
| 1:AA:355:C:N4 | 1:AA:356:A:H62 | 2.09 | 0.51 |
| 1:AA:384:G:H2' | 1:AA:385:C:H6 | 1.74 | 0.51 |
| 1:AA:839:U:O2 | 1:AA:839:U:H2' | 2.11 | 0.51 |
| 6:AF:44:GLY:O | 6:AF:60:PHE:N | 2.43 | 0.51 |
| 7:AG:75:VAL:O | 7:AG:75:VAL:HG23 | 2.11 | 0.51 |
| 8:AH:116:LYS:CD | 8:AH:127:LEU:HD12 | 2.41 | 0.51 |
| 9:AI:43:ALA:O | 9:AI:45:ALA:N | 2.44 | 0.51 |
| 15:AO:65:ARG:HH11 | 15:AO:65:ARG:HG2 | 1.76 | 0.51 |
| 20:AT:74:LYS:HG2 | 20:AT:75:ASN:H | 1.74 | 0.51 |
| 1:AA:927:G:O3' | 23:AX:15:A:H2 | 1.93 | 0.51 |
| 25:AZ:356:PRO:HB3 | 25:AZ:357:PRO:HD2 | 1.93 | 0.51 |
| 26:B0:67:VAL:HG12 | 26:B0:68:GLU:H | 1.75 | 0.51 |
| 36:BA:1244:G:H2' | 36:BA:1245:G:O4' | 2.11 | 0.51 |
| 36:BA:1327:C:H2' | 36:BA:1328:G:O4' | 2.10 | 0.51 |
| 36:BA:1354:A:H2' | 36:BA:1355:G:O4' | 2.11 | 0.51 |
| 36:BA:272(H):C:H2' | 36:BA:272(I):U:C5' | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:310:A:OP1 | 57:BY:18:GLY:HA2 | 2.11 | 0.51 |
| 33:B7:5:TRP:CZ3 | 36:BA:464:U:H4' | 2.45 | 0.51 |
| 36:BA:491:G:H2' | 36:BA:492:A:C8 | 2.46 | 0.51 |
| 36:BA:761:A:C3' | 36:BA:761:A:C8 | 2.93 | 0.51 |
| 36:BA:2170:A:H4' | 38:BC:133:PRO:HB3 | 1.92 | 0.51 |
| 41:BF:154:VAL:CG1 | 41:BF:193:VAL:HG23 | 2.40 | 0.51 |
| 42:BG:73:ALA:H | 42:BG:87:PRO:CG | 2.24 | 0.51 |
| 46:BN:62:VAL:CG2 | 46:BN:66:LYS:HB2 | 2.41 | 0.51 |
| 48:BP:111:ARG:NE | 48:BP:149:GLU:HG3 | 2.26 | 0.51 |
| 51:BS:66:ALA:CA | 51:BS:69:VAL:HG12 | 2.41 | 0.51 |
| 52:BT:13:ARG:HH12 | 52:BT:15:VAL:CG1 | 2.19 | 0.51 |
| 52:BT:83:ILE:HG13 | 52:BT:84:GLN:H | 1.70 | 0.51 |
| 53:BU:3:ARG:HG2 | 53:BU:3:ARG:HH11 | 1.76 | 0.51 |
| 53:BU:46:ALA:O | 53:BU:49:HIS:N | 2.44 | 0.51 |
| 56:BX:24:GLY:O | 56:BX:81:VAL:O | 2.29 | 0.51 |
| 58:BZ:44:PHE:CD1 | 58:BZ:44:PHE:C | 2.85 | 0.51 |
| 1:AA:259:G:O2' | 1:AA:260:G:H5' | 2.10 | 0.50 |
| 2:AB:8:LYS:HE2 | 2:AB:217:ARG:CZ | 2.41 | 0.50 |
| 9:AI:121:ARG:HG2 | 9:AI:121:ARG:HH11 | 1.75 | 0.50 |
| 11:AK:52:GLY:H | 11:AK:55:LYS:HE2 | 1.73 | 0.50 |
| 11:AK:25:TYR:HE1 | 11:AK:87:THR:HB | 1.75 | 0.50 |
| 12:AL:33:ARG:HB3 | 12:AL:60:LEU:HD12 | 1.93 | 0.50 |
| 20:AT:97:ALA:O | 20:AT:99:LEU:N | 2.44 | 0.50 |
| 25:AZ:352:VAL:O | 25:AZ:372:VAL:HG23 | 2.11 | 0.50 |
| 36:BA:2111:C:N3 | 36:BA:2145:C:H2' | 2.25 | 0.50 |
| 36:BA:2491:U:O2' | 36:BA:2492:U:H5' | 2.11 | 0.50 |
| 36:BA:1637:A:H4' | 36:BA:2711:A:O2' | 2.11 | 0.50 |
| 36:BA:2758:A:O2' | 36:BA:2759:G:H8 | 1.94 | 0.50 |
| 36:BA:2791:C:H4' | 36:BA:2792:G:O5' | 2.12 | 0.50 |
| 36:BA:686:G:N2 | 36:BA:788:A:N6 | 2.59 | 0.50 |
| 28:B2:14:ARG:NH2 | 36:BA:77:C:O3' | 2.37 | 0.50 |
| 39:BD:166:GLN:HE21 | 39:BD:166:GLN:CA | 2.19 | 0.50 |
| 36:BA:1826:G:H4' | 39:BD:242:ARG:NH2 | 2.26 | 0.50 |
| 39:BD:266:SER:O | 39:BD:267:SER:O | 2.29 | 0.50 |
| 47:BO:9:GLU:O | 47:BO:83:ALA:HA | 2.12 | 0.50 |
| 50:BR:114:VAL:HG23 | 50:BR:114:VAL:O | 2.12 | 0.50 |
| 50:BR:72:ASP:HB3 | 50:BR:75:LEU:HB2 | 1.92 | 0.50 |
| 50:BR:53:HIS:HD2 | 50:BR:94:TYR:OH | 1.94 | 0.50 |
| 52:BT:131:ALA:C | 52:BT:133:GLU:N | 2.61 | 0.50 |
| 52:BT:78:LEU:O | 52:BT:79:HIS:CG | 2.64 | 0.50 |
| 54:BV:17:GLY:C | 54:BV:18:LEU:HD13 | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BX:27:THR:HG22 | 56:BX:80:ILE:CG2 | 2.39 | 0.50 |
| 58:BZ:86:VAL:O | 58:BZ:87:ASP:OD1 | 2.29 | 0.50 |
| 1:AA:495:A:H1' | 1:AA:496:A:C8 | 2.45 | 0.50 |
| 1:AA:737:A:O2' | 1:AA:738:C:H5' | 2.11 | 0.50 |
| 2:AB:42:ILE:HD12 | 2:AB:202:PRO:C | 2.32 | 0.50 |
| 8:AH:103:VAL:HB | 8:AH:109:ILE:N | 2.26 | 0.50 |
| 9:AI:57:GLY:O | 9:AI:58:ARG:CB | 2.58 | 0.50 |
| 1:AA:1060:C:O2' | 10:AJ:56:HIS:HD2 | 1.94 | 0.50 |
| 19:AS:6:LYS:CD | 19:AS:6:LYS:N | 2.54 | 0.50 |
| 25:AZ:181:GLN:OE1 | 25:AZ:193:ASN:OD1 | 2.29 | 0.50 |
| 25:AZ:34:VAL:HG11 | 25:AZ:199:ILE:HG22 | 1.93 | 0.50 |
| 32:B6:11:LEU:HD11 | 32:B6:51:GLU:CG | 2.42 | 0.50 |
| 36:BA:1301:A:HO2' | 36:BA:1302:A:H2' | 1.69 | 0.50 |
| 36:BA:1645:G:H5'' | 36:BA:1646:C:H5' | 1.93 | 0.50 |
| 36:BA:2464:C:O2' | 36:BA:2465:C:P | 2.69 | 0.50 |
| 36:BA:276:A:O2' | 36:BA:277:C:H5' | 2.10 | 0.50 |
| 36:BA:363(E):U:H3' | 36:BA:363(F):A:O4' | 2.11 | 0.50 |
| 38:BC:14:VAL:HG12 | 38:BC:14:VAL:O | 2.10 | 0.50 |
| 38:BC:190:ARG:O | 38:BC:194:ARG:HG3 | 2.10 | 0.50 |
| 36:BA:2591:C:P | 39:BD:239:ARG:HB2 | 2.51 | 0.50 |
| 39:BD:244:ARG:HG2 | 39:BD:245:PRO:HD3 | 1.93 | 0.50 |
| 40:BE:134:ILE:C | 40:BE:134:ILE:HD12 | 2.31 | 0.50 |
| 40:BE:132:HIS:CA | 40:BE:135:HIS:HE1 | 2.23 | 0.50 |
| 46:BN:62:VAL:HG13 | 46:BN:62:VAL:O | 2.11 | 0.50 |
| 48:BP:17:LYS:O | 48:BP:17:LYS:HG2 | 2.12 | 0.50 |
| 50:BR:18:LEU:HD13 | 50:BR:18:LEU:C | 2.32 | 0.50 |
| 50:BR:80:PHE:O | 50:BR:85:PRO:HD3 | 2.11 | 0.50 |
| 51:BS:17:ARG:O | 51:BS:20:ARG:N | 2.38 | 0.50 |
| 57:BY:67:LEU:HD23 | 57:BY:68:HIS:N | 2.25 | 0.50 |
| 57:BY:88:LYS:NZ | 57:BY:93:GLY:N | 2.58 | 0.50 |
| 58:BZ:19:ARG:HH12 | 58:BZ:84:GLU:CB | 2.23 | 0.50 |
| 1:AA:232:G:H1' | 1:AA:262:A:N1 | 2.26 | 0.50 |
| 1:AA:882:C:O2' | 1:AA:883:C:H5' | 2.12 | 0.50 |
| 5:AE:76:ILE:HG12 | 5:AE:93:PRO:HG3 | 1.93 | 0.50 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:CD1 | 2.47 | 0.50 |
| 12:AL:41:ARG:HH12 | 12:AL:57:LYS:HZ3 | 1.59 | 0.50 |
| 20:AT:57:ARG:NH1 | 20:AT:103:GLY:N | 2.59 | 0.50 |
| 20:AT:41:ILE:HG21 | 20:AT:87:LYS:CG | 2.41 | 0.50 |
| 20:AT:53:LEU:H | 20:AT:53:LEU:HD12 | 1.76 | 0.50 |
| 21:AU:24:ARG:O | 21:AU:25:LYS:CB | 2.59 | 0.50 |
| 25:AZ:162:GLU:OE2 | 25:AZ:162:GLU:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:185:ASN:OD1 | 25:AZ:188:THR:HG21 | 2.12 | 0.50 |
| 27:B1:27:GLU:CG | 27:B1:28:GLY:N | 2.74 | 0.50 |
| 31:B5:20:ARG:HA | 31:B5:23:HIS:CE1 | 2.47 | 0.50 |
| 32:B6:16:CYS:SG | 32:B6:48:VAL:HG22 | 2.51 | 0.50 |
| 32:B6:42:TRP:HA | 32:B6:42:TRP:CE3 | 2.47 | 0.50 |
| 32:B6:10:LEU:HD12 | 34:B8:34:TRP:HD1 | 1.76 | 0.50 |
| 36:BA:1227:G:O2' | 36:BA:1228:G:H5' | 2.10 | 0.50 |
| 36:BA:1654:A:OP1 | 50:BR:3:HIS:N | 2.45 | 0.50 |
| 36:BA:2308:G:C2' | 36:BA:2309:A:C8 | 2.95 | 0.50 |
| 36:BA:251:A:H5' | 48:BP:51:PHE:CZ | 2.46 | 0.50 |
| 36:BA:308:G:H1' | 36:BA:501:A:OP1 | 2.12 | 0.50 |
| 36:BA:560:C:H4' | 53:BU:52:ARG:NH2 | 2.26 | 0.50 |
| 36:BA:673:C:P | 41:BF:81:PRO:HG3 | 2.52 | 0.50 |
| 36:BA:776:G:H4' | 36:BA:777:A:O5' | 2.12 | 0.50 |
| 36:BA:898:C:H2' | 36:BA:899:A:C5' | 2.36 | 0.50 |
| 38:BC:100:ILE:HG23 | 38:BC:127:LEU:CD1 | 2.42 | 0.50 |
| 38:BC:200:LYS:HG3 | 38:BC:208:PHE:CD1 | 2.46 | 0.50 |
| 38:BC:43:VAL:HG22 | 38:BC:214:VAL:HG13 | 1.92 | 0.50 |
| 39:BD:35:LYS:HB2 | 39:BD:63:ARG:HG2 | 1.93 | 0.50 |
| 43:BH:46:GLU:OE1 | 43:BH:50:VAL:HG13 | 2.11 | 0.50 |
| 43:BH:64:LEU:O | 43:BH:67:LEU:HB3 | 2.11 | 0.50 |
| 46:BN:103:VAL:O | 46:BN:104:LYS:C | 2.50 | 0.50 |
| 48:BP:57:THR:C | 48:BP:59:LEU:H | 2.14 | 0.50 |
| 54:BV:3:ALA:CB | 54:BV:14:VAL:HG23 | 2.41 | 0.50 |
| 54:BV:19:LYS:HB2 | 54:BV:96:ILE:HD11 | 1.93 | 0.50 |
| 56:BX:21:PHE:O | 56:BX:22:ALA:C | 2.49 | 0.50 |
| 57:BY:54:LYS:HE3 | 57:BY:55:TYR:HE1 | 1.73 | 0.50 |
| 57:BY:8:LYS:HE2 | 57:BY:72:VAL:HG23 | 1.92 | 0.50 |
| 1:AA:1191:A:OP2 | 3:AC:3:ASN:ND2 | 2.45 | 0.50 |
| 1:AA:532:A:H2 | 1:AA:1206:G:H21 | 1.57 | 0.50 |
| 1:AA:1242:C:O2' | 1:AA:1243:C:H5' | 2.12 | 0.50 |
| 1:AA:1392:G:H21 | 1:AA:1502:A:H8 | 1.56 | 0.50 |
| 1:AA:174:C:O5' | 1:AA:174:C:H6 | 1.94 | 0.50 |
| 1:AA:268:C:O2' | 1:AA:269:C:H5' | 2.11 | 0.50 |
| 1:AA:691:G:O2' | 1:AA:797:C:H4' | 2.11 | 0.50 |
| 2:AB:195:ASP:O | 8:AH:68:ARG:NH2 | 2.40 | 0.50 |
| 6:AF:41:GLU:H | 6:AF:62:TRP:HE3 | 1.60 | 0.50 |
| 13:AM:66:LEU:O | 13:AM:70:LEU:HB2 | 2.11 | 0.50 |
| 15:AO:28:GLN:O | 15:AO:32:LEU:HG | 2.12 | 0.50 |
| 18:AR:56:THR:HB | 18:AR:58:LEU:HD12 | 1.92 | 0.50 |
| 26:B0:2:ALA:HB3 | 36:BA:2602:A:N1 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:B0:56:ASP:OD2 | 36:BA:2364:C:C5' | 2.60 | 0.50 |
| 26:B0:52:GLY:N | 26:B0:62:LEU:HD21 | 2.26 | 0.50 |
| 27:B1:53:VAL:CG2 | 27:B1:74:VAL:HG13 | 2.40 | 0.50 |
| 31:B5:44:THR:HG21 | 50:BR:101:ALA:CB | 2.28 | 0.50 |
| 34:B8:6:THR:CG2 | 34:B8:63:PRO:HD3 | 2.42 | 0.50 |
| 36:BA:1178:C:H2' | 36:BA:1179:C:H6 | 1.76 | 0.50 |
| 36:BA:1270:C:H5'' | 36:BA:1271:G:C5' | 2.41 | 0.50 |
| 36:BA:2290:G:H2' | 36:BA:2291:U:O4' | 2.12 | 0.50 |
| 36:BA:2330:G:H2' | 36:BA:2331:G:O4' | 2.12 | 0.50 |
| 36:BA:2724:C:H2' | 36:BA:2725:A:C8 | 2.46 | 0.50 |
| 36:BA:485:C:O2' | 36:BA:486:C:H5' | 2.11 | 0.50 |
| 36:BA:933:A:H2' | 36:BA:934:G:O4' | 2.11 | 0.50 |
| 46:BN:102:ALA:O | 46:BN:106:MET:HG3 | 2.12 | 0.50 |
| 48:BP:47:ASP:HB3 | 48:BP:48:PRO:C | 2.32 | 0.50 |
| 51:BS:12:PHE:CD2 | 51:BS:12:PHE:N | 2.78 | 0.50 |
| 51:BS:12:PHE:O | 51:BS:14:VAL:N | 2.44 | 0.50 |
| 56:BX:10:ALA:O | 56:BX:28:PHE:CB | 2.59 | 0.50 |
| 1:AA:1124:G:H2' | 1:AA:1145:C:H41 | 1.75 | 0.50 |
| 1:AA:16:A:N1 | 1:AA:919:A:H2 | 2.08 | 0.50 |
| 1:AA:9:G:OP2 | 5:AE:121:LYS:HD2 | 2.12 | 0.50 |
| 2:AB:145:LEU:CD1 | 2:AB:149:LEU:HD12 | 2.41 | 0.50 |
| 4:AD:150:GLU:CD | 4:AD:151:LYS:H | 2.11 | 0.50 |
| 9:AI:11:LYS:O | 9:AI:11:LYS:HG2 | 2.11 | 0.50 |
| 13:AM:65:LYS:CE | 13:AM:73:GLU:HG3 | 2.42 | 0.50 |
| 20:AT:93:GLU:OE2 | 20:AT:94:ALA:N | 2.44 | 0.50 |
| 22:AV:5:G:H8 | 22:AV:5:G:H5' | 1.76 | 0.50 |
| 24:AY:42:G:O2' | 24:AY:43:G:H5' | 2.11 | 0.50 |
| 24:AY:75:C:H1' | 25:AZ:231:ILE:HD13 | 1.92 | 0.50 |
| 25:AZ:16:THR:HG23 | 25:AZ:81:ASP:HA | 1.93 | 0.50 |
| 25:AZ:4:GLU:O | 25:AZ:6:ILE:HD12 | 2.12 | 0.50 |
| 36:BA:1140:C:H5' | 36:BA:1141:U:OP2 | 2.11 | 0.50 |
| 36:BA:142:A:H1' | 36:BA:1408:C:O4' | 2.11 | 0.50 |
| 36:BA:1862:G:O2' | 36:BA:1863:G:H5' | 2.12 | 0.50 |
| 36:BA:1973:G:H2' | 36:BA:1974:C:C6 | 2.46 | 0.50 |
| 36:BA:2297:C:C2' | 36:BA:2298:A:H5' | 2.42 | 0.50 |
| 36:BA:2394:C:C2' | 36:BA:2395:C:H5' | 2.42 | 0.50 |
| 36:BA:335:C:H2' | 36:BA:336:C:H6 | 1.73 | 0.50 |
| 36:BA:498:G:H2' | 36:BA:499:U:H6 | 1.76 | 0.50 |
| 36:BA:679:C:O2' | 36:BA:680:G:H5' | 2.10 | 0.50 |
| 36:BA:71:A:C2 | 56:BX:31:HIS:HE1 | 2.30 | 0.50 |
| 36:BA:845:G:O2' | 36:BA:846:C:H5 | 1.95 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:2152:G:OP1 | 38:BC:1:PRO:HA | 2.11 | 0.50 |
| 41:BF:36:VAL:HG11 | 41:BF:183:VAL:HG21 | 1.93 | 0.50 |
| 42:BG:115:ARG:HG3 | 42:BG:137:GLU:OE1 | 2.12 | 0.50 |
| 43:BH:87:LEU:CD2 | 43:BH:164:TYR:HA | 2.40 | 0.50 |
| 44:BJ:23:UNK:O | 44:BJ:86:UNK:HA | 2.11 | 0.50 |
| 48:BP:30:THR:CG2 | 48:BP:31:ALA:H | 2.25 | 0.50 |
| 48:BP:23:PRO:C | 48:BP:33:ARG:NE | 2.65 | 0.50 |
| 50:BR:63:ARG:HA | 50:BR:80:PHE:CZ | 2.46 | 0.50 |
| 57:BY:20:TYR:N | 57:BY:20:TYR:CD1 | 2.79 | 0.50 |
| 57:BY:37:VAL:HG23 | 57:BY:38:ILE:N | 2.26 | 0.50 |
| 36:BA:336:C:H4' | 57:BY:7:VAL:HG21 | 1.94 | 0.50 |
| 58:BZ:155:LEU:CD2 | 58:BZ:155:LEU:N | 2.74 | 0.50 |
| 1:AA:1128:C:H41 | 1:AA:1139:G:H2' | 1.76 | 0.50 |
| 1:AA:1368:G:OP2 | 9:AI:112:LYS:CD | 2.59 | 0.50 |
| 1:AA:838:G:C2' | 1:AA:839:U:H5'' | 2.42 | 0.50 |
| 7:AG:54:THR:O | 7:AG:56:GLN:N | 2.44 | 0.50 |
| 1:AA:189(F):U:O4 | 17:AQ:62:SER:HB3 | 2.12 | 0.50 |
| 17:AQ:86:GLU:OE1 | 17:AQ:86:GLU:HA | 2.11 | 0.50 |
| 25:AZ:338:TYR:O | 25:AZ:353:VAL:HG23 | 2.11 | 0.50 |
| 27:B1:11:ARG:NH1 | 27:B1:11:ARG:HB3 | 2.27 | 0.50 |
| 30:B4:14:ILE:HG13 | 30:B4:31:ILE:CB | 2.41 | 0.50 |
| 36:BA:1061:U:H4' | 36:BA:1070:A:C1' | 2.42 | 0.50 |
| 36:BA:990:A:C6 | 36:BA:1186:G:H1' | 2.47 | 0.50 |
| 36:BA:2372:G:O2' | 36:BA:2373:G:H5' | 2.12 | 0.50 |
| 36:BA:265:A:C8 | 36:BA:266:G:H1' | 2.46 | 0.50 |
| 36:BA:2723:C:H4' | 50:BR:2:ARG:NE | 2.25 | 0.50 |
| 37:BB:82:G:H2' | 37:BB:83:G:H8 | 1.76 | 0.50 |
| 38:BC:72:VAL:O | 38:BC:157:LYS:HD3 | 2.11 | 0.50 |
| 39:BD:161:THR:O | 39:BD:196:VAL:HG23 | 2.11 | 0.50 |
| 41:BF:43:LYS:HB2 | 41:BF:98:SER:CB | 2.42 | 0.50 |
| 42:BG:101:ILE:HG22 | 42:BG:105:LYS:NZ | 2.26 | 0.50 |
| 42:BG:76:SER:HA | 42:BG:83:ARG:HA | 1.94 | 0.50 |
| 43:BH:147:ASN:HD22 | 43:BH:147:ASN:N | 2.08 | 0.50 |
| 46:BN:97:ARG:O | 46:BN:101:HIS:HB2 | 2.12 | 0.50 |
| 46:BN:39:ARG:O | 46:BN:41:ASP:N | 2.43 | 0.50 |
| 1:AA:1442(B):A:H5' | 52:BT:122:ASP:OD1 | 2.11 | 0.50 |
| 52:BT:16:ARG:HH12 | 52:BT:19:LEU:HD21 | 1.76 | 0.50 |
| 52:BT:45:PHE:CE1 | 52:BT:74:ARG:HG3 | 2.46 | 0.50 |
| 55:BW:3:ALA:O | 55:BW:107:LEU:HD12 | 2.12 | 0.50 |
| 57:BY:42:VAL:HG21 | 57:BY:67:LEU:CD1 | 2.40 | 0.50 |
| 58:BZ:70:LEU:HD23 | 58:BZ:70:LEU:H | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:1169:A:H2' | 1:AA:1170:A:C8 | 2.47 | 0.50 |
| 1:AA:1468:A:H2' | 1:AA:1469:G:O4' | 2.12 | 0.50 |
| 1:AA:156:G:C6 | 1:AA:166:G:C6 | 3.00 | 0.50 |
| 1:AA:18:C:H5'' | 5:AE:127:ASN:ND2 | 2.26 | 0.50 |
| 1:AA:686:U:O4 | 1:AA:703:G:H1' | 2.11 | 0.50 |
| 2:AB:17:PHE:HB2 | 2:AB:44:LEU:HD11 | 1.93 | 0.50 |
| 4:AD:31:CYS:C | 4:AD:33:MET:H | 2.14 | 0.50 |
| 6:AF:14:LEU:HD13 | 6:AF:18:GLN:HB2 | 1.94 | 0.50 |
| 6:AF:53:ALA:O | 6:AF:54:LYS:HG2 | 2.11 | 0.50 |
| 12:AL:119:LYS:O | 12:AL:120:TYR:CD1 | 2.65 | 0.50 |
| 12:AL:6:THR:O | 12:AL:9:GLN:N | 2.45 | 0.50 |
| 25:AZ:225:VAL:HG23 | 25:AZ:302:GLN:O | 2.11 | 0.50 |
| 26:B0:24:LYS:O | 26:B0:25:ARG:HG2 | 2.11 | 0.50 |
| 28:B2:21:LEU:O | 28:B2:24:LEU:HB3 | 2.12 | 0.50 |
| 36:BA:2142:C:H2' | 36:BA:2143:C:C6 | 2.47 | 0.50 |
| 36:BA:215:G:H4' | 36:BA:216:A:H4' | 1.92 | 0.50 |
| 36:BA:2392:A:H2 | 36:BA:2424:C:N4 | 2.09 | 0.50 |
| 36:BA:2801(A):A:H1' | 36:BA:2803:C:C5 | 2.47 | 0.50 |
| 37:BB:22:U:H2' | 37:BB:23:G:C8 | 2.47 | 0.50 |
| 37:BB:53:A:C5 | 37:BB:54:G:N7 | 2.80 | 0.50 |
| 39:BD:12:SER:HB2 | 39:BD:208:LYS:HB3 | 1.94 | 0.50 |
| 39:BD:147:LEU:HD11 | 39:BD:183:ARG:HD3 | 1.94 | 0.50 |
| 41:BF:110:LEU:HA | 41:BF:183:VAL:CG1 | 2.42 | 0.50 |
| 41:BF:65:TRP:HZ3 | 41:BF:73:ALA:O | 1.94 | 0.50 |
| 42:BG:34:LEU:HA | 42:BG:161:THR:HG22 | 1.93 | 0.50 |
| 43:BH:86:GLU:OE2 | 43:BH:86:GLU:N | 2.44 | 0.50 |
| 46:BN:18:ALA:CB | 46:BN:26:LEU:HD22 | 2.41 | 0.50 |
| 46:BN:56:ASN:H | 46:BN:125:GLY:N | 2.10 | 0.50 |
| 48:BP:27:HIS:HA | 48:BP:30:THR:OG1 | 2.12 | 0.50 |
| 51:BS:106:ARG:HD2 | 51:BS:107:GLU:O | 2.12 | 0.50 |
| 52:BT:27:THR:O | 52:BT:28:VAL:HG23 | 2.12 | 0.50 |
| 54:BV:12:TYR:HE2 | 54:BV:22:VAL:HG12 | 1.77 | 0.50 |
| 54:BV:2:PHE:CE1 | 54:BV:13:ARG:NH1 | 2.79 | 0.50 |
| 56:BX:11:PRO:HG2 | 56:BX:13:LEU:HG | 1.92 | 0.50 |
| 57:BY:87:LYS:HG3 | 57:BY:88:LYS:N | 2.27 | 0.50 |
| 58:BZ:60:GLU:O | 58:BZ:65:GLN:O | 2.29 | 0.50 |
| 58:BZ:79:ARG:O | 58:BZ:80:ARG:C | 2.49 | 0.50 |
| 1:AA:1322:C:H6 | 1:AA:1322:C:OP1 | 1.94 | 0.50 |
| 1:AA:310:G:H2' | 1:AA:311:C:C6 | 2.46 | 0.50 |
| 1:AA:355:C:C4 | 1:AA:356:A:N7 | 2.79 | 0.50 |
| 1:AA:952:U:H2' | 1:AA:953:G:H8 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:AG:91:VAL:O | 7:AG:91:VAL:HG13 | 2.12 | 0.50 |
| 12:AL:89:ARG:HH11 | 12:AL:91:LYS:CA | 2.13 | 0.50 |
| 14:AN:32:SER:O | 14:AN:40:CYS:HA | 2.12 | 0.50 |
| 16:AP:74:LEU:HD22 | 16:AP:79:VAL:HG21 | 1.94 | 0.50 |
| 22:AV:68:C:O2' | 22:AV:69:G:H5'' | 2.11 | 0.50 |
| 25:AZ:143:ASP:O | 25:AZ:144:PRO:C | 2.50 | 0.50 |
| 26:B0:70:GLN:NE2 | 26:B0:80:HIS:NE2 | 2.60 | 0.50 |
| 30:B4:7:PRO:HD2 | 42:BG:65:GLY:O | 2.12 | 0.50 |
| 34:B8:44:LYS:HD2 | 34:B8:44:LYS:N | 2.27 | 0.50 |
| 36:BA:1677:A:H2' | 36:BA:1678:G:H8 | 1.77 | 0.50 |
| 36:BA:1947:C:C2' | 36:BA:1948:G:C5' | 2.82 | 0.50 |
| 36:BA:2078:C:H2' | 36:BA:2079:U:H6 | 1.75 | 0.50 |
| 36:BA:848:G:H5' | 36:BA:848:G:H8 | 1.76 | 0.50 |
| 36:BA:951:C:O2' | 36:BA:952:G:H5' | 2.12 | 0.50 |
| 40:BE:77:ILE:CG2 | 40:BE:78:LEU:H | 1.98 | 0.50 |
| 41:BF:185:ASP:HA | 41:BF:188:ARG:CG | 2.41 | 0.50 |
| 43:BH:85:LYS:NZ | 43:BH:133:VAL:H | 2.07 | 0.50 |
| 48:BP:111:ARG:N | 48:BP:111:ARG:HD2 | 2.27 | 0.50 |
| 50:BR:34:ILE:HG22 | 50:BR:36:THR:HG23 | 1.94 | 0.50 |
| 50:BR:37:THR:HG23 | 50:BR:40:LYS:HE2 | 1.93 | 0.50 |
| 51:BS:47:THR:HG22 | 51:BS:49:VAL:O | 2.12 | 0.50 |
| 52:BT:48:ILE:O | 52:BT:63:VAL:HA | 2.11 | 0.50 |
| 54:BV:79:VAL:HG12 | 54:BV:79:VAL:O | 2.12 | 0.50 |
| 57:BY:20:TYR:CZ | 57:BY:42:VAL:HA | 2.47 | 0.50 |
| 58:BZ:177:PRO:O | 58:BZ:178:GLU:HG2 | 2.11 | 0.50 |
| 1:AA:1171:G:O2' | 1:AA:1172:C:H5' | 2.12 | 0.50 |
| 1:AA:978:A:C5 | 1:AA:1319:A:C2 | 3.00 | 0.50 |
| 1:AA:255:G:O6 | 1:AA:266:G:O6 | 2.29 | 0.50 |
| 2:AB:235:SER:O | 2:AB:237:ALA:N | 2.45 | 0.50 |
| 3:AC:101:LEU:C | 3:AC:101:LEU:HD23 | 2.32 | 0.50 |
| 3:AC:188:LEU:HD11 | 3:AC:195:VAL:HG11 | 1.93 | 0.50 |
| 4:AD:108:LEU:HD13 | 4:AD:174:LEU:HD13 | 1.94 | 0.50 |
| 5:AE:82:VAL:CG1 | 5:AE:83:GLU:N | 2.74 | 0.50 |
| 6:AF:33:TYR:CE2 | 6:AF:75:LEU:HA | 2.46 | 0.50 |
| 12:AL:102:ARG:HH11 | 12:AL:102:ARG:CG | 2.25 | 0.50 |
| 14:AN:23:ARG:HH11 | 14:AN:30:ALA:HB2 | 1.76 | 0.50 |
| 20:AT:26:ASN:N | 20:AT:26:ASN:ND2 | 2.58 | 0.50 |
| 22:AW:38:A:H3' | 22:AW:39:U:H5'' | 1.94 | 0.50 |
| 25:AZ:338:TYR:HB3 | 25:AZ:353:VAL:HB | 1.94 | 0.50 |
| 33:B7:21:ARG:O | 33:B7:27:GLY:HA3 | 2.12 | 0.50 |
| 36:BA:1054:A:H2' | 36:BA:1054:A:N3 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:1425:G:H2' | 36:BA:1426:G:C8 | 2.47 | 0.50 |
| 36:BA:1714:G:H2' | 36:BA:1717:G:O4' | 2.11 | 0.50 |
| 36:BA:2085:C:OP1 | 39:BD:261:LYS:NZ | 2.43 | 0.50 |
| 36:BA:212:G:O2' | 36:BA:213:A:H5' | 2.11 | 0.50 |
| 36:BA:2350:C:O2' | 36:BA:2351:G:H5' | 2.12 | 0.50 |
| 36:BA:264:C:H4' | 36:BA:428:A:N1 | 2.27 | 0.50 |
| 36:BA:997:G:OP1 | 53:BU:93:LYS:HD3 | 2.12 | 0.50 |
| 36:BA:782:A:N1 | 39:BD:226:MET:CE | 2.75 | 0.50 |
| 40:BE:105:THR:OG1 | 40:BE:166:THR:HG23 | 2.12 | 0.50 |
| 41:BF:20:LEU:HD12 | 41:BF:203:GLN:HE22 | 1.76 | 0.50 |
| 42:BG:109:VAL:O | 42:BG:111:LEU:N | 2.39 | 0.50 |
| 46:BN:120:LEU:CD1 | 46:BN:122:VAL:HG23 | 2.42 | 0.50 |
| 48:BP:16:ARG:CA | 48:BP:16:ARG:HH11 | 2.24 | 0.50 |
| 53:BU:79:PHE:CD1 | 53:BU:80:ILE:HD13 | 2.46 | 0.50 |
| 58:BZ:28:MET:HE1 | 58:BZ:33:LEU:HD21 | 1.93 | 0.50 |
| 58:BZ:45:ASP:OD2 | 58:BZ:49:ARG:HG2 | 2.12 | 0.50 |
| 1:AA:1319:A:H2' | 1:AA:1323:G:N7 | 2.27 | 0.49 |
| 1:AA:849:C:O2' | 1:AA:850:U:H5' | 2.12 | 0.49 |
| 2:AB:22:LYS:HE2 | 2:AB:22:LYS:N | 2.27 | 0.49 |
| 2:AB:7:VAL:O | 2:AB:7:VAL:HG12 | 2.10 | 0.49 |
| 3:AC:113:ALA:HB1 | 3:AC:185:GLY:N | 2.27 | 0.49 |
| 6:AF:40:VAL:HG23 | 6:AF:62:TRP:O | 2.11 | 0.49 |
| 7:AG:137:LYS:O | 7:AG:138:LYS:C | 2.49 | 0.49 |
| 10:AJ:50:ILE:HG13 | 14:AN:41:ARG:CZ | 2.42 | 0.49 |
| 17:AQ:56:VAL:O | 17:AQ:76:LEU:HD12 | 2.12 | 0.49 |
| 1:AA:324:G:OP1 | 20:AT:70:SER:HB2 | 2.12 | 0.49 |
| 22:AW:38:A:H2' | 22:AW:39:U:C5' | 2.39 | 0.49 |
| 25:AZ:156:ASP:O | 25:AZ:160:GLN:HB2 | 2.12 | 0.49 |
| 36:BA:1478:G:HO2' | 36:BA:1558:A:H2 | 1.60 | 0.49 |
| 36:BA:1310:G:H1 | 36:BA:1604:C:H42 | 1.60 | 0.49 |
| 36:BA:1802:A:H2' | 36:BA:1803:A:C8 | 2.47 | 0.49 |
| 36:BA:2097:C:H6 | 36:BA:2097:C:O5' | 1.94 | 0.49 |
| 36:BA:2134:A:H1' | 36:BA:2159:G:N3 | 2.27 | 0.49 |
| 36:BA:2159:G:C3' | 36:BA:2160:G:H5'' | 2.42 | 0.49 |
| 36:BA:2287:A:C2 | 36:BA:2346:A:N1 | 2.68 | 0.49 |
| 36:BA:2364:C:C2' | 36:BA:2365:G:H5' | 2.42 | 0.49 |
| 36:BA:2392:A:H2' | 36:BA:2393:A:O4' | 2.12 | 0.49 |
| 37:BB:14:U:OP2 | 37:BB:71:C:H5' | 2.12 | 0.49 |
| 38:BC:156:ILE:HA | 38:BC:160:ARG:HB3 | 1.93 | 0.49 |
| 40:BE:199:ARG:NH1 | 40:BE:199:ARG:CB | 2.75 | 0.49 |
| 40:BE:38:THR:C | 40:BE:40:GLU:H | 2.15 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BH:68:THR:O | 43:BH:70:THR:N | 2.45 | 0.49 |
| 47:BO:24:VAL:HG23 | 47:BO:24:VAL:O | 2.12 | 0.49 |
| 48:BP:113:LYS:HE2 | 48:BP:131:SER:HB3 | 1.93 | 0.49 |
| 52:BT:11:GLU:C | 52:BT:13:ARG:H | 2.15 | 0.49 |
| 54:BV:18:LEU:HD22 | 54:BV:18:LEU:N | 2.27 | 0.49 |
| 56:BX:51:VAL:CG1 | 56:BX:54:VAL:HG23 | 2.42 | 0.49 |
| 1:AA:223:U:H2' | 1:AA:224:C:H6 | 1.77 | 0.49 |
| 2:AB:187:LEU:CD1 | 2:AB:205:ASP:HB3 | 2.42 | 0.49 |
| 4:AD:168:ARG:N | 4:AD:168:ARG:HD2 | 2.27 | 0.49 |
| 10:AJ:46:ARG:HG2 | 10:AJ:46:ARG:NH1 | 2.27 | 0.49 |
| 1:AA:1060:C:O2' | 10:AJ:56:HIS:CD2 | 2.65 | 0.49 |
| 10:AJ:57:LYS:CE | 10:AJ:60:ARG:NH2 | 2.75 | 0.49 |
| 10:AJ:4:ILE:HB | 10:AJ:74:ILE:HD11 | 1.94 | 0.49 |
| 13:AM:25:ILE:HG13 | 13:AM:66:LEU:HD23 | 1.95 | 0.49 |
| 20:AT:41:ILE:HG21 | 20:AT:87:LYS:HG2 | 1.93 | 0.49 |
| 27:B1:76:ARG:HB3 | 36:BA:271(R):G:OP1 | 2.12 | 0.49 |
| 30:B4:24:THR:HG21 | 42:BG:104:GLU:HG2 | 1.92 | 0.49 |
| 32:B6:12:GLU:OE1 | 32:B6:53:LYS:O | 2.30 | 0.49 |
| 36:BA:1241:A:N6 | 36:BA:1242:A:N6 | 2.60 | 0.49 |
| 36:BA:1336:A:H2' | 36:BA:1337:G:H8 | 1.77 | 0.49 |
| 36:BA:2295:C:C2 | 36:BA:2296:U:C5 | 3.00 | 0.49 |
| 36:BA:727:A:O2' | 36:BA:728:G:H5' | 2.12 | 0.49 |
| 38:BC:6:ARG:O | 38:BC:10:LEU:HD23 | 2.12 | 0.49 |
| 42:BG:103:LEU:HD23 | 42:BG:103:LEU:O | 2.12 | 0.49 |
| 46:BN:48:MET:N | 46:BN:48:MET:HE3 | 2.27 | 0.49 |
| 47:BO:8:LEU:HD13 | 47:BO:8:LEU:N | 2.26 | 0.49 |
| 52:BT:67:SER:O | 52:BT:68:TYR:HB2 | 2.12 | 0.49 |
| 40:BE:181:LEU:HD21 | 52:BT:7:ILE:CG2 | 2.42 | 0.49 |
| 53:BU:46:ALA:O | 53:BU:47:TYR:C | 2.51 | 0.49 |
| 56:BX:3:THR:HA | 56:BX:6:ASP:OD2 | 2.12 | 0.49 |
| 1:AA:1286:A:O2' | 1:AA:1287:A:C5' | 2.60 | 0.49 |
| 1:AA:1491:G:C5 | 59:AA:1601:PAR:H21 | 2.48 | 0.49 |
| 1:AA:441:A:H3' | 1:AA:442:C:H6 | 1.77 | 0.49 |
| 1:AA:681:C:C2' | 1:AA:682:G:H5' | 2.42 | 0.49 |
| 1:AA:789:U:H2' | 1:AA:791:G:OP2 | 2.13 | 0.49 |
| 3:AC:23:TYR:CG | 3:AC:24:ALA:N | 2.80 | 0.49 |
| 5:AE:102:ALA:CB | 5:AE:120:THR:HG21 | 2.42 | 0.49 |
| 25:AZ:140:MET:HE1 | 61:AZ:501:GCP:HN21 | 1.76 | 0.49 |
| 36:BA:1208:C:C4 | 36:BA:1209:G:N7 | 2.80 | 0.49 |
| 36:BA:1231:G:H2' | 36:BA:1232:G:C8 | 2.40 | 0.49 |
| 36:BA:2360:A:C2 | 36:BA:2361:A:H1' | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:2383:G:O2' | 36:BA:2384:G:H5' | 2.12 | 0.49 |
| 36:BA:2554:U:H2' | 36:BA:2555:U:H6 | 1.77 | 0.49 |
| 36:BA:2712:U:H1' | 36:BA:2712(A):A:H8 | 1.74 | 0.49 |
| 36:BA:303:U:O2' | 36:BA:304:G:H5' | 2.12 | 0.49 |
| 38:BC:99:ILE:HG22 | 38:BC:99:ILE:O | 2.12 | 0.49 |
| 39:BD:24:ILE:CD1 | 39:BD:25:THR:N | 2.67 | 0.49 |
| 39:BD:65:ILE:HD13 | 39:BD:65:ILE:N | 2.27 | 0.49 |
| 40:BE:142:GLY:C | 40:BE:143:ASN:HD22 | 2.14 | 0.49 |
| 36:BA:2680:C:H5' | 40:BE:189:PRO:HA | 1.93 | 0.49 |
| 40:BE:35:GLN:CG | 40:BE:36:ARG:H | 2.21 | 0.49 |
| 40:BE:47:VAL:HG21 | 40:BE:85:ASN:HA | 1.93 | 0.49 |
| 41:BF:119:ARG:NH1 | 41:BF:119:ARG:HG2 | 2.27 | 0.49 |
| 41:BF:150:GLY:HA2 | 41:BF:172:TRP:CE3 | 2.46 | 0.49 |
| 42:BG:34:LEU:HD13 | 42:BG:99:MET:SD | 2.52 | 0.49 |
| 47:BO:20:MET:CE | 47:BO:44:LYS:HE3 | 2.43 | 0.49 |
| 48:BP:122:PRO:HB3 | 48:BP:141:ALA:HB1 | 1.93 | 0.49 |
| 48:BP:38:GLN:CG | 48:BP:39:LYS:H | 2.18 | 0.49 |
| 48:BP:71:VAL:H | 48:BP:72:PRO:HD2 | 1.74 | 0.49 |
| 49:BQ:78:PRO:O | 49:BQ:81:VAL:CG1 | 2.59 | 0.49 |
| 57:BY:67:LEU:HD21 | 57:BY:71:LYS:CE | 2.42 | 0.49 |
| 58:BZ:34:ASN:O | 58:BZ:35:ARG:NE | 2.44 | 0.49 |
| 1:AA:1309:G:C6 | 1:AA:1329:A:C2 | 3.00 | 0.49 |
| 1:AA:511:C:C2 | 1:AA:512:U:C5 | 3.00 | 0.49 |
| 1:AA:853:G:O2' | 1:AA:854:G:H5' | 2.12 | 0.49 |
| 4:AD:17:VAL:HG11 | 4:AD:197:PRO:CB | 2.42 | 0.49 |
| 9:AI:118:LYS:O | 9:AI:119:ALA:HB2 | 2.11 | 0.49 |
| 1:AA:1228:C:O2' | 13:AM:118:ALA:HB2 | 2.13 | 0.49 |
| 1:AA:974:A:P | 14:AN:29:ARG:HH22 | 2.35 | 0.49 |
| 25:AZ:217:VAL:HA | 25:AZ:245:GLY:HA2 | 1.93 | 0.49 |
| 32:B6:20:ASN:C | 32:B6:21:TYR:CD1 | 2.86 | 0.49 |
| 36:BA:1625:C:O2' | 36:BA:1626:G:H5' | 2.13 | 0.49 |
| 36:BA:2033:A:O2' | 36:BA:2034:U:P | 2.71 | 0.49 |
| 36:BA:2188:C:H2' | 36:BA:2189:U:N1 | 2.26 | 0.49 |
| 36:BA:2543:G:H2' | 36:BA:2544:G:C8 | 2.48 | 0.49 |
| 36:BA:2839:G:H5' | 50:BR:46:GLY:HA2 | 1.93 | 0.49 |
| 36:BA:325:G:O2' | 36:BA:326:G:H5' | 2.11 | 0.49 |
| 36:BA:500:G:H22 | 36:BA:503:A:P | 2.36 | 0.49 |
| 36:BA:635:C:O2' | 36:BA:639:U:H5'' | 2.12 | 0.49 |
| 36:BA:635:C:H2' | 36:BA:636:G:O4' | 2.12 | 0.49 |
| 36:BA:67:U:H2' | 36:BA:68:G:C8 | 2.47 | 0.49 |
| 39:BD:96:HIS:CE1 | 39:BD:102:LYS:HZ3 | 2.29 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:BG:172:LEU:HD23 | 42:BG:172:LEU:O | 2.13 | 0.49 |
| 42:BG:85:GLY:C | 42:BG:87:PRO:CD | 2.80 | 0.49 |
| 42:BG:85:GLY:C | 42:BG:87:PRO:HD3 | 2.32 | 0.49 |
| 45:BK:86:UNK:O | 45:BK:87:UNK:CB | 2.59 | 0.49 |
| 48:BP:111:ARG:HG2 | 48:BP:111:ARG:NH2 | 2.26 | 0.49 |
| 49:BQ:140:ALA:HB1 | 58:BZ:99:TYR:CB | 2.42 | 0.49 |
| 1:AA:242:C:H2' | 1:AA:243:A:H5' | 1.94 | 0.49 |
| 1:AA:277:C:O2' | 1:AA:278:G:H5' | 2.12 | 0.49 |
| 1:AA:642:A:N3 | 8:AH:113:SER:OG | 2.44 | 0.49 |
| 4:AD:170:VAL:HG12 | 4:AD:174:LEU:HB2 | 1.93 | 0.49 |
| 5:AE:12:LEU:HD22 | 5:AE:12:LEU:C | 2.32 | 0.49 |
| 5:AE:6:PHE:HB2 | 5:AE:34:VAL:CG2 | 2.42 | 0.49 |
| 6:AF:52:ILE:O | 6:AF:53:ALA:HB3 | 2.12 | 0.49 |
| 7:AG:37:ASN:HD21 | 9:AI:40:LEU:HA | 1.77 | 0.49 |
| 1:AA:35:G:N2 | 12:AL:118:SER:OG | 2.39 | 0.49 |
| 16:AP:53:VAL:CG2 | 16:AP:54:GLU:H | 2.22 | 0.49 |
| 16:AP:74:LEU:HB3 | 16:AP:79:VAL:HG21 | 1.93 | 0.49 |
| 20:AT:57:ARG:NH1 | 20:AT:102:GLY:HA3 | 2.27 | 0.49 |
| 25:AZ:221:PHE:CE2 | 25:AZ:304:LEU:O | 2.65 | 0.49 |
| 27:B1:58:ILE:HD11 | 27:B1:91:LYS:CB | 2.43 | 0.49 |
| 28:B2:33:MET:HG3 | 28:B2:37:PHE:CE1 | 2.48 | 0.49 |
| 30:B4:31:ILE:HG22 | 30:B4:33:VAL:HG23 | 1.94 | 0.49 |
| 34:B8:38:GLY:O | 34:B8:42:ARG:HB2 | 2.12 | 0.49 |
| 36:BA:1337:G:H2' | 36:BA:1338:G:H8 | 1.78 | 0.49 |
| 36:BA:1859:A:N6 | 36:BA:1883:G:O2' | 2.46 | 0.49 |
| 36:BA:2360:A:O2' | 36:BA:2361:A:C5' | 2.61 | 0.49 |
| 36:BA:323:G:C8 | 41:BF:171:PRO:HG3 | 2.47 | 0.49 |
| 36:BA:587:C:C5 | 48:BP:33:ARG:HG2 | 2.47 | 0.49 |
| 36:BA:652:C:O2' | 36:BA:653:A:O5' | 2.30 | 0.49 |
| 36:BA:658:C:H2' | 36:BA:659:C:H6 | 1.76 | 0.49 |
| 36:BA:85:G:O5' | 57:BY:30:VAL:HB | 2.11 | 0.49 |
| 37:BB:71:C:C2' | 37:BB:72:G:H5' | 2.42 | 0.49 |
| 40:BE:171:GLU:O | 40:BE:184:VAL:HA | 2.12 | 0.49 |
| 42:BG:52:ILE:HD13 | 42:BG:52:ILE:N | 2.23 | 0.49 |
| 47:BO:107:ARG:HA | 47:BO:112:MET:HE2 | 1.93 | 0.49 |
| 47:BO:35:VAL:CG2 | 47:BO:69:ILE:HD11 | 2.43 | 0.49 |
| 49:BQ:45:GLN:NE2 | 49:BQ:45:GLN:H | 2.10 | 0.49 |
| 49:BQ:58:PHE:O | 49:BQ:58:PHE:HD1 | 1.96 | 0.49 |
| 50:BR:32:GLY:O | 50:BR:115:GLU:HA | 2.13 | 0.49 |
| 50:BR:67:LEU:HD11 | 50:BR:71:GLN:O | 2.12 | 0.49 |
| 56:BX:51:VAL:HG11 | 56:BX:54:VAL:HG23 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:BY:31:LEU:HG | 57:BY:34:LYS:HB2 | 1.95 | 0.49 |
| 57:BY:86:ARG:NH2 | 57:BY:95:LYS:HZ3 | 2.11 | 0.49 |
| 58:BZ:96:VAL:O | 58:BZ:127:LYS:HA | 2.13 | 0.49 |
| 1:AA:1216:G:O2' | 1:AA:1217:C:H5' | 2.12 | 0.49 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:H8 | 1.75 | 0.49 |
| 1:AA:386:C:H2' | 1:AA:387:U:H5' | 1.94 | 0.49 |
| 1:AA:697:U:C2' | 1:AA:698:G:H5' | 2.42 | 0.49 |
| 5:AE:20:GLN:HE22 | 5:AE:25:ARG:CZ | 2.24 | 0.49 |
| 15:AO:61:GLY:O | 15:AO:65:ARG:HG3 | 2.12 | 0.49 |
| 19:AS:16:LEU:C | 19:AS:18:LYS:N | 2.65 | 0.49 |
| 1:AA:186:C:O3' | 20:AT:82:SER:HB3 | 2.13 | 0.49 |
| 23:AX:26:A:C3' | 23:AX:27:A:C5' | 2.90 | 0.49 |
| 25:AZ:164:PRO:O | 25:AZ:168:VAL:HG23 | 2.12 | 0.49 |
| 32:B6:20:ASN:CG | 32:B6:21:TYR:N | 2.65 | 0.49 |
| 36:BA:1103:A:H5' | 36:BA:1104:C:OP2 | 2.12 | 0.49 |
| 36:BA:1169:G:H1 | 36:BA:1180:C:N4 | 2.04 | 0.49 |
| 36:BA:1678:G:H8 | 36:BA:1678:G:O5' | 1.95 | 0.49 |
| 36:BA:416:C:N4 | 36:BA:2407:G:H1 | 2.06 | 0.49 |
| 36:BA:2631:G:N3 | 36:BA:2810:A:H2 | 2.10 | 0.49 |
| 36:BA:29:U:O2' | 36:BA:30:G:H5' | 2.13 | 0.49 |
| 36:BA:660:G:C5' | 41:BF:99:TYR:CE2 | 2.95 | 0.49 |
| 38:BC:14:VAL:HA | 38:BC:20:TYR:OH | 2.12 | 0.49 |
| 39:BD:131:LEU:CD1 | 39:BD:131:LEU:N | 2.73 | 0.49 |
| 39:BD:60:ARG:CG | 39:BD:86:PRO:HB2 | 2.38 | 0.49 |
| 49:BQ:74:TYR:C | 49:BQ:74:TYR:CD1 | 2.86 | 0.49 |
| 49:BQ:74:TYR:HD1 | 49:BQ:74:TYR:C | 2.16 | 0.49 |
| 53:BU:83:LEU:HD12 | 53:BU:83:LEU:H | 1.77 | 0.49 |
| 1:AA:109:A:H2' | 1:AA:326:G:N2 | 2.27 | 0.49 |
| 1:AA:1152:A:H2' | 1:AA:1153:C:C6 | 2.47 | 0.49 |
| 1:AA:1316:G:O3' | 14:AN:18:VAL:HG22 | 2.12 | 0.49 |
| 1:AA:1478:C:H2' | 1:AA:1479:C:C6 | 2.48 | 0.49 |
| 1:AA:149:A:H2' | 1:AA:150:C:C6 | 2.47 | 0.49 |
| 1:AA:580:U:H2' | 1:AA:581:G:O4' | 2.12 | 0.49 |
| 1:AA:992:U:H4' | 1:AA:993:G:O5' | 2.13 | 0.49 |
| 3:AC:95:THR:O | 3:AC:97:LYS:N | 2.46 | 0.49 |
| 4:AD:74:GLN:HE22 | 4:AD:100:ARG:HH22 | 1.59 | 0.49 |
| 12:AL:5:PRO:HG2 | 12:AL:10:LEU:CD2 | 2.42 | 0.49 |
| 17:AQ:58:GLU:O | 17:AQ:59:ILE:HD13 | 2.13 | 0.49 |
| 19:AS:25:LYS:HB3 | 19:AS:27:GLU:OE2 | 2.13 | 0.49 |
| 19:AS:48:THR:O | 19:AS:48:THR:HG22 | 2.13 | 0.49 |
| 21:AU:8:THR:O | 21:AU:12:LYS:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:AZ:72:THR:C | 25:AZ:74:LYS:N | 2.65 | 0.49 |
| 25:AZ:75:ARG:NH2 | 25:AZ:211:PRO:O | 2.46 | 0.49 |
| 36:BA:1638:C:H4' | 36:BA:2710:C:O2 | 2.13 | 0.49 |
| 36:BA:197:A:H8 | 36:BA:197:A:H5' | 1.76 | 0.49 |
| 36:BA:2137:C:O2' | 36:BA:2138:C:H5' | 2.11 | 0.49 |
| 36:BA:2297:C:O2' | 36:BA:2298:A:H5' | 2.13 | 0.49 |
| 36:BA:2520:C:C6 | 36:BA:2567:G:H1' | 2.47 | 0.49 |
| 36:BA:271(J):C:H2' | 36:BA:271(J):C:O2 | 2.12 | 0.49 |
| 36:BA:2777:G:C5' | 36:BA:2778:A:H5' | 2.42 | 0.49 |
| 36:BA:2821:A:H2' | 36:BA:2822:G:C8 | 2.48 | 0.49 |
| 36:BA:534:U:O2' | 53:BU:49:HIS:CD2 | 2.65 | 0.49 |
| 36:BA:600:G:H1 | 36:BA:657:U:H3 | 1.61 | 0.49 |
| 36:BA:969:U:H6 | 36:BA:969:U:O5' | 1.96 | 0.49 |
| 47:BO:98:VAL:O | 47:BO:119:PRO:HD3 | 2.11 | 0.49 |
| 36:BA:2562:U:H1' | 47:BO:23:ARG:HH11 | 1.78 | 0.49 |
| 49:BQ:111:GLU:O | 49:BQ:115:MET:HG2 | 2.12 | 0.49 |
| 26:B0:5:LYS:HG3 | 49:BQ:80:GLU:HB3 | 1.94 | 0.49 |
| 52:BT:41:ARG:NH1 | 52:BT:41:ARG:HG2 | 2.27 | 0.49 |
| 53:BU:85:LYS:HD3 | 53:BU:117:GLN:NE2 | 2.25 | 0.49 |
| 57:BY:17:SER:OG | 57:BY:18:GLY:N | 2.43 | 0.49 |
| 57:BY:90:LEU:HD23 | 57:BY:90:LEU:H | 1.78 | 0.49 |
| 58:BZ:74:VAL:HG12 | 58:BZ:74:VAL:O | 2.12 | 0.49 |
| 1:AA:115:G:H1' | 1:AA:116:A:N7 | 2.28 | 0.49 |
| 1:AA:126:G:H5' | 1:AA:633:G:N2 | 2.28 | 0.49 |
| 1:AA:625:G:O2' | 1:AA:626:U:H5' | 2.12 | 0.49 |
| 3:AC:15:THR:HG23 | 3:AC:181:ASN:HB2 | 1.95 | 0.49 |
| 5:AE:46:GLY:HA3 | 5:AE:58:ALA:HB2 | 1.95 | 0.49 |
| 6:AF:98:LEU:H | 6:AF:98:LEU:HD12 | 1.76 | 0.49 |
| 7:AG:78:ARG:CG | 7:AG:78:ARG:O | 2.60 | 0.49 |
| 8:AH:120:THR:OG1 | 8:AH:123:GLU:HG3 | 2.12 | 0.49 |
| 8:AH:101:PRO:HG2 | 8:AH:133:LEU:HD21 | 1.94 | 0.49 |
| 10:AJ:39:PRO:HA | 10:AJ:70:ARG:HD3 | 1.94 | 0.49 |
| 13:AM:23:TYR:C | 13:AM:23:TYR:CD1 | 2.86 | 0.49 |
| 13:AM:83:ASP:OD2 | 13:AM:84:ILE:N | 2.46 | 0.49 |
| 26:B0:27:GLU:HG3 | 26:B0:69:PHE:CD1 | 2.37 | 0.49 |
| 32:B6:35:GLU:HB3 | 32:B6:51:GLU:HB2 | 1.94 | 0.49 |
| 36:BA:1166:C:H2' | 36:BA:1167:U:C6 | 2.48 | 0.49 |
| 36:BA:528:A:C2 | 36:BA:2042:A:H2' | 2.48 | 0.49 |
| 36:BA:2159:G:H2' | 36:BA:2160:G:C4' | 2.42 | 0.49 |
| 36:BA:271(J):C:H2' | 36:BA:271(K):U:H5'' | 1.94 | 0.49 |
| 36:BA:882:G:N2 | 36:BA:894:C:H42 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BC:10:LEU:HD12 | 38:BC:32:LEU:CA | 2.21 | 0.49 |
| 38:BC:217:THR:HG22 | 38:BC:218:MET:N | 2.27 | 0.49 |
| 38:BC:4:GLY:O | 38:BC:8:ARG:HG3 | 2.12 | 0.49 |
| 39:BD:181:GLU:HA | 39:BD:272:ALA:O | 2.13 | 0.49 |
| 40:BE:132:HIS:CD2 | 40:BE:135:HIS:CE1 | 3.00 | 0.49 |
| 42:BG:131:TYR:HB3 | 42:BG:159:VAL:CG1 | 2.42 | 0.49 |
| 47:BO:43:VAL:HG23 | 47:BO:56:ASP:O | 2.13 | 0.49 |
| 36:BA:2684:U:O4' | 47:BO:70:LYS:HD2 | 2.13 | 0.49 |
| 52:BT:30:VAL:HG21 | 52:BT:84:GLN:HG3 | 1.94 | 0.49 |
| 55:BW:29:LEU:CD2 | 55:BW:33:ARG:HH11 | 2.26 | 0.49 |
| 58:BZ:109:ALA:HB3 | 58:BZ:144:LEU:O | 2.12 | 0.49 |
| 58:BZ:72:ARG:NH2 | 58:BZ:97:GLU:O | 2.45 | 0.49 |
| 1:AA:1240:U:OP1 | 7:AG:116:ALA:HB2 | 2.12 | 0.49 |
| 1:AA:294:U:H2' | 1:AA:295:C:H6 | 1.77 | 0.49 |
| 1:AA:379:C:C2' | 1:AA:380:G:H5' | 2.43 | 0.49 |
| 1:AA:975:A:H8 | 1:AA:975:A:H5' | 1.77 | 0.49 |
| 2:AB:189:ASP:O | 2:AB:191:ASP:N | 2.46 | 0.49 |
| 2:AB:212:GLN:NE2 | 2:AB:216:SER:HB2 | 2.26 | 0.49 |
| 5:AE:80:ILE:HD11 | 5:AE:138:ALA:CA | 2.42 | 0.49 |
| 7:AG:88:PRO:O | 7:AG:89:MET:HB3 | 2.13 | 0.49 |
| 8:AH:9:MET:HG3 | 8:AH:26:VAL:HG11 | 1.95 | 0.49 |
| 9:AI:29:ASN:OD1 | 9:AI:65:VAL:N | 2.46 | 0.49 |
| 9:AI:50:LEU:HG | 9:AI:81:ILE:HG21 | 1.95 | 0.49 |
| 11:AK:34:ASP:OD2 | 11:AK:34:ASP:C | 2.51 | 0.49 |
| 13:AM:65:LYS:HE2 | 13:AM:73:GLU:HG3 | 1.95 | 0.49 |
| 15:AO:74:ASP:OD2 | 15:AO:76:GLU:HB3 | 2.13 | 0.49 |
| 20:AT:89:ARG:NH2 | 20:AT:104:LEU:CD2 | 2.75 | 0.49 |
| 20:AT:89:ARG:HD2 | 20:AT:104:LEU:HD21 | 1.95 | 0.49 |
| 25:AZ:258:LEU:CD2 | 25:AZ:349:VAL:HG11 | 2.43 | 0.49 |
| 25:AZ:359:VAL:O | 25:AZ:361:MET:N | 2.46 | 0.49 |
| 36:BA:1578:U:H2' | 36:BA:1579:A:H5'' | 1.95 | 0.49 |
| 36:BA:1757:U:O4 | 36:BA:1762:A:C2 | 2.65 | 0.49 |
| 36:BA:2092:U:H4' | 36:BA:2093:G:H5'' | 1.95 | 0.49 |
| 36:BA:2130:U:OP2 | 38:BC:5:LYS:HG2 | 2.12 | 0.49 |
| 36:BA:258:G:O2' | 36:BA:259:G:H5' | 2.13 | 0.49 |
| 36:BA:580:C:H2' | 36:BA:581:C:C6 | 2.48 | 0.49 |
| 36:BA:937:U:C2 | 36:BA:938:G:C8 | 3.00 | 0.49 |
| 36:BA:1827:C:OP2 | 39:BD:222:ARG:HD2 | 2.12 | 0.49 |
| 39:BD:35:LYS:CD | 39:BD:36:PRO:N | 2.69 | 0.49 |
| 40:BE:132:HIS:CD2 | 40:BE:135:HIS:HE2 | 2.30 | 0.49 |
| 40:BE:169:ASN:C | 40:BE:169:ASN:HD22 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BE:167:VAL:HG11 | 40:BE:187:ALA:O | 2.11 | 0.49 |
| 40:BE:22:PRO:O | 40:BE:185:LYS:O | 2.31 | 0.49 |
| 41:BF:135:LYS:HB3 | 41:BF:138:GLU:CG | 2.37 | 0.49 |
| 42:BG:100:TRP:O | 42:BG:104:GLU:N | 2.45 | 0.49 |
| 43:BH:86:GLU:O | 43:BH:87:LEU:HD23 | 2.13 | 0.49 |
| 46:BN:61:ARG:HH11 | 46:BN:61:ARG:HG3 | 1.76 | 0.49 |
| 46:BN:78:TYR:N | 46:BN:78:TYR:HD1 | 2.10 | 0.49 |
| 47:BO:19:ILE:HB | 47:BO:41:ALA:HB1 | 1.95 | 0.49 |
| 50:BR:10:LEU:HA | 50:BR:17:ARG:HD3 | 1.94 | 0.49 |
| 50:BR:29:LEU:HD22 | 50:BR:70:LEU:HD11 | 1.95 | 0.49 |
| 51:BS:98:VAL:O | 51:BS:99:LYS:HB2 | 2.12 | 0.49 |
| 54:BV:15:GLU:O | 54:BV:96:ILE:HB | 2.13 | 0.49 |
| 57:BY:80:GLY:O | 57:BY:81:LYS:O | 2.31 | 0.49 |
| 1:AA:1047:G:C2' | 1:AA:1048:G:H5' | 2.43 | 0.49 |
| 1:AA:1217:C:OP1 | 14:AN:9:LYS:HE3 | 2.13 | 0.49 |
| 1:AA:1286:A:O2' | 1:AA:1287:A:OP2 | 2.29 | 0.49 |
| 1:AA:173:U:C5' | 1:AA:197:A:O4' | 2.55 | 0.49 |
| 1:AA:245:C:O2 | 1:AA:283:C:N3 | 2.46 | 0.49 |
| 1:AA:738:C:H2' | 1:AA:739:C:H6 | 1.78 | 0.49 |
| 1:AA:966:G:O2' | 1:AA:967:C:C5' | 2.61 | 0.49 |
| 4:AD:88:VAL:O | 4:AD:92:VAL:HG23 | 2.13 | 0.49 |
| 4:AD:91:SER:O | 4:AD:92:VAL:C | 2.51 | 0.49 |
| 5:AE:64:ARG:CZ | 5:AE:64:ARG:HB2 | 2.43 | 0.49 |
| 22:AW:48:C:H2' | 22:AW:59:U:H1' | 1.94 | 0.49 |
| 25:AZ:249:VAL:HG22 | 25:AZ:269:GLY:HA2 | 1.94 | 0.49 |
| 28:B2:32:LEU:HD23 | 28:B2:32:LEU:C | 2.34 | 0.49 |
| 36:BA:1131:G:C2 | 36:BA:1132:A:C5 | 3.00 | 0.49 |
| 36:BA:1376:C:O2' | 36:BA:1377:G:H5' | 2.12 | 0.49 |
| 36:BA:1642:G:O2' | 36:BA:1643:G:H5' | 2.13 | 0.49 |
| 36:BA:2366:A:H2' | 36:BA:2367:G:O4' | 2.12 | 0.49 |
| 36:BA:2653:U:H5'' | 36:BA:2654:A:H2' | 1.94 | 0.49 |
| 36:BA:271(A):A:H5' | 36:BA:271(B):C:OP2 | 2.13 | 0.49 |
| 36:BA:370:G:H4' | 36:BA:371:A:OP2 | 2.13 | 0.49 |
| 36:BA:631:A:H2' | 36:BA:632:A:O4' | 2.13 | 0.49 |
| 39:BD:10:THR:HG23 | 39:BD:13:ARG:HB2 | 1.94 | 0.49 |
| 40:BE:13:ARG:O | 52:BT:57:PHE:CE1 | 2.66 | 0.49 |
| 36:BA:2679:A:H4' | 40:BE:165:VAL:HG11 | 1.95 | 0.49 |
| 42:BG:128:ARG:O | 42:BG:129:GLY:O | 2.31 | 0.49 |
| 42:BG:139:LEU:HA | 42:BG:144:ILE:HD13 | 1.94 | 0.49 |
| 43:BH:137:ASP:OD2 | 43:BH:140:LYS:HE3 | 2.13 | 0.49 |
| 49:BQ:141:GLN:OE1 | 58:BZ:72:ARG:HD3 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:BR:7:GLY:O | 50:BR:8:ARG:CZ | 2.61 | 0.49 |
| 52:BT:129:ARG:HG3 | 52:BT:129:ARG:HH11 | 1.78 | 0.49 |
| 53:BU:82:GLY:O | 53:BU:85:LYS:N | 2.46 | 0.49 |
| 57:BY:84:ARG:HG2 | 57:BY:85:VAL:H | 1.78 | 0.49 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:H8 | 1.75 | 0.48 |
| 1:AA:1478:C:H2' | 1:AA:1479:C:H6 | 1.78 | 0.48 |
| 1:AA:433:C:H2' | 1:AA:434:U:C6 | 2.48 | 0.48 |
| 1:AA:567:G:H2' | 1:AA:568:G:O4' | 2.13 | 0.48 |
| 1:AA:78:G:H2' | 1:AA:79:G:H4' | 1.95 | 0.48 |
| 2:AB:42:ILE:CD1 | 2:AB:202:PRO:C | 2.81 | 0.48 |
| 3:AC:70:VAL:HG12 | 3:AC:71:ALA:N | 2.28 | 0.48 |
| 12:AL:5:PRO:CG | 12:AL:10:LEU:HD21 | 2.42 | 0.48 |
| 13:AM:82:MET:CG | 13:AM:82:MET:O | 2.60 | 0.48 |
| 17:AQ:55:ASP:O | 17:AQ:57:VAL:HG13 | 2.13 | 0.48 |
| 18:AR:45:SER:N | 18:AR:51:LEU:HG | 2.21 | 0.48 |
| 20:AT:100:ILE:O | 20:AT:102:GLY:N | 2.43 | 0.48 |
| 20:AT:57:ARG:HH11 | 20:AT:57:ARG:HB2 | 1.77 | 0.48 |
| 25:AZ:130:TYR:CG | 25:AZ:211:PRO:HD3 | 2.48 | 0.48 |
| 25:AZ:89:ILE:HD13 | 25:AZ:389:ARG:NH1 | 2.28 | 0.48 |
| 30:B4:12:ALA:CB | 30:B4:29:PRO:HA | 2.42 | 0.48 |
| 32:B6:32:ASN:O | 32:B6:33:LYS:HB2 | 2.13 | 0.48 |
| 36:BA:1087:G:H2' | 36:BA:1088:A:H4' | 1.95 | 0.48 |
| 36:BA:1417:C:H2' | 36:BA:1418:G:O4' | 2.12 | 0.48 |
| 36:BA:2320:A:C2 | 36:BA:2333:A:C8 | 3.01 | 0.48 |
| 36:BA:271(H):G:N2 | 36:BA:271(I):G:H1' | 2.28 | 0.48 |
| 36:BA:2820:A:O3' | 50:BR:5:LYS:HE2 | 2.13 | 0.48 |
| 36:BA:27:G:O2' | 36:BA:28:A:OP2 | 2.30 | 0.48 |
| 36:BA:331:A:H1' | 36:BA:332:A:OP1 | 2.13 | 0.48 |
| 36:BA:68:G:H2' | 36:BA:69:C:C6 | 2.47 | 0.48 |
| 36:BA:708:C:N4 | 36:BA:723:G:H1 | 2.04 | 0.48 |
| 37:BB:87:G:H3' | 37:BB:88:C:C5' | 2.40 | 0.48 |
| 22:AW:56:C:H5'' | 38:BC:137:LEU:HG | 1.95 | 0.48 |
| 39:BD:117:VAL:HG21 | 39:BD:128:GLY:HA3 | 1.94 | 0.48 |
| 39:BD:25:THR:CG2 | 39:BD:26:LYS:HD2 | 2.41 | 0.48 |
| 39:BD:57:GLY:HA2 | 39:BD:214:TRP:O | 2.13 | 0.48 |
| 40:BE:116:VAL:CG2 | 40:BE:122:PHE:CD2 | 2.96 | 0.48 |
| 41:BF:135:LYS:CB | 41:BF:138:GLU:HG3 | 2.36 | 0.48 |
| 41:BF:148:LEU:C | 41:BF:150:GLY:H | 2.16 | 0.48 |
| 47:BO:1:MET:HE2 | 47:BO:32:TYR:CD2 | 2.48 | 0.48 |
| 49:BQ:63:LYS:HD3 | 49:BQ:65:PHE:CZ | 2.48 | 0.48 |
| 50:BR:87:TYR:O | 50:BR:89:ASP:N | 2.41 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:BT:109:GLU:OE2 | 52:BT:112:ARG:NH2 | 2.45 | 0.48 |
| 56:BX:51:VAL:HG11 | 56:BX:54:VAL:CG2 | 2.42 | 0.48 |
| 56:BX:50:LYS:HG2 | 56:BX:84:ALA:HB2 | 1.94 | 0.48 |
| 57:BY:2:ARG:HD3 | 57:BY:3:VAL:HG23 | 1.95 | 0.48 |
| 58:BZ:35:ARG:NE | 58:BZ:35:ARG:CA | 2.75 | 0.48 |
| 1:AA:102:G:C4 | 1:AA:103:C:C6 | 3.01 | 0.48 |
| 1:AA:114:U:H2' | 1:AA:115:G:C8 | 2.48 | 0.48 |
| 1:AA:145:G:H2' | 1:AA:146:G:O4' | 2.13 | 0.48 |
| 1:AA:501:C:H2' | 1:AA:502:G:C8 | 2.48 | 0.48 |
| 3:AC:103:VAL:HG12 | 3:AC:103:VAL:O | 2.13 | 0.48 |
| 5:AE:82:VAL:HG12 | 5:AE:83:GLU:N | 2.27 | 0.48 |
| 6:AF:40:VAL:HG13 | 6:AF:40:VAL:O | 2.13 | 0.48 |
| 7:AG:65:ALA:HB3 | 7:AG:124:LEU:HD23 | 1.95 | 0.48 |
| 10:AJ:35:SER:O | 10:AJ:36:GLY:O | 2.31 | 0.48 |
| 13:AM:14:ARG:H | 13:AM:44:ARG:NH1 | 2.08 | 0.48 |
| 21:AU:3:LYS:HD3 | 21:AU:14:TRP:CD1 | 2.47 | 0.48 |
| 25:AZ:113:MET:HB3 | 25:AZ:114:PRO:CD | 2.43 | 0.48 |
| 25:AZ:176:LEU:O | 25:AZ:180:GLU:HG3 | 2.13 | 0.48 |
| 36:BA:1435:G:H2' | 36:BA:1436:G:O4' | 2.12 | 0.48 |
| 36:BA:2689:U:H4' | 36:BA:2690:C:C6 | 2.48 | 0.48 |
| 36:BA:2758:A:HO2' | 36:BA:2759:G:H8 | 1.61 | 0.48 |
| 36:BA:2861:G:O2' | 36:BA:2862:G:H5' | 2.13 | 0.48 |
| 36:BA:594:U:H3 | 36:BA:663:G:H1 | 1.61 | 0.48 |
| 36:BA:904:C:H2' | 36:BA:905:U:C6 | 2.47 | 0.48 |
| 37:BB:66:A:N6 | 37:BB:108:U:C6 | 2.82 | 0.48 |
| 38:BC:47:LEU:HD12 | 38:BC:47:LEU:N | 2.28 | 0.48 |
| 38:BC:75:LEU:HD12 | 38:BC:76:ALA:N | 2.28 | 0.48 |
| 39:BD:230:ASP:O | 39:BD:231:HIS:HB2 | 2.12 | 0.48 |
| 36:BA:1824:G:OP1 | 39:BD:52:ARG:NH1 | 2.46 | 0.48 |
| 39:BD:97:TYR:HE1 | 39:BD:103:ARG:HD3 | 1.76 | 0.48 |
| 41:BF:60:SER:OG | 41:BF:61:GLY:N | 2.46 | 0.48 |
| 42:BG:16:ARG:NE | 42:BG:31:VAL:HG11 | 2.28 | 0.48 |
| 43:BH:85:LYS:NZ | 43:BH:132:ARG:HA | 2.28 | 0.48 |
| 52:BT:38:ASN:O | 52:BT:40:THR:N | 2.43 | 0.48 |
| 52:BT:41:ARG:HG2 | 52:BT:41:ARG:HH11 | 1.78 | 0.48 |
| 53:BU:25:TRP:CD1 | 53:BU:26:GLY:N | 2.81 | 0.48 |
| 55:BW:64:MET:O | 55:BW:65:LEU:O | 2.31 | 0.48 |
| 56:BX:63:LYS:HE2 | 56:BX:72:LYS:HG2 | 1.94 | 0.48 |
| 56:BX:88:LYS:HB2 | 56:BX:93:GLU:OE2 | 2.13 | 0.48 |
| 58:BZ:17:ALA:HA | 58:BZ:20:ARG:CD | 2.43 | 0.48 |
| 1:AA:674:G:O2' | 1:AA:675:A:H5' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:729:A:H2' | 1:AA:730:G:O4' | 2.14 | 0.48 |
| 1:AA:952:U:H2' | 1:AA:953:G:C8 | 2.49 | 0.48 |
| 2:AB:75:LYS:HD3 | 2:AB:75:LYS:O | 2.13 | 0.48 |
| 2:AB:88:ALA:HB2 | 2:AB:219:VAL:HG13 | 1.95 | 0.48 |
| 4:AD:64:LEU:O | 4:AD:67:ILE:HB | 2.14 | 0.48 |
| 13:AM:22:ILE:CG2 | 13:AM:66:LEU:HD23 | 2.39 | 0.48 |
| 14:AN:29:ARG:NH1 | 14:AN:29:ARG:CG | 2.75 | 0.48 |
| 22:AV:61:C:O2 | 22:AV:61:C:H2' | 2.12 | 0.48 |
| 25:AZ:102:ALA:HB2 | 25:AZ:128:VAL:HG11 | 1.94 | 0.48 |
| 25:AZ:272:MET:HB2 | 25:AZ:277:LEU:HD23 | 1.95 | 0.48 |
| 26:B0:40:GLN:NE2 | 26:B0:43:THR:HA | 2.28 | 0.48 |
| 29:B3:28:LEU:CD2 | 29:B3:28:LEU:N | 2.69 | 0.48 |
| 29:B3:3:ARG:HB2 | 29:B3:59:VAL:O | 2.12 | 0.48 |
| 36:BA:1332:G:H5' | 36:BA:1333:C:H5 | 1.78 | 0.48 |
| 36:BA:1378:A:O2' | 36:BA:1379:A:C5' | 2.54 | 0.48 |
| 36:BA:1536:C:H2' | 36:BA:1537:G:H4' | 1.95 | 0.48 |
| 36:BA:2866:U:O2 | 36:BA:2866:U:H2' | 2.13 | 0.48 |
| 36:BA:329:G:N7 | 57:BY:71:LYS:HE3 | 2.28 | 0.48 |
| 36:BA:61:G:H8 | 36:BA:61:G:O5' | 1.96 | 0.48 |
| 38:BC:215:THR:HB | 38:BC:221:SER:N | 2.28 | 0.48 |
| 42:BG:91:ARG:HG3 | 42:BG:91:ARG:HH11 | 1.78 | 0.48 |
| 43:BH:85:LYS:O | 43:BH:132:ARG:HB2 | 2.13 | 0.48 |
| 50:BR:48:VAL:O | 50:BR:51:LEU:HB2 | 2.13 | 0.48 |
| 51:BS:35:ILE:CD1 | 51:BS:99:LYS:HE3 | 2.43 | 0.48 |
| 52:BT:55:ASN:H | 52:BT:59:THR:CG2 | 2.09 | 0.48 |
| 53:BU:21:ALA:HB1 | 53:BU:24:TYR:HD1 | 1.75 | 0.48 |
| 36:BA:535:C:O3' | 53:BU:53:ARG:NH1 | 2.47 | 0.48 |
| 53:BU:57:PHE:CD2 | 53:BU:60:LEU:HD12 | 2.49 | 0.48 |
| 53:BU:92:ARG:HH22 | 54:BV:10:LYS:HG2 | 1.77 | 0.48 |
| 57:BY:64:GLU:O | 57:BY:65:ALA:CB | 2.61 | 0.48 |
| 57:BY:75:ILE:HG13 | 57:BY:76:CYS:N | 2.28 | 0.48 |
| 57:BY:95:LYS:HG3 | 57:BY:101:LYS:H | 1.77 | 0.48 |
| 1:AA:1108:G:H5' | 3:AC:176:HIS:CD2 | 2.48 | 0.48 |
| 1:AA:1306:A:H61 | 1:AA:1331:G:H1' | 1.77 | 0.48 |
| 1:AA:189(C):C:H2' | 1:AA:189(D):C:O4' | 2.13 | 0.48 |
| 1:AA:376:G:O2' | 1:AA:377:G:H5' | 2.13 | 0.48 |
| 1:AA:429:U:H4' | 1:AA:430:A:O5' | 2.13 | 0.48 |
| 1:AA:64:G:H4' | 1:AA:65:U:C5' | 2.44 | 0.48 |
| 3:AC:167:TRP:CD1 | 3:AC:168:ALA:N | 2.81 | 0.48 |
| 3:AC:15:THR:CG2 | 3:AC:181:ASN:HA | 2.43 | 0.48 |
| 4:AD:171:GLY:O | 4:AD:173:TRP:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:199:ASN:OD1 | 4:AD:201:GLN:HB2 | 2.13 | 0.48 |
| 5:AE:75:THR:OG1 | 5:AE:76:ILE:N | 2.45 | 0.48 |
| 8:AH:13:ILE:O | 8:AH:17:THR:HG23 | 2.13 | 0.48 |
| 12:AL:110:VAL:HG23 | 12:AL:120:TYR:HB3 | 1.95 | 0.48 |
| 15:AO:25:THR:O | 15:AO:26:GLU:C | 2.51 | 0.48 |
| 15:AO:4:THR:OG1 | 15:AO:7:GLU:HB2 | 2.14 | 0.48 |
| 17:AQ:17:LYS:HA | 17:AQ:49:GLU:HG2 | 1.95 | 0.48 |
| 20:AT:26:ASN:HB2 | 20:AT:71:THR:CG2 | 2.33 | 0.48 |
| 25:AZ:75:ARG:HD2 | 25:AZ:77:TYR:CZ | 2.48 | 0.48 |
| 32:B6:12:GLU:HA | 32:B6:23:THR:HA | 1.94 | 0.48 |
| 36:BA:1344:G:H4' | 36:BA:1384:A:C5 | 2.48 | 0.48 |
| 36:BA:2187:G:H2' | 36:BA:2188:C:H5' | 1.94 | 0.48 |
| 36:BA:2238:G:H2' | 36:BA:2238:G:N3 | 2.28 | 0.48 |
| 36:BA:2369:A:H2' | 36:BA:2370:G:C8 | 2.48 | 0.48 |
| 36:BA:247:G:H4' | 36:BA:386:G:C5 | 2.48 | 0.48 |
| 36:BA:2543:G:H8 | 36:BA:2543:G:H5' | 1.78 | 0.48 |
| 36:BA:2715:C:O2' | 36:BA:2716:U:H5' | 2.13 | 0.48 |
| 36:BA:2740:A:H2' | 36:BA:2741:A:C8 | 2.48 | 0.48 |
| 31:B5:13:LYS:NZ | 36:BA:517:C:OP2 | 2.36 | 0.48 |
| 36:BA:528:A:OP2 | 46:BN:114:ARG:NH1 | 2.43 | 0.48 |
| 36:BA:628:G:C2' | 36:BA:629:G:C5' | 2.86 | 0.48 |
| 36:BA:914:C:C2' | 36:BA:915:C:H5' | 2.33 | 0.48 |
| 39:BD:165:ILE:HG23 | 39:BD:173:VAL:HG21 | 1.94 | 0.48 |
| 45:BK:55:UNK:CB | 45:BK:69:UNK:HA | 2.43 | 0.48 |
| 46:BN:27:ALA:HB1 | 46:BN:103:VAL:HG22 | 1.94 | 0.48 |
| 48:BP:92:GLU:HA | 48:BP:123:LEU:HD13 | 1.93 | 0.48 |
| 52:BT:28:VAL:HB | 52:BT:88:ILE:HG12 | 1.95 | 0.48 |
| 54:BV:47:VAL:C | 54:BV:49:THR:H | 2.16 | 0.48 |
| 56:BX:18:TYR:C | 56:BX:20:GLY:H | 2.16 | 0.48 |
| 57:BY:31:LEU:HD23 | 57:BY:36:ALA:H | 1.79 | 0.48 |
| 58:BZ:6:LYS:N | 58:BZ:6:LYS:CD | 2.77 | 0.48 |
| 1:AA:108:G:H5' | 1:AA:109:A:H5'' | 1.93 | 0.48 |
| 1:AA:1053:G:O6 | 1:AA:1199:U:H2' | 2.14 | 0.48 |
| 2:AB:108:ILE:C | 2:AB:110:GLN:H | 2.17 | 0.48 |
| 2:AB:8:LYS:HE2 | 2:AB:217:ARG:NH1 | 2.27 | 0.48 |
| 3:AC:154:SER:H | 3:AC:157:ILE:HD11 | 1.79 | 0.48 |
| 4:AD:147:ALA:HB2 | 4:AD:182:LYS:HA | 1.94 | 0.48 |
| 5:AE:31:LEU:HD23 | 5:AE:45:PHE:CD1 | 2.41 | 0.48 |
| 12:AL:33:ARG:NE | 12:AL:62:SER:HB3 | 2.29 | 0.48 |
| 13:AM:32:GLU:O | 13:AM:35:GLU:HG2 | 2.13 | 0.48 |
| 14:AN:19:ARG:O | 14:AN:20:ALA:HB3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:AO:62:GLN:NE2 | 15:AO:62:GLN:HA | 2.27 | 0.48 |
| 12:AL:7:ILE:HG21 | 17:AQ:34:LYS:HB2 | 1.96 | 0.48 |
| 22:AV:18:G:H4' | 22:AV:60:U:O2 | 2.14 | 0.48 |
| 25:AZ:46:ASP:O | 25:AZ:50:ILE:HG12 | 2.13 | 0.48 |
| 32:B6:13:CYS:HA | 32:B6:50:ARG:O | 2.13 | 0.48 |
| 36:BA:1517:G:H5' | 36:BA:1517:G:H8 | 1.78 | 0.48 |
| 36:BA:1567:A:C5' | 39:BD:58:HIS:CD2 | 2.97 | 0.48 |
| 36:BA:1598:C:C5' | 56:BX:36:LYS:HD2 | 2.43 | 0.48 |
| 36:BA:2295:C:O2' | 36:BA:2296:U:H5' | 2.14 | 0.48 |
| 36:BA:301:G:H1' | 36:BA:302:C:C6 | 2.49 | 0.48 |
| 36:BA:497:A:H2' | 36:BA:498:G:H8 | 1.79 | 0.48 |
| 36:BA:523:C:C2' | 36:BA:524:U:H5' | 2.44 | 0.48 |
| 36:BA:534:U:H5' | 53:BU:42:ALA:CB | 2.43 | 0.48 |
| 36:BA:970:C:H2' | 36:BA:971:C:C6 | 2.48 | 0.48 |
| 38:BC:77:ILE:HB | 38:BC:115:ALA:HA | 1.95 | 0.48 |
| 38:BC:37:PHE:CZ | 38:BC:39:GLU:HG3 | 2.49 | 0.48 |
| 39:BD:129:ASN:O | 39:BD:193:VAL:HG12 | 2.13 | 0.48 |
| 39:BD:35:LYS:HG3 | 39:BD:63:ARG:CG | 2.43 | 0.48 |
| 40:BE:3:GLY:O | 40:BE:4:ILE:CB | 2.61 | 0.48 |
| 42:BG:41:GLN:C | 42:BG:43:LEU:H | 2.16 | 0.48 |
| 47:BO:32:TYR:CD1 | 47:BO:32:TYR:N | 2.81 | 0.48 |
| 47:BO:68:GLU:OE2 | 47:BO:78:ARG:HD3 | 2.13 | 0.48 |
| 36:BA:2413:G:H21 | 48:BP:70:GLN:NE2 | 2.06 | 0.48 |
| 53:BU:92:ARG:O | 53:BU:94:ASN:N | 2.46 | 0.48 |
| 57:BY:95:LYS:HE3 | 57:BY:100:ALA:HA | 1.94 | 0.48 |
| 57:BY:2:ARG:C | 57:BY:4:LYS:N | 2.67 | 0.48 |
| 57:BY:17:SER:HA | 57:BY:71:LYS:HD2 | 1.95 | 0.48 |
| 58:BZ:7:ALA:HB3 | 58:BZ:61:LEU:HD23 | 1.96 | 0.48 |
| 1:AA:348:G:H2' | 1:AA:349:A:H5' | 1.96 | 0.48 |
| 1:AA:633:G:H5' | 1:AA:634:C:OP2 | 2.13 | 0.48 |
| 1:AA:84:U:O2' | 1:AA:88:A:H5' | 2.14 | 0.48 |
| 1:AA:858:G:C6 | 1:AA:869:G:C8 | 3.01 | 0.48 |
| 2:AB:8:LYS:C | 2:AB:10:LEU:N | 2.64 | 0.48 |
| 3:AC:16:ARG:NH1 | 3:AC:16:ARG:HB2 | 2.29 | 0.48 |
| 3:AC:60:ALA:CB | 3:AC:63:ASN:HD21 | 2.25 | 0.48 |
| 7:AG:85:TYR:CD1 | 7:AG:154:TYR:CE1 | 3.02 | 0.48 |
| 10:AJ:8:LEU:HD22 | 10:AJ:20:ALA:HB2 | 1.95 | 0.48 |
| 12:AL:41:ARG:HH22 | 12:AL:57:LYS:CE | 2.26 | 0.48 |
| 15:AO:70:LEU:O | 15:AO:72:ARG:N | 2.46 | 0.48 |
| 16:AP:19:ILE:HG22 | 16:AP:36:ILE:HG13 | 1.95 | 0.48 |
| 20:AT:99:LEU:HB3 | 20:AT:100:ILE:HD12 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AV:5:G:O2' | 22:AV:6:G:H5' | 2.13 | 0.48 |
| 25:AZ:222:LEU:CD1 | 25:AZ:303:VAL:HG11 | 2.44 | 0.48 |
| 33:B7:47:ARG:HG3 | 33:B7:48:LYS:N | 2.28 | 0.48 |
| 36:BA:1224:C:C5 | 36:BA:1225:G:C6 | 3.01 | 0.48 |
| 36:BA:139(A):G:H22 | 56:BX:44:GLU:CD | 2.17 | 0.48 |
| 36:BA:1682:G:H5' | 36:BA:1762:A:O2' | 2.14 | 0.48 |
| 36:BA:2234:G:O2' | 36:BA:2235:G:H5' | 2.13 | 0.48 |
| 36:BA:2580:U:H5' | 40:BE:131:ALA:CB | 2.43 | 0.48 |
| 36:BA:2580:U:P | 40:BE:131:ALA:HB2 | 2.53 | 0.48 |
| 36:BA:521:G:O2' | 36:BA:522:G:H5' | 2.13 | 0.48 |
| 38:BC:42:GLU:N | 38:BC:215:THR:O | 2.35 | 0.48 |
| 38:BC:22:ILE:HD13 | 38:BC:190:ARG:HG2 | 1.95 | 0.48 |
| 39:BD:26:LYS:HA | 39:BD:26:LYS:HZ3 | 1.79 | 0.48 |
| 48:BP:147:LEU:O | 48:BP:148:LEU:HB2 | 2.14 | 0.48 |
| 49:BQ:79:LEU:O | 49:BQ:80:GLU:HB2 | 2.14 | 0.48 |
| 50:BR:14:SER:HA | 50:BR:17:ARG:NH2 | 2.29 | 0.48 |
| 50:BR:45:ARG:O | 50:BR:48:VAL:HG12 | 2.13 | 0.48 |
| 36:BA:2880:C:O3' | 50:BR:90:ARG:NH1 | 2.47 | 0.48 |
| 51:BS:34:HIS:HB3 | 51:BS:53:SER:HB3 | 1.95 | 0.48 |
| 1:AA:1442(A):G:C8 | 52:BT:118:ARG:NH2 | 2.82 | 0.48 |
| 52:BT:28:VAL:O | 52:BT:29:ARG:CB | 2.60 | 0.48 |
| 53:BU:92:ARG:CB | 54:BV:11:GLN:NE2 | 2.76 | 0.48 |
| 55:BW:70:TYR:CZ | 55:BW:72:LYS:HG2 | 2.49 | 0.48 |
| 58:BZ:127:LYS:HD2 | 58:BZ:162:GLU:OE2 | 2.13 | 0.48 |
| 1:AA:1122:U:O2' | 1:AA:1123:A:H5' | 2.13 | 0.48 |
| 1:AA:1166:G:H22 | 1:AA:1169:A:H3' | 1.79 | 0.48 |
| 1:AA:1423:G:H2' | 1:AA:1424:C:H6 | 1.79 | 0.48 |
| 1:AA:123:C:OP1 | 1:AA:312:C:H5' | 2.14 | 0.48 |
| 1:AA:415:A:H2' | 1:AA:416:G:C8 | 2.48 | 0.48 |
| 1:AA:495:A:H61 | 4:AD:119:GLN:NE2 | 2.12 | 0.48 |
| 1:AA:975:A:H4' | 1:AA:976:G:C5' | 2.37 | 0.48 |
| 2:AB:160:ASP:O | 2:AB:183:PRO:HD2 | 2.13 | 0.48 |
| 2:AB:59:GLU:CB | 2:AB:221:LEU:HD11 | 2.43 | 0.48 |
| 3:AC:173:VAL:HG12 | 3:AC:175:LEU:CD1 | 2.43 | 0.48 |
| 4:AD:129:ASN:HD21 | 4:AD:145:GLU:N | 2.01 | 0.48 |
| 4:AD:31:CYS:O | 4:AD:32:ALA:HB3 | 2.13 | 0.48 |
| 6:AF:76:ALA:O | 6:AF:80:ARG:HG3 | 2.14 | 0.48 |
| 7:AG:54:THR:HG23 | 7:AG:54:THR:O | 2.13 | 0.48 |
| 16:AP:75:ARG:HG3 | 16:AP:75:ARG:HH11 | 1.79 | 0.48 |
| 20:AT:81:LYS:C | 20:AT:83:ARG:H | 2.16 | 0.48 |
| 22:AW:29:G:H1 | 22:AW:41:C:N4 | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:AZ:129:PRO:O | 25:AZ:130:TYR:CB | 2.62 | 0.48 |
| 30:B4:35:VAL:HG12 | 30:B4:36:CYS:N | 2.29 | 0.48 |
| 36:BA:1141:U:C5' | 36:BA:1142(A):A:O4' | 2.61 | 0.48 |
| 36:BA:1215:G:O2' | 36:BA:1216:G:H5' | 2.14 | 0.48 |
| 27:B1:41:ARG:NH2 | 36:BA:1365:A:OP1 | 2.34 | 0.48 |
| 36:BA:1670:C:H2' | 36:BA:1671:U:O4' | 2.13 | 0.48 |
| 36:BA:1809:A:H2' | 36:BA:1810:A:C8 | 2.48 | 0.48 |
| 36:BA:1809:A:C6 | 36:BA:1810:A:C6 | 3.01 | 0.48 |
| 36:BA:1885:A:H8 | 36:BA:1885:A:H5' | 1.78 | 0.48 |
| 36:BA:198:C:O5' | 36:BA:198:C:H6 | 1.97 | 0.48 |
| 36:BA:2009:G:O2' | 36:BA:2010:G:H5' | 2.13 | 0.48 |
| 36:BA:2360:A:O2' | 36:BA:2361:A:P | 2.72 | 0.48 |
| 36:BA:2658:C:N4 | 36:BA:2664:G:N2 | 2.62 | 0.48 |
| 31:B5:52:TYR:HH | 36:BA:2884:U:H1' | 1.79 | 0.48 |
| 36:BA:606:U:H2' | 36:BA:607:U:O4' | 2.14 | 0.48 |
| 36:BA:623:G:H2' | 36:BA:624:C:H6 | 1.78 | 0.48 |
| 36:BA:654(L):G:H3' | 36:BA:654(L):G:N3 | 2.28 | 0.48 |
| 36:BA:605:C:H1' | 36:BA:657:U:O2' | 2.14 | 0.48 |
| 36:BA:833:U:H2' | 36:BA:834:C:C6 | 2.48 | 0.48 |
| 39:BD:21:PHE:HB3 | 39:BD:24:ILE:HG21 | 1.96 | 0.48 |
| 39:BD:35:LYS:HZ2 | 39:BD:36:PRO:CD | 2.27 | 0.48 |
| 40:BE:150:VAL:HG13 | 40:BE:154:LYS:HD3 | 1.95 | 0.48 |
| 42:BG:111:LEU:CB | 42:BG:112:PRO:HD3 | 2.43 | 0.48 |
| 42:BG:31:VAL:O | 42:BG:31:VAL:HG13 | 2.13 | 0.48 |
| 46:BN:10:GLU:HG3 | 46:BN:11:PRO:HD2 | 1.95 | 0.48 |
| 46:BN:72:TYR:CE1 | 46:BN:87:LEU:HD23 | 2.48 | 0.48 |
| 48:BP:93:GLY:O | 48:BP:123:LEU:HD12 | 2.13 | 0.48 |
| 49:BQ:14:ARG:HG2 | 49:BQ:14:ARG:HH11 | 1.79 | 0.48 |
| 50:BR:78:LYS:O | 50:BR:83:ILE:HG12 | 2.13 | 0.48 |
| 58:BZ:11:GLU:OE2 | 58:BZ:13:GLU:HG3 | 2.14 | 0.48 |
| 58:BZ:9:TYR:CE2 | 58:BZ:61:LEU:HD13 | 2.48 | 0.48 |
| 1:AA:1217:C:O2' | 1:AA:1218:C:H5' | 2.14 | 0.48 |
| 1:AA:266:G:H5' | 1:AA:267:C:C5 | 2.48 | 0.48 |
| 1:AA:591:U:H2' | 1:AA:592:G:C8 | 2.49 | 0.48 |
| 2:AB:15:VAL:O | 2:AB:15:VAL:HG23 | 2.14 | 0.48 |
| 3:AC:15:THR:HG21 | 3:AC:181:ASN:HA | 1.95 | 0.48 |
| 3:AC:58:GLU:C | 3:AC:59:ARG:HG2 | 2.34 | 0.48 |
| 13:AM:97:PRO:N | 13:AM:110:ARG:HD3 | 2.28 | 0.48 |
| 13:AM:63:THR:HG22 | 13:AM:64:TRP:N | 2.28 | 0.48 |
| 22:AV:69:G:C8 | 22:AV:69:G:H5' | 2.41 | 0.48 |
| 25:AZ:104:LEU:N | 25:AZ:132:VAL:O | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:272:MET:O | 25:AZ:273:HIS:HB2 | 2.14 | 0.48 |
| 25:AZ:335:PHE:C | 25:AZ:337:GLY:H | 2.16 | 0.48 |
| 27:B1:33:LYS:N | 27:B1:33:LYS:CD | 2.73 | 0.48 |
| 28:B2:34:GLU:O | 28:B2:38:GLN:HG2 | 2.13 | 0.48 |
| 31:B5:49:CYS:O | 31:B5:56:LYS:HB2 | 2.14 | 0.48 |
| 32:B6:11:LEU:HD21 | 32:B6:51:GLU:OE2 | 2.13 | 0.48 |
| 34:B8:4:MET:SD | 34:B8:61:LEU:CD2 | 3.02 | 0.48 |
| 36:BA:1431:U:H2' | 36:BA:1432:C:C6 | 2.49 | 0.48 |
| 36:BA:1858:G:N2 | 36:BA:1883:G:H2' | 2.26 | 0.48 |
| 31:B5:2:ALA:HA | 36:BA:2015:A:O2' | 2.14 | 0.48 |
| 36:BA:2050:C:H2' | 36:BA:2051:A:O4' | 2.14 | 0.48 |
| 36:BA:2289:G:C8 | 36:BA:2289:G:O5' | 2.66 | 0.48 |
| 36:BA:2533:A:C2' | 36:BA:2534:A:H5' | 2.44 | 0.48 |
| 36:BA:539:G:H2' | 36:BA:540:C:H6 | 1.79 | 0.48 |
| 38:BC:43:VAL:CG2 | 38:BC:214:VAL:HG13 | 2.44 | 0.48 |
| 39:BD:24:ILE:HG23 | 39:BD:25:THR:H | 1.79 | 0.48 |
| 40:BE:80:GLU:O | 40:BE:81:ILE:HD13 | 2.14 | 0.48 |
| 41:BF:36:VAL:CG1 | 41:BF:183:VAL:HG21 | 2.43 | 0.48 |
| 41:BF:185:ASP:HA | 41:BF:188:ARG:CD | 2.44 | 0.48 |
| 41:BF:53:THR:HG23 | 41:BF:56:GLU:HG3 | 1.96 | 0.48 |
| 43:BH:83:TYR:HB2 | 43:BH:134:SER:HA | 1.94 | 0.48 |
| 43:BH:53:GLU:C | 43:BH:54:ARG:HG3 | 2.33 | 0.48 |
| 36:BA:1131:G:OP1 | 46:BN:80:GLY:N | 2.47 | 0.48 |
| 41:BF:31:HIS:CE1 | 48:BP:13:ASN:HB2 | 2.49 | 0.48 |
| 48:BP:126:VAL:HG22 | 48:BP:145:PRO:HG2 | 1.95 | 0.48 |
| 49:BQ:12:GLN:OE1 | 49:BQ:72:LYS:HG3 | 2.13 | 0.48 |
| 50:BR:13:HIS:HE1 | 50:BR:15:SER:OG | 1.96 | 0.48 |
| 50:BR:4:LEU:O | 50:BR:5:LYS:HD2 | 2.14 | 0.48 |
| 50:BR:83:ILE:HA | 50:BR:86:ARG:HD3 | 1.95 | 0.48 |
| 36:BA:2845:G:H5" | 52:BT:54:ARG:O | 2.13 | 0.48 |
| 57:BY:77:PRO:O | 57:BY:78:ALA:HB2 | 2.14 | 0.48 |
| 58:BZ:77:ASP:O | 58:BZ:79:ARG:N | 2.46 | 0.48 |
| 1:AA:1250:A:H2' | 1:AA:1251:A:C8 | 2.49 | 0.48 |
| 1:AA:1442(A):G:H5' | 1:AA:1442(B):A:OP2 | 2.13 | 0.48 |
| 2:AB:209:ARG:HD3 | 2:AB:239:VAL:HG11 | 1.95 | 0.48 |
| 2:AB:215:LEU:O | 2:AB:219:VAL:N | 2.42 | 0.48 |
| 12:AL:53:ARG:HD2 | 12:AL:53:ARG:N | 2.26 | 0.48 |
| 17:AQ:22:LEU:HD12 | 17:AQ:41:LYS:CG | 2.44 | 0.48 |
| 25:AZ:324:LYS:CG | 25:AZ:364:PRO:HB3 | 2.34 | 0.48 |
| 29:B3:5:LYS:HB3 | 29:B3:57:GLU:HB3 | 1.96 | 0.48 |
| 30:B4:37:SER:O | 30:B4:38:LYS:CB | 2.62 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:B5:16:ARG:HH11 | 31:B5:20:ARG:NH1 | 2.11 | 0.48 |
| 32:B6:33:LYS:HA | 32:B6:33:LYS:CE | 2.26 | 0.48 |
| 35:B9:7:VAL:HG22 | 35:B9:34:GLN:CG | 2.42 | 0.48 |
| 36:BA:814:C:H1' | 36:BA:1225:G:N2 | 2.29 | 0.48 |
| 36:BA:2223:G:O2' | 36:BA:2224:G:H5' | 2.14 | 0.48 |
| 32:B6:25:LYS:NZ | 36:BA:2284:C:H41 | 2.11 | 0.48 |
| 36:BA:2533:A:OP1 | 36:BA:2665:A:H1' | 2.14 | 0.48 |
| 36:BA:321:G:N3 | 41:BF:165:ARG:HD3 | 2.28 | 0.48 |
| 36:BA:359:A:H2' | 36:BA:360:G:O4' | 2.13 | 0.48 |
| 36:BA:548:A:C2' | 36:BA:549:G:H5' | 2.41 | 0.48 |
| 36:BA:752:A:H4' | 36:BA:753:C:O5' | 2.13 | 0.48 |
| 37:BB:71:C:H2' | 37:BB:72:G:H5' | 1.96 | 0.48 |
| 38:BC:78:ALA:HB1 | 38:BC:83:ILE:HA | 1.95 | 0.48 |
| 40:BE:167:VAL:HG12 | 40:BE:189:PRO:HD3 | 1.95 | 0.48 |
| 40:BE:197:ILE:O | 40:BE:197:ILE:CG1 | 2.62 | 0.48 |
| 40:BE:50:GLY:HA2 | 40:BE:78:LEU:CB | 2.29 | 0.48 |
| 41:BF:20:LEU:HB2 | 41:BF:23:ASP:OD2 | 2.14 | 0.48 |
| 41:BF:51:THR:CB | 41:BF:88:VAL:HG11 | 2.44 | 0.48 |
| 42:BG:138:GLN:HG3 | 42:BG:139:LEU:H | 1.79 | 0.48 |
| 44:BJ:64:UNK:HA | 44:BJ:67:UNK:CB | 2.44 | 0.48 |
| 46:BN:56:ASN:H | 46:BN:125:GLY:H | 1.62 | 0.48 |
| 46:BN:65:LYS:HZ3 | 46:BN:65:LYS:HB3 | 1.78 | 0.48 |
| 48:BP:110:TYR:HE1 | 48:BP:149:GLU:OE1 | 1.97 | 0.48 |
| 34:B8:13:ARG:HA | 48:BP:63:PRO:HA | 1.96 | 0.48 |
| 48:BP:91:PHE:N | 48:BP:91:PHE:CD1 | 2.81 | 0.48 |
| 51:BS:27:SER:O | 51:BS:37:ALA:HA | 2.14 | 0.48 |
| 53:BU:8:VAL:CG2 | 53:BU:11:ARG:HH21 | 2.23 | 0.48 |
| 36:BA:534:U:H5' | 53:BU:42:ALA:HB1 | 1.96 | 0.48 |
| 53:BU:47:TYR:HE2 | 54:BV:74:LYS:NZ | 2.10 | 0.48 |
| 57:BY:29:GLU:OE1 | 57:BY:29:GLU:N | 2.47 | 0.48 |
| 58:BZ:71:VAL:HA | 58:BZ:87:ASP:O | 2.14 | 0.48 |
| 49:BQ:25:ASP:OD2 | 58:BZ:78:LYS:HD3 | 2.13 | 0.48 |
| 1:AA:122:G:O2' | 1:AA:123:C:H5' | 2.13 | 0.48 |
| 1:AA:1247:U:H1' | 1:AA:1291:G:N2 | 2.29 | 0.48 |
| 1:AA:137:C:O2 | 1:AA:137:C:H2' | 2.14 | 0.48 |
| 1:AA:1510:U:H2' | 1:AA:1511:G:H8 | 1.76 | 0.48 |
| 1:AA:555:C:H2' | 1:AA:556:C:C6 | 2.49 | 0.48 |
| 2:AB:129:GLU:O | 2:AB:130:ARG:O | 2.31 | 0.48 |
| 2:AB:95:GLN:O | 2:AB:96:ARG:HD2 | 2.14 | 0.48 |
| 3:AC:188:LEU:HD13 | 3:AC:195:VAL:HG13 | 1.96 | 0.48 |
| 1:AA:409:G:H5' | 4:AD:25:ARG:HB2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:63:ARG:HG2 | 5:AE:66:MET:HE1 | 1.95 | 0.48 |
| 9:AI:53:VAL:HG13 | 9:AI:95:LYS:HZ1 | 1.79 | 0.48 |
| 12:AL:45:PRO:HG2 | 12:AL:51:ALA:HB3 | 1.96 | 0.48 |
| 13:AM:87:TYR:CE1 | 19:AS:81:ARG:NH2 | 2.82 | 0.48 |
| 27:B1:86:SER:O | 27:B1:90:ILE:HG12 | 2.14 | 0.48 |
| 34:B8:5:LYS:HG2 | 36:BA:254:G:O6 | 2.14 | 0.48 |
| 36:BA:1142:U:H3' | 36:BA:1142:U:H6 | 1.78 | 0.48 |
| 36:BA:1210:A:O2' | 36:BA:1211:U:OP2 | 2.27 | 0.48 |
| 36:BA:1550:C:O2' | 36:BA:1551:C:H5' | 2.14 | 0.48 |
| 36:BA:1757:U:O4 | 36:BA:1762:A:H2 | 1.97 | 0.48 |
| 36:BA:2229:C:O2' | 36:BA:2230:G:H5' | 2.14 | 0.48 |
| 36:BA:2582:G:OP2 | 36:BA:2583:G:OP2 | 2.30 | 0.48 |
| 36:BA:2760:C:C3' | 36:BA:2761:G:H5'' | 2.43 | 0.48 |
| 33:B7:11:LYS:HE2 | 36:BA:686:G:C5' | 2.42 | 0.48 |
| 36:BA:744:G:C2' | 36:BA:745:G:H5' | 2.43 | 0.48 |
| 36:BA:860:U:H2' | 36:BA:861:A:H8 | 1.79 | 0.48 |
| 22:AW:56:C:H5'' | 38:BC:137:LEU:CB | 2.43 | 0.48 |
| 38:BC:186:ALA:HB1 | 38:BC:190:ARG:HH22 | 1.77 | 0.48 |
| 36:BA:2572:A:C2 | 40:BE:144:ARG:NH1 | 2.82 | 0.48 |
| 40:BE:38:THR:O | 40:BE:42:ASP:HB2 | 2.12 | 0.48 |
| 41:BF:107:LYS:C | 41:BF:109:GLY:H | 2.17 | 0.48 |
| 41:BF:157:VAL:HG12 | 41:BF:176:LEU:HB2 | 1.95 | 0.48 |
| 43:BH:150:ALA:O | 43:BH:152:ARG:N | 2.46 | 0.48 |
| 49:BQ:21:THR:C | 49:BQ:23:GLY:H | 2.17 | 0.48 |
| 50:BR:29:LEU:HD11 | 50:BR:52:ILE:HD11 | 1.95 | 0.48 |
| 54:BV:33:VAL:O | 54:BV:59:ALA:O | 2.32 | 0.48 |
| 55:BW:12:ILE:CG1 | 55:BW:42:ARG:HH12 | 2.27 | 0.48 |
| 58:BZ:168:GLU:O | 58:BZ:169:GLU:C | 2.51 | 0.48 |
| 58:BZ:60:GLU:C | 58:BZ:61:LEU:HG | 2.35 | 0.48 |
| 1:AA:1137:C:O2' | 1:AA:1138:G:N2 | 2.47 | 0.47 |
| 1:AA:1310:G:H2' | 1:AA:1311:G:H8 | 1.79 | 0.47 |
| 1:AA:434:U:H2' | 1:AA:435:C:C6 | 2.49 | 0.47 |
| 1:AA:779:C:H2' | 1:AA:780:A:O4' | 2.14 | 0.47 |
| 1:AA:792:A:H4' | 1:AA:793:U:O5' | 2.14 | 0.47 |
| 2:AB:59:GLU:HA | 2:AB:221:LEU:HD11 | 1.95 | 0.47 |
| 4:AD:13:ARG:HD2 | 4:AD:38:TYR:O | 2.14 | 0.47 |
| 7:AG:100:ALA:O | 7:AG:104:LEU:HD22 | 2.14 | 0.47 |
| 7:AG:30:ILE:HD13 | 7:AG:105:VAL:HG22 | 1.96 | 0.47 |
| 1:AA:539:A:OP2 | 12:AL:115:LYS:HE3 | 2.13 | 0.47 |
| 12:AL:27:LEU:C | 12:AL:29:GLY:N | 2.66 | 0.47 |
| 13:AM:42:ALA:O | 13:AM:43:THR:C | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:AP:21:VAL:HG13 | 16:AP:34:GLU:H | 1.78 | 0.47 |
| 1:AA:1321:C:HO2' | 19:AS:77:THR:HG21 | 1.78 | 0.47 |
| 20:AT:51:GLU:HA | 20:AT:54:LYS:CE | 2.39 | 0.47 |
| 1:AA:1505:G:H4' | 23:AX:16:A:N6 | 2.29 | 0.47 |
| 24:AY:20:H2U:H4' | 24:AY:21:A:H5' | 1.96 | 0.47 |
| 24:AY:70:C:H2' | 24:AY:71:C:C6 | 2.49 | 0.47 |
| 25:AZ:109:ALA:HB3 | 25:AZ:137:LYS:HE2 | 1.95 | 0.47 |
| 27:B1:84:GLY:C | 27:B1:86:SER:H | 2.15 | 0.47 |
| 28:B2:53:LEU:O | 28:B2:53:LEU:HD23 | 2.13 | 0.47 |
| 32:B6:5:VAL:HB | 36:BA:2284:C:OP2 | 2.13 | 0.47 |
| 36:BA:1064:C:H4' | 45:BK:87:UNK:CB | 2.44 | 0.47 |
| 36:BA:1407:C:H5' | 36:BA:1408:C:OP2 | 2.13 | 0.47 |
| 36:BA:1450(A):C:N4 | 36:BA:1451:C:H41 | 2.12 | 0.47 |
| 36:BA:2189:U:H3' | 36:BA:2190:G:H5'' | 1.95 | 0.47 |
| 36:BA:2654:A:N1 | 36:BA:2665:A:H5'' | 2.29 | 0.47 |
| 36:BA:90:U:O2 | 36:BA:90:U:C2' | 2.61 | 0.47 |
| 37:BB:73:A:H2' | 37:BB:74:U:C5' | 2.44 | 0.47 |
| 39:BD:112:GLN:HG3 | 39:BD:115:GLN:NE2 | 2.29 | 0.47 |
| 39:BD:227:ASN:HB3 | 39:BD:228:PRO:HD2 | 1.96 | 0.47 |
| 39:BD:24:ILE:HD13 | 39:BD:25:THR:CA | 2.42 | 0.47 |
| 40:BE:5:LEU:HB2 | 40:BE:51:PHE:CD2 | 2.49 | 0.47 |
| 46:BN:21:LYS:HD3 | 46:BN:22:THR:H | 1.79 | 0.47 |
| 48:BP:91:PHE:CE2 | 48:BP:95:VAL:HG12 | 2.48 | 0.47 |
| 49:BQ:141:GLN:OXT | 58:BZ:53:ILE:O | 2.32 | 0.47 |
| 51:BS:39:ILE:HD12 | 51:BS:73:LEU:CD2 | 2.44 | 0.47 |
| 51:BS:82:ILE:O | 51:BS:82:ILE:HG22 | 2.14 | 0.47 |
| 54:BV:95:LEU:C | 54:BV:95:LEU:HD23 | 2.34 | 0.47 |
| 1:AA:537:G:H2' | 1:AA:538:G:C8 | 2.49 | 0.47 |
| 1:AA:620:C:H2' | 1:AA:621:A:O4' | 2.13 | 0.47 |
| 1:AA:668:G:O2' | 15:AO:46:HIS:HD2 | 1.97 | 0.47 |
| 1:AA:713:G:H2' | 1:AA:714:G:C8 | 2.48 | 0.47 |
| 2:AB:51:LEU:CD2 | 2:AB:55:PHE:HE2 | 2.27 | 0.47 |
| 3:AC:101:LEU:HD23 | 3:AC:102:ASN:O | 2.14 | 0.47 |
| 3:AC:188:LEU:CD1 | 3:AC:195:VAL:HG13 | 2.45 | 0.47 |
| 7:AG:15:ASP:OD1 | 7:AG:18:TYR:HD1 | 1.96 | 0.47 |
| 9:AI:121:ARG:NH1 | 9:AI:122:ALA:O | 2.47 | 0.47 |
| 16:AP:20:VAL:CG2 | 16:AP:32:TYR:HB2 | 2.44 | 0.47 |
| 16:AP:59:TRP:O | 16:AP:62:VAL:HG23 | 2.14 | 0.47 |
| 17:AQ:83:ASP:O | 17:AQ:86:GLU:HB2 | 2.13 | 0.47 |
| 6:AF:99:ALA:HB3 | 18:AR:29:PHE:CE2 | 2.49 | 0.47 |
| 18:AR:47:THR:O | 18:AR:83:GLU:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AU:13:ILE:O | 21:AU:16:GLY:N | 2.41 | 0.47 |
| 24:AY:1:A:H5' | 25:AZ:90:LYS:HZ1 | 1.71 | 0.47 |
| 25:AZ:19:HIS:ND1 | 25:AZ:115:GLN:HB2 | 2.29 | 0.47 |
| 28:B2:64:LEU:CD2 | 28:B2:68:ARG:HD2 | 2.45 | 0.47 |
| 28:B2:69:ARG:NH2 | 36:BA:111:A:H4' | 2.29 | 0.47 |
| 30:B4:45:GLY:O | 30:B4:46:GLN:HB2 | 2.12 | 0.47 |
| 32:B6:11:LEU:O | 32:B6:23:THR:HB | 2.14 | 0.47 |
| 36:BA:1264:G:C3' | 36:BA:1265:A:H5'' | 2.42 | 0.47 |
| 36:BA:1471:A:H2' | 36:BA:1472:A:H8 | 1.77 | 0.47 |
| 36:BA:1798:U:H5'' | 39:BD:259:THR:HG22 | 1.93 | 0.47 |
| 36:BA:1800:C:OP1 | 39:BD:266:SER:OG | 2.33 | 0.47 |
| 36:BA:2051:A:H5' | 36:BA:2578:G:O4' | 2.15 | 0.47 |
| 36:BA:2590:A:H2' | 36:BA:2591:C:H6 | 1.78 | 0.47 |
| 36:BA:2880:C:O2' | 50:BR:90:ARG:HD3 | 2.13 | 0.47 |
| 36:BA:336:C:O3' | 57:BY:7:VAL:HG22 | 2.14 | 0.47 |
| 36:BA:36:G:H2' | 36:BA:37:C:H6 | 1.79 | 0.47 |
| 36:BA:869:G:O2' | 36:BA:870:A:H5' | 2.14 | 0.47 |
| 38:BC:147:PHE:C | 38:BC:149:ILE:N | 2.65 | 0.47 |
| 39:BD:126:GLN:HG2 | 39:BD:129:ASN:HD21 | 1.77 | 0.47 |
| 39:BD:3:VAL:HG11 | 39:BD:17:THR:HB | 1.95 | 0.47 |
| 39:BD:127:VAL:HA | 39:BD:193:VAL:HG13 | 1.96 | 0.47 |
| 36:BA:1826:G:H4' | 39:BD:242:ARG:HH21 | 1.79 | 0.47 |
| 39:BD:34:VAL:HG23 | 39:BD:35:LYS:H | 1.78 | 0.47 |
| 39:BD:35:LYS:O | 39:BD:37:LEU:HB2 | 2.13 | 0.47 |
| 39:BD:30:GLU:CG | 39:BD:63:ARG:NE | 2.65 | 0.47 |
| 40:BE:32:PRO:O | 40:BE:33:VAL:C | 2.52 | 0.47 |
| 40:BE:3:GLY:HA3 | 40:BE:81:ILE:HG21 | 1.96 | 0.47 |
| 36:BA:2635:C:OP1 | 40:BE:77:ILE:HD13 | 2.14 | 0.47 |
| 48:BP:106:LEU:O | 48:BP:107:LYS:HG2 | 2.14 | 0.47 |
| 49:BQ:35:VAL:HG12 | 49:BQ:130:LYS:O | 2.13 | 0.47 |
| 50:BR:18:LEU:CD1 | 50:BR:22:ARG:NE | 2.72 | 0.47 |
| 52:BT:47:GLY:HA3 | 52:BT:63:VAL:HG12 | 1.95 | 0.47 |
| 53:BU:92:ARG:HH22 | 54:BV:10:LYS:HA | 1.77 | 0.47 |
| 55:BW:31:GLU:O | 55:BW:34:ASN:HB2 | 2.14 | 0.47 |
| 55:BW:72:LYS:HE3 | 55:BW:108:GLY:CA | 2.35 | 0.47 |
| 56:BX:39:ILE:O | 56:BX:43:VAL:HG23 | 2.13 | 0.47 |
| 57:BY:13:VAL:CG2 | 57:BY:73:ARG:C | 2.82 | 0.47 |
| 57:BY:40:GLU:HA | 57:BY:40:GLU:OE2 | 2.14 | 0.47 |
| 58:BZ:126:VAL:HA | 58:BZ:163:LEU:HB2 | 1.96 | 0.47 |
| 1:AA:1150:U:C4 | 1:AA:1151:A:N7 | 2.82 | 0.47 |
| 1:AA:1201:A:H4' | 1:AA:1202:G:H5'' | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:169:C:C2' | 1:AA:170:U:H5' | 2.44 | 0.47 |
| 1:AA:179:A:H2' | 1:AA:180:U:C6 | 2.49 | 0.47 |
| 1:AA:222:U:C2 | 1:AA:223:U:C5 | 3.02 | 0.47 |
| 1:AA:413:G:N2 | 1:AA:428:G:H1' | 2.29 | 0.47 |
| 1:AA:477:A:O2' | 1:AA:479:C:H5' | 2.14 | 0.47 |
| 2:AB:61:LEU:HD12 | 2:AB:64:ARG:CD | 2.41 | 0.47 |
| 9:AI:16:ARG:HG3 | 9:AI:16:ARG:NH1 | 2.27 | 0.47 |
| 12:AL:87:GLY:HA2 | 12:AL:98:TYR:CD2 | 2.50 | 0.47 |
| 25:AZ:133:VAL:HB | 25:AZ:170:VAL:HG22 | 1.96 | 0.47 |
| 28:B2:7:ARG:O | 28:B2:11:GLU:HG3 | 2.14 | 0.47 |
| 32:B6:10:LEU:HD12 | 34:B8:34:TRP:HB2 | 1.95 | 0.47 |
| 36:BA:1141:U:H5'' | 36:BA:1142(A):A:O4' | 2.15 | 0.47 |
| 36:BA:1512:U:O2 | 36:BA:1512:U:C2' | 2.59 | 0.47 |
| 36:BA:1523:U:H2' | 36:BA:1524:G:C8 | 2.49 | 0.47 |
| 36:BA:1406:U:N3 | 36:BA:1597:A:C2 | 2.83 | 0.47 |
| 36:BA:2128:C:O2' | 36:BA:2129:C:O5' | 2.31 | 0.47 |
| 36:BA:2320:A:H2' | 36:BA:2320:A:N3 | 2.29 | 0.47 |
| 36:BA:2422:A:H4' | 36:BA:2423:U:OP1 | 2.14 | 0.47 |
| 36:BA:2476:A:H2' | 36:BA:2476:A:N3 | 2.29 | 0.47 |
| 36:BA:287:C:N4 | 36:BA:354:G:H1 | 2.11 | 0.47 |
| 36:BA:482:A:H62 | 36:BA:506:G:H1' | 1.79 | 0.47 |
| 31:B5:13:LYS:HZ1 | 36:BA:516:C:C5' | 2.27 | 0.47 |
| 36:BA:539:G:H2' | 36:BA:540:C:C6 | 2.50 | 0.47 |
| 36:BA:552:G:H1' | 36:BA:1220:A:C2 | 2.49 | 0.47 |
| 36:BA:693:C:H2' | 36:BA:694:U:H6 | 1.79 | 0.47 |
| 36:BA:814:C:H2' | 36:BA:815:C:C6 | 2.50 | 0.47 |
| 38:BC:11:LEU:CD2 | 38:BC:220:PRO:HB3 | 2.45 | 0.47 |
| 38:BC:98:GLU:O | 38:BC:98:GLU:HG3 | 2.15 | 0.47 |
| 39:BD:61:LEU:O | 39:BD:63:ARG:NH1 | 2.47 | 0.47 |
| 39:BD:96:HIS:HE1 | 39:BD:102:LYS:HZ3 | 1.60 | 0.47 |
| 43:BH:149:ARG:HD3 | 43:BH:164:TYR:CE1 | 2.49 | 0.47 |
| 46:BN:23:LEU:HB3 | 46:BN:60:ILE:CG2 | 2.45 | 0.47 |
| 46:BN:91:LEU:HA | 46:BN:95:PRO:HA | 1.96 | 0.47 |
| 53:BU:88:ILE:HB | 53:BU:90:VAL:CG2 | 2.42 | 0.47 |
| 36:BA:996:A:H4' | 53:BU:92:ARG:CZ | 2.45 | 0.47 |
| 55:BW:107:LEU:N | 55:BW:107:LEU:HD12 | 2.24 | 0.47 |
| 55:BW:52:GLU:C | 55:BW:54:ALA:N | 2.67 | 0.47 |
| 57:BY:13:VAL:HG12 | 57:BY:28:LYS:HD3 | 1.96 | 0.47 |
| 57:BY:46:LYS:O | 57:BY:47:LYS:HD2 | 2.14 | 0.47 |
| 57:BY:86:ARG:NH2 | 57:BY:95:LYS:HZ2 | 2.11 | 0.47 |
| 58:BZ:28:MET:O | 58:BZ:34:ASN:HA | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BZ:5:LEU:C | 58:BZ:6:LYS:HD3 | 2.34 | 0.47 |
| 1:AA:102:G:O2' | 1:AA:103:C:H5' | 2.13 | 0.47 |
| 1:AA:254:G:O2' | 1:AA:255:G:H5' | 2.13 | 0.47 |
| 1:AA:432:A:H2' | 1:AA:433:C:H5' | 1.96 | 0.47 |
| 1:AA:475:G:H2' | 1:AA:476:G:C8 | 2.47 | 0.47 |
| 1:AA:858:G:C8 | 1:AA:858:G:O5' | 2.67 | 0.47 |
| 2:AB:229:VAL:HG12 | 2:AB:230:VAL:N | 2.28 | 0.47 |
| 2:AB:22:LYS:HZ1 | 2:AB:40:HIS:CE1 | 2.32 | 0.47 |
| 2:AB:52:GLU:OE1 | 2:AB:56:ARG:NH2 | 2.47 | 0.47 |
| 10:AJ:58:ASP:O | 10:AJ:59:SER:O | 2.32 | 0.47 |
| 13:AM:23:TYR:HB3 | 13:AM:67:GLU:HB2 | 1.97 | 0.47 |
| 15:AO:10:LYS:CA | 15:AO:10:LYS:HE3 | 2.42 | 0.47 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:HB2 | 1.94 | 0.47 |
| 17:AQ:76:LEU:HD12 | 17:AQ:77:VAL:N | 2.25 | 0.47 |
| 22:AV:66:U:O2' | 22:AV:67:C:H5' | 2.14 | 0.47 |
| 22:AV:74:C:O2 | 22:AV:74:C:H2' | 2.15 | 0.47 |
| 26:B0:14:ARG:CG | 26:B0:14:ARG:HH11 | 2.24 | 0.47 |
| 29:B3:56:VAL:O | 29:B3:57:GLU:HB2 | 2.14 | 0.47 |
| 36:BA:2026:C:C4 | 36:BA:2027:G:N7 | 2.82 | 0.47 |
| 36:BA:2124:G:H5'' | 38:BC:174:PRO:HG3 | 1.96 | 0.47 |
| 36:BA:2485:G:O2' | 36:BA:2486:G:H5' | 2.14 | 0.47 |
| 36:BA:2629:A:N3 | 36:BA:2629:A:H2' | 2.29 | 0.47 |
| 36:BA:2695:C:O2' | 36:BA:2696:U:H5' | 2.14 | 0.47 |
| 36:BA:271(C):C:H2' | 36:BA:271(D):G:H8 | 1.79 | 0.47 |
| 35:B9:35:ARG:NH1 | 36:BA:2741:A:O3' | 2.48 | 0.47 |
| 36:BA:565:C:H5'' | 54:BV:80:GLN:HE22 | 1.80 | 0.47 |
| 38:BC:33:ALA:HB2 | 38:BC:216:THR:HG21 | 1.97 | 0.47 |
| 39:BD:35:LYS:CA | 39:BD:63:ARG:HA | 2.44 | 0.47 |
| 41:BF:131:GLY:HA3 | 41:BF:138:GLU:O | 2.14 | 0.47 |
| 52:BT:61:PHE:N | 52:BT:61:PHE:CD2 | 2.81 | 0.47 |
| 52:BT:64:ARG:HB2 | 52:BT:73:GLU:HG2 | 1.96 | 0.47 |
| 52:BT:50:ILE:HA | 52:BT:99:LEU:CD1 | 2.44 | 0.47 |
| 53:BU:92:ARG:O | 53:BU:93:LYS:C | 2.52 | 0.47 |
| 55:BW:84:ARG:HH11 | 55:BW:84:ARG:HG2 | 1.79 | 0.47 |
| 57:BY:85:VAL:HG12 | 57:BY:86:ARG:H | 1.79 | 0.47 |
| 58:BZ:34:ASN:C | 58:BZ:35:ARG:HE | 2.17 | 0.47 |
| 1:AA:106:C:HO2' | 1:AA:107:G:H5' | 1.80 | 0.47 |
| 1:AA:1269:A:C8 | 1:AA:1326:C:O4' | 2.68 | 0.47 |
| 2:AB:61:LEU:HD13 | 2:AB:64:ARG:NH1 | 2.28 | 0.47 |
| 3:AC:16:ARG:HH11 | 3:AC:16:ARG:HB2 | 1.80 | 0.47 |
| 1:AA:619:U:N3 | 4:AD:134:ASP:OD1 | 2.42 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:AD:159:ARG:HG3 | 4:AD:159:ARG:NH1 | 2.28 | 0.47 |
| 4:AD:25:ARG:O | 4:AD:28:SER:HB2 | 2.15 | 0.47 |
| 4:AD:78:LEU:CD2 | 4:AD:96:LEU:HB3 | 2.44 | 0.47 |
| 5:AE:6:PHE:HB2 | 5:AE:34:VAL:HG22 | 1.92 | 0.47 |
| 10:AJ:85:LEU:C | 10:AJ:87:THR:H | 2.18 | 0.47 |
| 12:AL:41:ARG:HG2 | 12:AL:42:THR:N | 2.20 | 0.47 |
| 3:AC:34:LEU:CG | 14:AN:25:VAL:HG11 | 2.36 | 0.47 |
| 1:AA:390:C:O3' | 16:AP:28:ARG:NH1 | 2.47 | 0.47 |
| 1:AA:1318:A:H1' | 19:AS:37:ARG:HH21 | 1.80 | 0.47 |
| 25:AZ:181:GLN:OE1 | 25:AZ:193:ASN:ND2 | 2.46 | 0.47 |
| 27:B1:80:LEU:HD22 | 27:B1:82:LEU:CD2 | 2.41 | 0.47 |
| 27:B1:90:ILE:O | 27:B1:94:LEU:HD13 | 2.15 | 0.47 |
| 30:B4:6:HIS:HB3 | 42:BG:67:LYS:CE | 2.28 | 0.47 |
| 32:B6:15:GLU:O | 32:B6:16:CYS:C | 2.53 | 0.47 |
| 34:B8:50:LEU:C | 34:B8:52:LYS:H | 2.17 | 0.47 |
| 36:BA:1069:A:C1' | 36:BA:1070:A:P | 3.03 | 0.47 |
| 36:BA:1142(A):A:H5' | 36:BA:1142(A):A:H8 | 1.79 | 0.47 |
| 36:BA:839:U:H1' | 36:BA:1191:G:H1' | 1.96 | 0.47 |
| 36:BA:1210:A:H5'' | 36:BA:1212:G:H5' | 1.96 | 0.47 |
| 36:BA:1252:G:N3 | 53:BU:33:ARG:CD | 2.77 | 0.47 |
| 36:BA:2128:C:OP1 | 38:BC:36:LYS:N | 2.47 | 0.47 |
| 36:BA:2298:A:H62 | 36:BA:2318:G:H8 | 1.61 | 0.47 |
| 36:BA:2342:C:O2' | 36:BA:2374:C:H5'' | 2.14 | 0.47 |
| 36:BA:2538:C:O2' | 36:BA:2539:C:H5' | 2.15 | 0.47 |
| 36:BA:57:C:H2' | 36:BA:58:G:O4' | 2.14 | 0.47 |
| 36:BA:590:A:H2' | 36:BA:591:C:H6 | 1.79 | 0.47 |
| 42:BG:106:LEU:HD12 | 42:BG:110:ALA:HB3 | 1.96 | 0.47 |
| 42:BG:95:ARG:HH11 | 42:BG:95:ARG:HG2 | 1.79 | 0.47 |
| 43:BH:85:LYS:HZ1 | 43:BH:132:ARG:HA | 1.79 | 0.47 |
| 50:BR:118:GLU:HA | 50:BR:118:GLU:OE1 | 2.15 | 0.47 |
| 36:BA:1598:C:H5' | 56:BX:36:LYS:HD2 | 1.97 | 0.47 |
| 56:BX:41:ASN:HD22 | 56:BX:41:ASN:N | 2.12 | 0.47 |
| 58:BZ:149:SER:HB2 | 58:BZ:172:ALA:O | 2.15 | 0.47 |
| 58:BZ:19:ARG:C | 58:BZ:21:ALA:N | 2.65 | 0.47 |
| 58:BZ:48:PHE:O | 58:BZ:52:SER:N | 2.47 | 0.47 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:C8 | 2.56 | 0.47 |
| 1:AA:1286:A:O2' | 1:AA:1287:A:H5'' | 2.14 | 0.47 |
| 1:AA:1526:G:O2' | 1:AA:1527:C:H5' | 2.15 | 0.47 |
| 1:AA:501:C:H2' | 1:AA:502:G:H8 | 1.79 | 0.47 |
| 13:AM:36:LYS:HG3 | 13:AM:59:TYR:CE2 | 2.49 | 0.47 |
| 13:AM:78:ILE:O | 13:AM:81:LEU:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:AJ:50:ILE:CD1 | 14:AN:41:ARG:HD2 | 2.42 | 0.47 |
| 20:AT:27:LYS:HD3 | 20:AT:27:LYS:C | 2.34 | 0.47 |
| 1:AA:927:G:HO2' | 23:AX:15:A:H2 | 1.61 | 0.47 |
| 24:AY:62:U:C5' | 24:AY:62:U:H6 | 2.24 | 0.47 |
| 25:AZ:359:VAL:C | 25:AZ:361:MET:H | 2.17 | 0.47 |
| 36:BA:1202:C:H2' | 36:BA:1203:G:H5' | 1.96 | 0.47 |
| 36:BA:1762:A:O5' | 36:BA:1762:A:C8 | 2.51 | 0.47 |
| 36:BA:793:A:OP2 | 36:BA:2072:G:H5' | 2.15 | 0.47 |
| 36:BA:2289:G:C1' | 36:BA:2346:A:H2 | 2.27 | 0.47 |
| 36:BA:2068:U:N3 | 36:BA:2430:A:H2 | 2.13 | 0.47 |
| 36:BA:310:A:C4 | 36:BA:312:G:C8 | 3.03 | 0.47 |
| 36:BA:548:A:H2' | 36:BA:549:G:C5' | 2.41 | 0.47 |
| 36:BA:839:U:H2' | 36:BA:840:C:C6 | 2.49 | 0.47 |
| 36:BA:887:A:H2' | 36:BA:887:A:N3 | 2.29 | 0.47 |
| 36:BA:943:U:OP2 | 48:BP:38:GLN:CD | 2.53 | 0.47 |
| 37:BB:10:C:O2' | 37:BB:11:C:H5' | 2.14 | 0.47 |
| 38:BC:65:PRO:CD | 38:BC:188:ASN:HA | 2.34 | 0.47 |
| 36:BA:2173:A:C2' | 38:BC:218:MET:HE1 | 2.45 | 0.47 |
| 39:BD:24:ILE:C | 39:BD:24:ILE:HD13 | 2.35 | 0.47 |
| 41:BF:120:GLU:CB | 41:BF:122:LYS:HE3 | 2.44 | 0.47 |
| 41:BF:57:VAL:HG12 | 41:BF:59:TYR:H | 1.79 | 0.47 |
| 48:BP:108:LYS:O | 48:BP:110:TYR:N | 2.41 | 0.47 |
| 48:BP:32:THR:O | 48:BP:33:ARG:O | 2.32 | 0.47 |
| 51:BS:42:ASP:O | 51:BS:43:GLU:HB3 | 2.14 | 0.47 |
| 54:BV:21:ARG:HG2 | 54:BV:91:TYR:CG | 2.49 | 0.47 |
| 56:BX:64:LYS:HZ2 | 56:BX:73:ARG:HH21 | 1.57 | 0.47 |
| 58:BZ:48:PHE:HE2 | 58:BZ:52:SER:O | 1.98 | 0.47 |
| 1:AA:986:A:C2 | 1:AA:1220:G:C2 | 3.02 | 0.47 |
| 1:AA:192:U:C4' | 20:AT:103:GLY:HA2 | 2.44 | 0.47 |
| 1:AA:271:C:O2' | 1:AA:272:C:H5' | 2.15 | 0.47 |
| 8:AH:9:MET:O | 8:AH:13:ILE:HG12 | 2.14 | 0.47 |
| 10:AJ:94:VAL:CG1 | 10:AJ:95:GLU:N | 2.77 | 0.47 |
| 11:AK:108:ILE:HD12 | 11:AK:108:ILE:H | 1.79 | 0.47 |
| 11:AK:27:ASN:HB2 | 11:AK:55:LYS:HB2 | 1.96 | 0.47 |
| 13:AM:113:PRO:O | 13:AM:114:ARG:C | 2.52 | 0.47 |
| 17:AQ:15:MET:HB2 | 17:AQ:18:THR:HB | 1.95 | 0.47 |
| 25:AZ:130:TYR:CZ | 25:AZ:211:PRO:HD3 | 2.49 | 0.47 |
| 26:B0:45:PHE:HB2 | 26:B0:59:LEU:HD11 | 1.97 | 0.47 |
| 30:B4:19:GLY:O | 30:B4:20:ASN:C | 2.52 | 0.47 |
| 31:B5:49:CYS:SG | 31:B5:50:GLY:N | 2.82 | 0.47 |
| 34:B8:2:PRO:HA | 36:BA:591:C:HI' | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:1020:A:N1 | 36:BA:1141:U:H1' | 2.29 | 0.47 |
| 36:BA:1205:U:H4' | 36:BA:1206:G:OP2 | 2.14 | 0.47 |
| 36:BA:1516:C:H2' | 36:BA:1517:G:C5' | 2.19 | 0.47 |
| 36:BA:1830:C:O2' | 36:BA:1831:G:H5' | 2.15 | 0.47 |
| 26:B0:56:ASP:OD2 | 36:BA:2364:C:H4' | 2.14 | 0.47 |
| 36:BA:2439:A:C8 | 36:BA:2439:A:H5' | 2.50 | 0.47 |
| 38:BC:120:MET:CE | 38:BC:123:VAL:HG21 | 2.44 | 0.47 |
| 38:BC:15:ASP:O | 38:BC:20:TYR:HE1 | 1.98 | 0.47 |
| 38:BC:30:LYS:N | 38:BC:30:LYS:HD2 | 2.29 | 0.47 |
| 39:BD:142:VAL:CG2 | 39:BD:191:ALA:HB1 | 2.45 | 0.47 |
| 40:BE:201:THR:C | 40:BE:202:LYS:HD2 | 2.35 | 0.47 |
| 40:BE:38:THR:HG22 | 40:BE:40:GLU:N | 2.30 | 0.47 |
| 42:BG:165:THR:OG1 | 42:BG:168:GLU:HG3 | 2.15 | 0.47 |
| 42:BG:47:LYS:HB3 | 42:BG:48:GLU:H | 1.48 | 0.47 |
| 43:BH:127:GLU:HB2 | 43:BH:130:ARG:HB2 | 1.96 | 0.47 |
| 46:BN:34:LEU:CD2 | 46:BN:120:LEU:HD23 | 2.43 | 0.47 |
| 48:BP:96:THR:HG22 | 48:BP:126:VAL:CG2 | 2.45 | 0.47 |
| 49:BQ:48:GLU:HG3 | 49:BQ:52:VAL:HG23 | 1.97 | 0.47 |
| 49:BQ:74:TYR:HD1 | 49:BQ:75:THR:N | 2.12 | 0.47 |
| 52:BT:82:LEU:O | 52:BT:82:LEU:HD13 | 2.15 | 0.47 |
| 57:BY:10:GLY:HA2 | 57:BY:27:VAL:HG13 | 1.96 | 0.47 |
| 57:BY:81:LYS:O | 57:BY:82:PRO:O | 2.33 | 0.47 |
| 1:AA:1030:C:H2' | 1:AA:1030(A):G:O4' | 2.14 | 0.47 |
| 1:AA:1153:C:O2' | 1:AA:1154:G:O5' | 2.33 | 0.47 |
| 1:AA:1320:C:H5' | 1:AA:1320:C:C6 | 2.35 | 0.47 |
| 1:AA:355:C:H42 | 1:AA:356:A:N6 | 2.13 | 0.47 |
| 1:AA:495:A:H61 | 4:AD:119:GLN:HE22 | 1.63 | 0.47 |
| 1:AA:404:U:C5' | 4:AD:122:ARG:HD3 | 2.44 | 0.47 |
| 4:AD:122:ARG:NH1 | 4:AD:134:ASP:O | 2.47 | 0.47 |
| 4:AD:187:ARG:HH11 | 4:AD:187:ARG:CB | 2.27 | 0.47 |
| 5:AE:147:ASP:OD2 | 5:AE:147:ASP:N | 2.48 | 0.47 |
| 7:AG:101:LEU:HA | 7:AG:104:LEU:HD23 | 1.96 | 0.47 |
| 10:AJ:83:GLU:HB3 | 10:AJ:84:GLN:H | 1.61 | 0.47 |
| 14:AN:15:LYS:O | 14:AN:16:PHE:O | 2.32 | 0.47 |
| 19:AS:8:GLY:O | 19:AS:9:VAL:HG23 | 2.15 | 0.47 |
| 29:B3:19:GLN:HE22 | 29:B3:52:HIS:CE1 | 2.31 | 0.47 |
| 32:B6:28:ARG:HH11 | 32:B6:28:ARG:HG2 | 1.80 | 0.47 |
| 32:B6:45:LYS:O | 32:B6:46:HIS:CB | 2.63 | 0.47 |
| 34:B8:51:ALA:N | 34:B8:53:PRO:HD2 | 2.30 | 0.47 |
| 36:BA:1315:C:O2' | 36:BA:1316:U:H5' | 2.15 | 0.47 |
| 36:BA:1572:A:O2' | 36:BA:1573:G:H5' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:1625:C:H2' | 36:BA:1626:G:C5' | 2.44 | 0.47 |
| 36:BA:1778:U:H2' | 36:BA:1784:A:N6 | 2.30 | 0.47 |
| 36:BA:2167:U:H2' | 36:BA:2168:G:H5' | 1.95 | 0.47 |
| 36:BA:2539:C:O2' | 36:BA:2540:C:H5' | 2.14 | 0.47 |
| 36:BA:2555:U:C2' | 36:BA:2556:C:H5' | 2.45 | 0.47 |
| 36:BA:2562:U:C2' | 36:BA:2563:U:H5' | 2.44 | 0.47 |
| 36:BA:2849:U:O4 | 52:BT:23:ARG:NH2 | 2.43 | 0.47 |
| 36:BA:363:G:H2' | 36:BA:363(A):A:H8 | 1.80 | 0.47 |
| 37:BB:87:G:N2 | 37:BB:89:G:H3' | 2.30 | 0.47 |
| 38:BC:6:ARG:O | 38:BC:10:LEU:HD21 | 2.15 | 0.47 |
| 36:BA:1566:A:OP1 | 39:BD:211:ARG:NH1 | 2.48 | 0.47 |
| 40:BE:144:ARG:HB3 | 40:BE:145:LYS:H | 1.55 | 0.47 |
| 40:BE:74:PRO:HG3 | 40:BE:77:ILE:O | 2.15 | 0.47 |
| 41:BF:29:ASN:N | 41:BF:112:MET:SD | 2.77 | 0.47 |
| 41:BF:205:ARG:C | 41:BF:206:ILE:HD13 | 2.35 | 0.47 |
| 49:BQ:48:GLU:O | 49:BQ:49:ALA:C | 2.52 | 0.47 |
| 26:B0:7:LEU:CD2 | 49:BQ:81:VAL:CG2 | 2.90 | 0.47 |
| 51:BS:14:VAL:HG12 | 51:BS:15:ARG:N | 2.29 | 0.47 |
| 52:BT:58:ASN:ND2 | 52:BT:58:ASN:N | 2.60 | 0.47 |
| 1:AA:1441:G:H1' | 1:AA:1460:A:H61 | 1.79 | 0.47 |
| 2:AB:101:MET:HA | 2:AB:108:ILE:HG13 | 1.96 | 0.47 |
| 2:AB:17:PHE:CD1 | 2:AB:44:LEU:HD11 | 2.50 | 0.47 |
| 3:AC:142:MET:CE | 3:AC:171:GLY:HA3 | 2.44 | 0.47 |
| 3:AC:203:PHE:CE1 | 3:AC:205:GLY:O | 2.67 | 0.47 |
| 7:AG:22:LEU:HD22 | 7:AG:62:PHE:CZ | 2.50 | 0.47 |
| 11:AK:54:ARG:O | 11:AK:57:THR:HB | 2.15 | 0.47 |
| 13:AM:70:LEU:HD23 | 13:AM:74:VAL:HG23 | 1.97 | 0.47 |
| 1:AA:1319:A:OP2 | 19:AS:5:LEU:HD21 | 2.15 | 0.47 |
| 20:AT:74:LYS:CG | 20:AT:75:ASN:N | 2.77 | 0.47 |
| 20:AT:73:HIS:CB | 20:AT:74:LYS:HD3 | 2.37 | 0.47 |
| 27:B1:66:HIS:C | 27:B1:68:PRO:HD2 | 2.35 | 0.47 |
| 28:B2:18:PRO:HG2 | 28:B2:19:VAL:N | 2.29 | 0.47 |
| 32:B6:42:TRP:HA | 32:B6:42:TRP:HE3 | 1.78 | 0.47 |
| 33:B7:12:ARG:HG3 | 33:B7:12:ARG:HH11 | 1.79 | 0.47 |
| 34:B8:52:LYS:O | 34:B8:55:ALA:HB3 | 2.15 | 0.47 |
| 36:BA:1665:A:H2' | 36:BA:1666:G:C5' | 2.21 | 0.47 |
| 36:BA:2111:C:H1' | 36:BA:2118:U:C4' | 2.45 | 0.47 |
| 36:BA:2175:C:H4' | 38:BC:221:SER:CB | 2.38 | 0.47 |
| 36:BA:225:A:C2' | 36:BA:226:G:H5' | 2.45 | 0.47 |
| 36:BA:2263:C:O2' | 36:BA:2264:C:H5' | 2.15 | 0.47 |
| 36:BA:2777:G:C4' | 36:BA:2778:A:H5' | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BB:65:C:H2' | 37:BB:109:C:N4 | 2.29 | 0.47 |
| 37:BB:21:G:H2' | 37:BB:22:U:O4' | 2.15 | 0.47 |
| 38:BC:14:VAL:HG21 | 38:BC:32:LEU:HD11 | 1.96 | 0.47 |
| 36:BA:773:U:H4' | 39:BD:47:GLY:HA3 | 1.97 | 0.47 |
| 39:BD:79:VAL:HG12 | 39:BD:113:VAL:HA | 1.97 | 0.47 |
| 40:BE:167:VAL:CG1 | 40:BE:189:PRO:HD3 | 2.45 | 0.47 |
| 40:BE:59:VAL:O | 40:BE:62:PRO:HG2 | 2.15 | 0.47 |
| 42:BG:76:SER:OG | 42:BG:83:ARG:HB3 | 2.15 | 0.47 |
| 43:BH:118:PRO:CG | 43:BH:121:ILE:HD12 | 2.45 | 0.47 |
| 46:BN:3:THR:C | 46:BN:4:TYR:CG | 2.88 | 0.47 |
| 55:BW:10:VAL:O | 55:BW:11:ARG:CB | 2.63 | 0.47 |
| 57:BY:3:VAL:O | 57:BY:3:VAL:HG12 | 2.15 | 0.47 |
| 57:BY:80:GLY:O | 57:BY:81:LYS:C | 2.53 | 0.47 |
| 36:BA:84:A:C5' | 57:BY:9:LYS:HB3 | 2.36 | 0.47 |
| 58:BZ:99:TYR:CD2 | 58:BZ:99:TYR:N | 2.83 | 0.47 |
| 1:AA:1278:U:H5'' | 1:AA:1279:A:O4' | 2.15 | 0.47 |
| 1:AA:369:C:HO2' | 1:AA:370:C:C5' | 2.28 | 0.47 |
| 1:AA:594:G:O2' | 1:AA:595:G:H5' | 2.14 | 0.47 |
| 1:AA:601:C:O2' | 1:AA:602:A:H5' | 2.14 | 0.47 |
| 1:AA:76:C:N4 | 1:AA:93:G:H1 | 2.13 | 0.47 |
| 1:AA:977:A:O2' | 1:AA:978:A:H5' | 2.12 | 0.47 |
| 2:AB:142:LEU:O | 2:AB:146:GLN:HB2 | 2.15 | 0.47 |
| 2:AB:72:GLY:CA | 2:AB:165:VAL:HG22 | 2.45 | 0.47 |
| 4:AD:127:THR:N | 4:AD:147:ALA:O | 2.48 | 0.47 |
| 4:AD:85:LYS:HD3 | 4:AD:92:VAL:HG11 | 1.96 | 0.47 |
| 5:AE:8:GLU:CA | 5:AE:34:VAL:HG23 | 2.45 | 0.47 |
| 7:AG:18:TYR:O | 7:AG:20:ASP:N | 2.48 | 0.47 |
| 8:AH:20:TYR:CE1 | 8:AH:76:PRO:HG2 | 2.49 | 0.47 |
| 8:AH:85:ARG:HG3 | 8:AH:85:ARG:HH11 | 1.80 | 0.47 |
| 10:AJ:96:ILE:N | 10:AJ:96:ILE:HD13 | 2.16 | 0.47 |
| 11:AK:103:LEU:H | 11:AK:103:LEU:HD22 | 1.79 | 0.47 |
| 12:AL:34:ARG:O | 12:AL:61:THR:HG23 | 2.13 | 0.47 |
| 1:AA:127:G:N2 | 17:AQ:61:GLU:OE1 | 2.46 | 0.47 |
| 1:AA:1503:A:C8 | 23:AX:15:A:C6 | 3.03 | 0.47 |
| 25:AZ:324:LYS:HE3 | 25:AZ:364:PRO:HB3 | 1.97 | 0.47 |
| 25:AZ:344:PHE:CE2 | 25:AZ:380:LEU:HD21 | 2.50 | 0.47 |
| 25:AZ:32:THR:HG22 | 25:AZ:44:VAL:HA | 1.97 | 0.47 |
| 25:AZ:92:MET:HE3 | 25:AZ:96:ALA:HB2 | 1.97 | 0.47 |
| 36:BA:1453:U:OP1 | 50:BR:77:ARG:HD3 | 2.14 | 0.47 |
| 36:BA:2275:C:O2 | 49:BQ:85:LYS:HD3 | 2.14 | 0.47 |
| 36:BA:479:A:O2' | 36:BA:481:G:H5' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:74:A:O2' | 36:BA:75:G:OP2 | 2.25 | 0.47 |
| 37:BB:70:C:HO2' | 37:BB:71:C:H5' | 1.80 | 0.47 |
| 37:BB:91:C:O2' | 37:BB:92:C:H5' | 2.15 | 0.47 |
| 39:BD:16:MET:HG3 | 39:BD:206:LEU:O | 2.15 | 0.47 |
| 40:BE:151:TYR:HB3 | 46:BN:79:PRO:HG3 | 1.96 | 0.47 |
| 40:BE:44:TYR:O | 40:BE:45:THR:CB | 2.62 | 0.47 |
| 41:BF:148:LEU:C | 41:BF:150:GLY:N | 2.67 | 0.47 |
| 43:BH:162:ILE:HG23 | 43:BH:162:ILE:O | 2.15 | 0.47 |
| 43:BH:167:GLU:HG2 | 43:BH:168:PRO:CD | 2.28 | 0.47 |
| 43:BH:24:VAL:HG12 | 43:BH:25:LYS:N | 2.29 | 0.47 |
| 44:BJ:27:UNK:O | 44:BJ:82:UNK:HA | 2.15 | 0.47 |
| 48:BP:115:LEU:H | 48:BP:115:LEU:HD23 | 1.79 | 0.47 |
| 49:BQ:63:LYS:NZ | 58:BZ:175:VAL:HG21 | 2.29 | 0.47 |
| 51:BS:12:PHE:N | 51:BS:12:PHE:HD2 | 2.13 | 0.47 |
| 51:BS:34:HIS:CB | 51:BS:36:TYR:HE1 | 2.28 | 0.47 |
| 51:BS:85:VAL:H | 51:BS:106:ARG:HA | 1.80 | 0.47 |
| 54:BV:1:MET:SD | 54:BV:43:GLU:HG2 | 2.54 | 0.47 |
| 56:BX:26:TYR:HD2 | 56:BX:92:LEU:CD1 | 2.28 | 0.47 |
| 58:BZ:19:ARG:HG3 | 58:BZ:20:ARG:N | 2.29 | 0.47 |
| 1:AA:946:A:C2 | 1:AA:1236:A:C2 | 3.03 | 0.47 |
| 1:AA:135:C:C2' | 1:AA:136:C:H5' | 2.45 | 0.47 |
| 1:AA:196:A:N3 | 1:AA:222:U:H1' | 2.30 | 0.47 |
| 1:AA:601:C:H2' | 1:AA:602:A:H8 | 1.80 | 0.47 |
| 2:AB:67:THR:HA | 2:AB:90:MET:HE1 | 1.97 | 0.47 |
| 3:AC:159:GLY:HA2 | 3:AC:193:TYR:CD1 | 2.50 | 0.47 |
| 3:AC:32:LEU:HB3 | 3:AC:59:ARG:HH21 | 1.80 | 0.47 |
| 3:AC:59:ARG:HD3 | 3:AC:64:VAL:HG13 | 1.96 | 0.47 |
| 8:AH:102:ARG:N | 8:AH:102:ARG:CD | 2.78 | 0.47 |
| 10:AJ:83:GLU:O | 10:AJ:84:GLN:C | 2.53 | 0.47 |
| 10:AJ:87:THR:OG1 | 10:AJ:88:LEU:N | 2.48 | 0.47 |
| 14:AN:41:ARG:NH2 | 14:AN:42:ILE:HD11 | 2.30 | 0.47 |
| 17:AQ:67:LYS:CA | 17:AQ:70:ARG:NH1 | 2.75 | 0.47 |
| 18:AR:44:LEU:HD21 | 18:AR:79:LEU:HD22 | 1.97 | 0.47 |
| 20:AT:25:ARG:CG | 20:AT:25:ARG:HH11 | 2.26 | 0.47 |
| 27:B1:20:ARG:HB3 | 27:B1:34:THR:HA | 1.96 | 0.47 |
| 28:B2:41:ILE:HD11 | 28:B2:44:LEU:HD12 | 1.96 | 0.47 |
| 36:BA:1248:G:C8 | 41:BF:92:PRO:HD3 | 2.50 | 0.47 |
| 36:BA:1416:G:O2' | 36:BA:1417:C:H5 | 1.95 | 0.47 |
| 36:BA:1485:G:H2' | 36:BA:1486:A:C8 | 2.50 | 0.47 |
| 36:BA:1502:C:H2' | 36:BA:1502:C:O2 | 2.13 | 0.47 |
| 36:BA:1511:C:C5 | 36:BA:1512:U:H5 | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:1890:A:C2' | 36:BA:1891:G:H5' | 2.44 | 0.47 |
| 36:BA:2231:C:H2' | 36:BA:2232:U:H6 | 1.79 | 0.47 |
| 36:BA:2286:A:H4' | 36:BA:2287:A:O4' | 2.14 | 0.47 |
| 36:BA:2872:G:H2' | 36:BA:2873:A:C8 | 2.50 | 0.47 |
| 36:BA:342:G:H2' | 36:BA:343:C:C6 | 2.50 | 0.47 |
| 36:BA:686:G:H21 | 36:BA:788:A:N6 | 2.12 | 0.47 |
| 36:BA:821:A:H5'' | 36:BA:822:U:H6 | 1.80 | 0.47 |
| 37:BB:5:C:O2' | 37:BB:27:C:O2 | 2.28 | 0.47 |
| 37:BB:98:G:C2' | 37:BB:99:G:H5' | 2.45 | 0.47 |
| 38:BC:161:ILE:HD12 | 38:BC:161:ILE:C | 2.35 | 0.47 |
| 36:BA:2124:G:H4' | 38:BC:174:PRO:HB3 | 1.96 | 0.47 |
| 38:BC:78:ALA:HB3 | 38:BC:95:GLY:N | 2.29 | 0.47 |
| 39:BD:96:HIS:HE1 | 39:BD:102:LYS:NZ | 2.09 | 0.47 |
| 39:BD:214:TRP:C | 39:BD:216:GLY:H | 2.18 | 0.47 |
| 41:BF:158:THR:HA | 41:BF:198:ALA:HB2 | 1.97 | 0.47 |
| 43:BH:28:GLY:HA3 | 43:BH:79:VAL:HB | 1.97 | 0.47 |
| 48:BP:83:VAL:CG2 | 48:BP:105:LEU:HD22 | 2.40 | 0.47 |
| 48:BP:111:ARG:NH1 | 48:BP:149:GLU:HG3 | 2.29 | 0.47 |
| 48:BP:126:VAL:HG22 | 48:BP:145:PRO:CG | 2.45 | 0.47 |
| 36:BA:661:C:H4' | 48:BP:18:ARG:HG2 | 1.96 | 0.47 |
| 50:BR:3:HIS:O | 50:BR:4:LEU:C | 2.52 | 0.47 |
| 52:BT:58:ASN:H | 52:BT:58:ASN:HD22 | 1.63 | 0.47 |
| 54:BV:12:TYR:CE2 | 54:BV:22:VAL:HG12 | 2.50 | 0.47 |
| 54:BV:34:GLU:HG2 | 54:BV:36:PRO:HD3 | 1.95 | 0.47 |
| 57:BY:20:TYR:CE1 | 57:BY:42:VAL:HG22 | 2.50 | 0.47 |
| 58:BZ:24:LEU:HD12 | 58:BZ:41:LEU:HA | 1.97 | 0.47 |
| 58:BZ:71:VAL:HG12 | 58:BZ:73:GLN:H | 1.80 | 0.47 |
| 1:AA:390:C:H4' | 16:AP:28:ARG:HH11 | 1.80 | 0.46 |
| 1:AA:585:G:H4' | 12:AL:8:ASN:ND2 | 2.29 | 0.46 |
| 2:AB:114:ARG:O | 2:AB:118:LEU:HD12 | 2.15 | 0.46 |
| 2:AB:115:LEU:HD13 | 2:AB:145:LEU:HD12 | 1.97 | 0.46 |
| 2:AB:51:LEU:CD2 | 2:AB:201:ILE:HD12 | 2.44 | 0.46 |
| 3:AC:8:ILE:O | 3:AC:11:ARG:N | 2.48 | 0.46 |
| 3:AC:148:GLY:HA3 | 3:AC:172:ARG:O | 2.15 | 0.46 |
| 5:AE:20:GLN:NE2 | 5:AE:25:ARG:NH2 | 2.59 | 0.46 |
| 11:AK:12:ARG:C | 11:AK:13:GLN:HG3 | 2.36 | 0.46 |
| 12:AL:26:ALA:O | 12:AL:27:LEU:O | 2.32 | 0.46 |
| 12:AL:74:GLY:O | 12:AL:102:ARG:NH2 | 2.47 | 0.46 |
| 18:AR:43:PHE:HD1 | 18:AR:66:LEU:HD11 | 1.80 | 0.46 |
| 32:B6:32:ASN:O | 32:B6:33:LYS:CB | 2.63 | 0.46 |
| 36:BA:1494:A:H2' | 36:BA:1495:A:C5' | 2.41 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:1654:A:H2 | 40:BE:113:PHE:CD2 | 2.33 | 0.46 |
| 36:BA:1988:C:O2' | 36:BA:1989:G:H5' | 2.15 | 0.46 |
| 36:BA:2134:A:H2' | 36:BA:2135:A:H8 | 1.80 | 0.46 |
| 36:BA:222:A:H5'' | 36:BA:421:U:OP1 | 2.15 | 0.46 |
| 36:BA:2679:A:O2' | 36:BA:2680:C:H5' | 2.16 | 0.46 |
| 38:BC:104:LEU:CD2 | 38:BC:127:LEU:HD21 | 2.45 | 0.46 |
| 38:BC:163:PHE:CE2 | 38:BC:192:PHE:HE1 | 2.33 | 0.46 |
| 38:BC:65:PRO:HG2 | 38:BC:187:ASP:O | 2.15 | 0.46 |
| 39:BD:237:GLU:HA | 39:BD:237:GLU:OE2 | 2.16 | 0.46 |
| 45:BK:123:UNK:C | 45:BK:125:UNK:N | 2.78 | 0.46 |
| 46:BN:10:GLU:CG | 46:BN:11:PRO:HD2 | 2.45 | 0.46 |
| 47:BO:35:VAL:HG23 | 47:BO:65:THR:HG23 | 1.95 | 0.46 |
| 48:BP:111:ARG:H | 48:BP:111:ARG:CD | 2.28 | 0.46 |
| 48:BP:24:GLY:HA3 | 48:BP:33:ARG:HH12 | 1.79 | 0.46 |
| 55:BW:1:MET:C | 55:BW:64:MET:HE3 | 2.36 | 0.46 |
| 56:BX:18:TYR:O | 56:BX:21:PHE:CD1 | 2.68 | 0.46 |
| 56:BX:27:THR:HG22 | 56:BX:80:ILE:CB | 2.44 | 0.46 |
| 1:AA:284:G:H2' | 1:AA:285:G:C8 | 2.50 | 0.46 |
| 1:AA:555:C:H2' | 1:AA:556:C:H6 | 1.81 | 0.46 |
| 2:AB:121:LEU:HA | 2:AB:124:SER:HB3 | 1.97 | 0.46 |
| 2:AB:71:VAL:HG12 | 2:AB:170:GLU:HG2 | 1.97 | 0.46 |
| 2:AB:80:ILE:HG12 | 2:AB:208:ILE:HG23 | 1.97 | 0.46 |
| 3:AC:16:ARG:NH2 | 3:AC:183:ASP:HA | 2.31 | 0.46 |
| 1:AA:1149:C:OP1 | 9:AI:9:ARG:NH1 | 2.48 | 0.46 |
| 15:AO:26:GLU:O | 15:AO:81:LEU:HD21 | 2.15 | 0.46 |
| 16:AP:50:LYS:O | 16:AP:51:VAL:HG23 | 2.14 | 0.46 |
| 22:AV:14:A:N6 | 22:AV:21:A:H2 | 2.12 | 0.46 |
| 31:B5:18:ALA:O | 31:B5:21:SER:HB3 | 2.15 | 0.46 |
| 33:B7:46:VAL:HG12 | 33:B7:47:ARG:N | 2.29 | 0.46 |
| 36:BA:1434:A:O2' | 36:BA:1435:G:H5' | 2.15 | 0.46 |
| 36:BA:1831:G:H2' | 36:BA:1832:C:H6 | 1.79 | 0.46 |
| 36:BA:1887:C:H2' | 36:BA:1888:G:H5'' | 1.96 | 0.46 |
| 36:BA:2087:G:O2' | 36:BA:2088:G:H5' | 2.15 | 0.46 |
| 36:BA:2697:G:H2' | 36:BA:2698:U:O4' | 2.15 | 0.46 |
| 36:BA:604:G:O2' | 36:BA:605:C:H5' | 2.15 | 0.46 |
| 36:BA:973:A:H5' | 36:BA:1188:U:H1' | 1.97 | 0.46 |
| 38:BC:110:PHE:O | 38:BC:111:ASP:HB2 | 2.14 | 0.46 |
| 39:BD:79:VAL:HG21 | 39:BD:111:LEU:HD21 | 1.96 | 0.46 |
| 39:BD:21:PHE:HB3 | 39:BD:24:ILE:CG2 | 2.45 | 0.46 |
| 42:BG:85:GLY:O | 42:BG:86:MET:CB | 2.63 | 0.46 |
| 48:BP:45:LEU:HD22 | 48:BP:46:LYS:H | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:BP:83:VAL:HA | 48:BP:105:LEU:HD22 | 1.96 | 0.46 |
| 52:BT:28:VAL:HG11 | 52:BT:46:GLU:OE1 | 2.15 | 0.46 |
| 53:BU:90:VAL:O | 53:BU:92:ARG:N | 2.48 | 0.46 |
| 58:BZ:146:ILE:O | 58:BZ:147:GLY:O | 2.32 | 0.46 |
| 1:AA:1396:A:O4' | 1:AA:1398:A:HI' | 2.15 | 0.46 |
| 1:AA:1459:C:H2' | 1:AA:1460:A:H8 | 1.80 | 0.46 |
| 1:AA:1521:G:H2' | 1:AA:1522:U:H6 | 1.79 | 0.46 |
| 1:AA:556:C:O2' | 1:AA:557:G:H5' | 2.14 | 0.46 |
| 2:AB:111:ARG:HG2 | 2:AB:111:ARG:NH1 | 2.31 | 0.46 |
| 3:AC:142:MET:C | 3:AC:144:SER:H | 2.17 | 0.46 |
| 3:AC:179:ARG:O | 3:AC:206:GLU:O | 2.33 | 0.46 |
| 3:AC:52:LEU:HD23 | 3:AC:52:LEU:O | 2.16 | 0.46 |
| 4:AD:170:VAL:HG11 | 4:AD:174:LEU:HB2 | 1.96 | 0.46 |
| 4:AD:108:LEU:HG | 4:AD:176:LEU:HD13 | 1.96 | 0.46 |
| 4:AD:83:SER:HA | 4:AD:89:THR:HG21 | 1.97 | 0.46 |
| 12:AL:64:TYR:N | 12:AL:64:TYR:CD1 | 2.83 | 0.46 |
| 19:AS:36:ARG:HB3 | 19:AS:51:VAL:HG13 | 1.97 | 0.46 |
| 1:AA:186:C:H5' | 20:AT:78:ALA:HB1 | 1.97 | 0.46 |
| 22:AV:21:A:O2' | 22:AV:22:G:H5'' | 2.16 | 0.46 |
| 7:AG:86:GLN:NE2 | 22:AW:39:U:H5 | 2.13 | 0.46 |
| 22:AW:71:G:C2' | 22:AW:72:C:H5' | 2.45 | 0.46 |
| 28:B2:32:LEU:HD23 | 28:B2:32:LEU:O | 2.14 | 0.46 |
| 31:B5:3:LYS:HD3 | 36:BA:747:U:OP1 | 2.15 | 0.46 |
| 34:B8:61:LEU:CD1 | 34:B8:62:LEU:N | 2.75 | 0.46 |
| 36:BA:1178:C:H2' | 36:BA:1179:C:C6 | 2.50 | 0.46 |
| 36:BA:1754:C:N3 | 36:BA:2716:U:O2' | 2.45 | 0.46 |
| 36:BA:1946:U:H2' | 36:BA:1947:C:H6 | 1.78 | 0.46 |
| 36:BA:1967:C:C2' | 36:BA:1968:G:H5' | 2.46 | 0.46 |
| 36:BA:2691:C:H5' | 36:BA:2691:C:H6 | 1.80 | 0.46 |
| 36:BA:2856:C:O2' | 36:BA:2857:G:H5' | 2.15 | 0.46 |
| 36:BA:693:C:O2' | 36:BA:694:U:H5' | 2.15 | 0.46 |
| 36:BA:718:A:C2' | 36:BA:719:C:H5' | 2.44 | 0.46 |
| 36:BA:921:G:H4' | 36:BA:2269:A:C5 | 2.51 | 0.46 |
| 37:BB:13:A:H2' | 37:BB:14:U:H5'' | 1.97 | 0.46 |
| 39:BD:273:ARG:O | 39:BD:274:ARG:CG | 2.64 | 0.46 |
| 41:BF:31:HIS:HB2 | 48:BP:13:ASN:OD1 | 2.14 | 0.46 |
| 49:BQ:21:THR:HG22 | 49:BQ:23:GLY:O | 2.15 | 0.46 |
| 36:BA:1075:C:OP1 | 49:BQ:59:ARG:NH2 | 2.49 | 0.46 |
| 52:BT:31:SER:HB2 | 52:BT:32:TYR:CD2 | 2.51 | 0.46 |
| 52:BT:50:ILE:HG23 | 52:BT:99:LEU:O | 2.16 | 0.46 |
| 53:BU:58:ARG:O | 53:BU:62:ILE:HG13 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:BU:76:TYR:O | 53:BU:80:ILE:HG12 | 2.14 | 0.46 |
| 55:BW:18:ARG:HG3 | 55:BW:18:ARG:HH11 | 1.80 | 0.46 |
| 55:BW:89:ALA:O | 55:BW:90:ARG:HB2 | 2.15 | 0.46 |
| 56:BX:54:VAL:HG21 | 56:BX:81:VAL:HG12 | 1.97 | 0.46 |
| 57:BY:74:PRO:HG2 | 57:BY:80:GLY:O | 2.14 | 0.46 |
| 58:BZ:63:ASP:C | 58:BZ:65:GLN:H | 2.16 | 0.46 |
| 1:AA:102:G:C4 | 1:AA:103:C:C5 | 3.04 | 0.46 |
| 1:AA:437:U:H2' | 1:AA:438:G:C8 | 2.50 | 0.46 |
| 1:AA:457:C:C2 | 1:AA:458:C:C5 | 3.04 | 0.46 |
| 1:AA:782:A:H4' | 1:AA:1514:C:O2' | 2.15 | 0.46 |
| 1:AA:930:C:O2' | 1:AA:931:C:H5' | 2.15 | 0.46 |
| 1:AA:954:G:H4' | 13:AM:120:LYS:HD2 | 1.97 | 0.46 |
| 3:AC:180:ALA:O | 3:AC:181:ASN:CB | 2.54 | 0.46 |
| 4:AD:126:ILE:HD12 | 4:AD:126:ILE:N | 2.30 | 0.46 |
| 4:AD:12:CYS:O | 4:AD:33:MET:CE | 2.62 | 0.46 |
| 4:AD:173:TRP:CD2 | 4:AD:189:PRO:HB3 | 2.50 | 0.46 |
| 7:AG:114:ARG:HG2 | 7:AG:114:ARG:H | 1.51 | 0.46 |
| 7:AG:86:GLN:NE2 | 22:AW:39:U:C5 | 2.84 | 0.46 |
| 8:AH:43:GLY:O | 8:AH:64:LYS:NZ | 2.37 | 0.46 |
| 13:AM:112:GLY:O | 13:AM:113:PRO:C | 2.53 | 0.46 |
| 14:AN:41:ARG:HH21 | 14:AN:42:ILE:HD11 | 1.80 | 0.46 |
| 15:AO:75:PRO:O | 15:AO:79:ARG:HG3 | 2.15 | 0.46 |
| 19:AS:43:GLU:HG2 | 19:AS:43:GLU:O | 2.14 | 0.46 |
| 23:AX:26:A:N3 | 23:AX:26:A:O2' | 2.38 | 0.46 |
| 36:BA:1270:C:H5'' | 36:BA:1271:G:H5' | 1.98 | 0.46 |
| 36:BA:1536:C:N3 | 36:BA:1537:G:H1' | 2.30 | 0.46 |
| 28:B2:47:ASN:ND2 | 36:BA:94(A):G:H21 | 2.14 | 0.46 |
| 36:BA:986:C:O2' | 36:BA:987:G:H5' | 2.15 | 0.46 |
| 38:BC:149:ILE:CG2 | 38:BC:150:GLY:N | 2.79 | 0.46 |
| 38:BC:14:VAL:CG1 | 38:BC:222:VAL:HG13 | 2.46 | 0.46 |
| 38:BC:75:LEU:HD11 | 38:BC:113:VAL:HG13 | 1.98 | 0.46 |
| 43:BH:33:LEU:HD21 | 43:BH:136:ILE:HG22 | 1.97 | 0.46 |
| 46:BN:94:HIS:N | 46:BN:95:PRO:CD | 2.78 | 0.46 |
| 48:BP:130:PHE:CB | 48:BP:135:LEU:HD23 | 2.46 | 0.46 |
| 48:BP:46:LYS:HG2 | 48:BP:52:GLU:OE2 | 2.16 | 0.46 |
| 50:BR:7:GLY:O | 50:BR:8:ARG:CB | 2.59 | 0.46 |
| 51:BS:30:ARG:NH2 | 51:BS:62:LYS:CD | 2.79 | 0.46 |
| 52:BT:22:PHE:CD1 | 52:BT:22:PHE:C | 2.89 | 0.46 |
| 58:BZ:125:LEU:HD23 | 58:BZ:164:ALA:O | 2.16 | 0.46 |
| 1:AA:1001(A):G:H8 | 1:AA:1002:G:C8 | 2.33 | 0.46 |
| 1:AA:155:C:O2' | 1:AA:156:G:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:186:C:C2 | 1:AA:187:C:H5 | 2.33 | 0.46 |
| 1:AA:349:A:O2' | 1:AA:350:G:H5' | 2.16 | 0.46 |
| 1:AA:625:G:H2' | 1:AA:626:U:H6 | 1.80 | 0.46 |
| 1:AA:671:G:H2' | 1:AA:672:U:C6 | 2.51 | 0.46 |
| 1:AA:684:A:N6 | 1:AA:685:G:C6 | 2.84 | 0.46 |
| 2:AB:179:LYS:O | 2:AB:179:LYS:HG2 | 2.15 | 0.46 |
| 3:AC:164:ARG:HH22 | 3:AC:166:GLU:CD | 2.18 | 0.46 |
| 7:AG:16:LEU:HA | 7:AG:16:LEU:HD23 | 1.80 | 0.46 |
| 9:AI:126:SER:O | 9:AI:127:LYS:HB3 | 2.15 | 0.46 |
| 9:AI:82:ALA:O | 9:AI:84:ALA:N | 2.49 | 0.46 |
| 9:AI:89:ASN:HB3 | 9:AI:92:TYR:CD1 | 2.50 | 0.46 |
| 10:AJ:40:LEU:CD2 | 10:AJ:40:LEU:H | 2.24 | 0.46 |
| 10:AJ:75:ILE:O | 10:AJ:77:PRO:HD3 | 2.16 | 0.46 |
| 1:AA:625:G:H4' | 16:AP:16:HIS:CD2 | 2.50 | 0.46 |
| 16:AP:4:ILE:HG23 | 16:AP:36:ILE:HD11 | 1.97 | 0.46 |
| 18:AR:44:LEU:O | 18:AR:45:SER:C | 2.54 | 0.46 |
| 19:AS:40:ILE:CG2 | 19:AS:67:VAL:HA | 2.45 | 0.46 |
| 25:AZ:138:VAL:HG21 | 25:AZ:173:GLY:N | 2.30 | 0.46 |
| 25:AZ:19:HIS:CG | 25:AZ:20:VAL:N | 2.84 | 0.46 |
| 25:AZ:29:ALA:O | 25:AZ:32:THR:HB | 2.14 | 0.46 |
| 36:BA:1060:U:H1' | 36:BA:1061:U:C5' | 2.46 | 0.46 |
| 36:BA:1582:C:O2' | 36:BA:1586:A:C8 | 2.66 | 0.46 |
| 36:BA:2131:G:H5'' | 36:BA:2132:U:C5' | 2.45 | 0.46 |
| 36:BA:2283:C:H2' | 36:BA:2284:C:C5' | 2.43 | 0.46 |
| 36:BA:2488:A:O2' | 36:BA:2489:G:H5' | 2.16 | 0.46 |
| 36:BA:2529:G:H5'' | 36:BA:2530:A:H5'' | 1.98 | 0.46 |
| 36:BA:2836:U:C4 | 36:BA:2883:A:N6 | 2.83 | 0.46 |
| 36:BA:483:A:H4' | 57:BY:48:ALA:O | 2.16 | 0.46 |
| 36:BA:654(S):G:H2' | 36:BA:654(T):C:O4' | 2.14 | 0.46 |
| 36:BA:92:A:H2' | 36:BA:93:G:O4' | 2.15 | 0.46 |
| 36:BA:948:G:O2' | 36:BA:949:C:H5' | 2.15 | 0.46 |
| 37:BB:32:C:O4' | 37:BB:53:A:N1 | 2.48 | 0.46 |
| 38:BC:163:PHE:CD1 | 38:BC:171:ILE:HD11 | 2.50 | 0.46 |
| 38:BC:25:ALA:O | 38:BC:29:VAL:HG22 | 2.14 | 0.46 |
| 39:BD:79:VAL:CG1 | 39:BD:113:VAL:HA | 2.46 | 0.46 |
| 39:BD:16:MET:CE | 39:BD:208:LYS:HD3 | 2.46 | 0.46 |
| 36:BA:2572:A:N7 | 40:BE:144:ARG:HD3 | 2.30 | 0.46 |
| 41:BF:156:LEU:HD21 | 41:BF:163:VAL:CG1 | 2.45 | 0.46 |
| 41:BF:157:VAL:O | 41:BF:157:VAL:HG23 | 2.16 | 0.46 |
| 42:BG:91:ARG:HG3 | 42:BG:91:ARG:NH1 | 2.31 | 0.46 |
| 43:BH:137:ASP:HB3 | 43:BH:140:LYS:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:832:G:H21 | 48:BP:53:GLY:CA | 2.28 | 0.46 |
| 36:BA:2876:G:OP1 | 52:BT:4:GLY:HA3 | 2.16 | 0.46 |
| 54:BV:2:PHE:O | 54:BV:3:ALA:HB2 | 2.15 | 0.46 |
| 54:BV:64:HIS:HA | 54:BV:92:THR:HG22 | 1.97 | 0.46 |
| 58:BZ:140:ASP:C | 58:BZ:141:VAL:HG23 | 2.36 | 0.46 |
| 58:BZ:29:TYR:HB3 | 58:BZ:34:ASN:HA | 1.96 | 0.46 |
| 2:AB:43:ASP:O | 2:AB:45:GLN:N | 2.49 | 0.46 |
| 2:AB:60:ASP:OD2 | 2:AB:60:ASP:O | 2.33 | 0.46 |
| 1:AA:427:U:OP1 | 4:AD:13:ARG:NH2 | 2.48 | 0.46 |
| 1:AA:921:U:O2 | 5:AE:19:MET:HB2 | 2.15 | 0.46 |
| 10:AJ:4:ILE:HA | 10:AJ:99:LYS:O | 2.16 | 0.46 |
| 11:AK:120:ARG:HG3 | 11:AK:120:ARG:NH1 | 2.28 | 0.46 |
| 14:AN:12:ARG:HB3 | 14:AN:12:ARG:HH11 | 1.81 | 0.46 |
| 22:AV:75:C:OP1 | 36:BA:2602:A:H5'' | 2.16 | 0.46 |
| 23:AX:26:A:H2' | 23:AX:27:A:O4' | 2.15 | 0.46 |
| 25:AZ:265:THR:CG2 | 25:AZ:266:VAL:H | 2.25 | 0.46 |
| 32:B6:8:LYS:CG | 32:B6:25:LYS:HD3 | 2.46 | 0.46 |
| 32:B6:26:ASN:ND2 | 32:B6:32:ASN:OD1 | 2.48 | 0.46 |
| 36:BA:1141:U:H6 | 46:BN:63:THR:HG21 | 1.81 | 0.46 |
| 36:BA:1368:G:O2' | 36:BA:1369:G:H5' | 2.16 | 0.46 |
| 36:BA:1385:G:O2' | 36:BA:1396:U:H6 | 1.98 | 0.46 |
| 36:BA:2107:C:H2' | 36:BA:2108:C:H6 | 1.81 | 0.46 |
| 36:BA:2094:G:N2 | 36:BA:2196:C:H1' | 2.31 | 0.46 |
| 36:BA:1889:A:N1 | 36:BA:2234:G:H1' | 2.31 | 0.46 |
| 36:BA:622:G:H2' | 36:BA:623:G:H8 | 1.81 | 0.46 |
| 38:BC:14:VAL:CG2 | 38:BC:28:LEU:HD21 | 2.45 | 0.46 |
| 38:BC:70:LYS:HE3 | 38:BC:70:LYS:HA | 1.97 | 0.46 |
| 39:BD:58:HIS:HD2 | 39:BD:59:LYS:O | 1.98 | 0.46 |
| 40:BE:198:VAL:CG1 | 40:BE:199:ARG:N | 2.79 | 0.46 |
| 36:BA:2787:C:H1' | 40:BE:61:ARG:HG3 | 1.98 | 0.46 |
| 41:BF:181:LEU:CD2 | 41:BF:202:PHE:HD1 | 2.28 | 0.46 |
| 47:BO:3:GLN:O | 47:BO:21:CYS:HB3 | 2.16 | 0.46 |
| 47:BO:34:THR:HG23 | 47:BO:35:VAL:N | 2.30 | 0.46 |
| 36:BA:811:U:H6 | 48:BP:24:GLY:O | 1.98 | 0.46 |
| 49:BQ:134:ARG:NH1 | 58:BZ:122:ARG:NH2 | 2.64 | 0.46 |
| 54:BV:17:GLY:O | 54:BV:18:LEU:HD13 | 2.15 | 0.46 |
| 55:BW:79:GLY:N | 55:BW:100:THR:O | 2.46 | 0.46 |
| 57:BY:50:ARG:CG | 57:BY:53:PRO:HA | 2.45 | 0.46 |
| 1:AA:1130:A:C2 | 1:AA:1146:A:C4 | 3.04 | 0.46 |
| 1:AA:344:A:H4' | 1:AA:345:C:OP2 | 2.15 | 0.46 |
| 2:AB:194:PRO:O | 2:AB:195:ASP:C | 2.52 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:112:SER:HB3 | 3:AC:115:LEU:HD12 | 1.98 | 0.46 |
| 4:AD:122:ARG:HA | 4:AD:122:ARG:HH11 | 1.79 | 0.46 |
| 5:AE:147:ASP:O | 5:AE:151:LEU:HG | 2.16 | 0.46 |
| 10:AJ:45:ARG:NE | 14:AN:36:PHE:CD2 | 2.84 | 0.46 |
| 17:AQ:34:LYS:HG2 | 17:AQ:35:VAL:N | 2.31 | 0.46 |
| 17:AQ:76:LEU:HD21 | 17:AQ:79:SER:HB2 | 1.98 | 0.46 |
| 25:AZ:98:GLN:O | 25:AZ:241:ARG:NH2 | 2.49 | 0.46 |
| 34:B8:46:ARG:HH11 | 34:B8:46:ARG:HG2 | 1.80 | 0.46 |
| 34:B8:53:PRO:O | 34:B8:54:GLU:C | 2.54 | 0.46 |
| 36:BA:1049:C:O2' | 36:BA:1050:A:H5' | 2.16 | 0.46 |
| 36:BA:1173:G:H5' | 36:BA:1174:A:P | 2.56 | 0.46 |
| 36:BA:1590:U:O2' | 36:BA:1591:G:H5'' | 2.16 | 0.46 |
| 36:BA:1625:C:H2' | 36:BA:1626:G:H5' | 1.98 | 0.46 |
| 36:BA:2461:C:H2' | 36:BA:2462:U:C6 | 2.51 | 0.46 |
| 36:BA:271(Q):G:O2' | 36:BA:271(R):G:OP2 | 2.31 | 0.46 |
| 38:BC:120:MET:SD | 38:BC:123:VAL:HG11 | 2.56 | 0.46 |
| 38:BC:74:VAL:HG21 | 38:BC:157:LYS:HG2 | 1.97 | 0.46 |
| 38:BC:21:THR:O | 38:BC:25:ALA:CB | 2.63 | 0.46 |
| 39:BD:53:PHE:CE2 | 39:BD:220:HIS:ND1 | 2.83 | 0.46 |
| 39:BD:35:LYS:HD2 | 39:BD:36:PRO:HA | 1.97 | 0.46 |
| 42:BG:133:LEU:C | 42:BG:133:LEU:HD12 | 2.36 | 0.46 |
| 48:BP:110:TYR:CD2 | 48:BP:111:ARG:HD3 | 2.51 | 0.46 |
| 48:BP:56:SER:C | 48:BP:57:THR:CG2 | 2.83 | 0.46 |
| 52:BT:115:ARG:NH1 | 52:BT:115:ARG:HG3 | 2.31 | 0.46 |
| 52:BT:87:ASP:O | 52:BT:87:ASP:OD2 | 2.33 | 0.46 |
| 53:BU:67:ALA:O | 53:BU:71:GLN:HB2 | 2.16 | 0.46 |
| 54:BV:52:VAL:HG22 | 54:BV:52:VAL:O | 2.16 | 0.46 |
| 57:BY:29:GLU:OE2 | 57:BY:38:ILE:HG21 | 2.15 | 0.46 |
| 57:BY:78:ALA:O | 57:BY:79:CYS:HB3 | 2.16 | 0.46 |
| 1:AA:1158:C:O2 | 1:AA:1158:C:C2' | 2.64 | 0.46 |
| 1:AA:22:G:H2' | 1:AA:23:C:H6 | 1.81 | 0.46 |
| 1:AA:35:G:H2' | 1:AA:36:C:H6 | 1.80 | 0.46 |
| 1:AA:379:C:O2' | 1:AA:380:G:H5' | 2.16 | 0.46 |
| 1:AA:841:U:O2' | 1:AA:848:C:H5' | 2.16 | 0.46 |
| 1:AA:981:U:H6 | 1:AA:981:U:O5' | 1.99 | 0.46 |
| 2:AB:136:VAL:O | 2:AB:140:HIS:HB2 | 2.16 | 0.46 |
| 2:AB:221:LEU:C | 2:AB:221:LEU:HD13 | 2.37 | 0.46 |
| 9:AI:73:GLN:O | 9:AI:76:ALA:HB3 | 2.15 | 0.46 |
| 1:AA:966:G:C4 | 22:AV:34:G:H4' | 2.51 | 0.46 |
| 25:AZ:303:VAL:CG1 | 25:AZ:304:LEU:N | 2.71 | 0.46 |
| 25:AZ:258:LEU:HD21 | 25:AZ:349:VAL:HG11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:AZ:40:PRO:HG2 | 25:AZ:41:ASN:OD1 | 2.16 | 0.46 |
| 26:B0:37:LEU:N | 26:B0:59:LEU:O | 2.48 | 0.46 |
| 36:BA:1062:G:C2 | 36:BA:1063:G:H1' | 2.51 | 0.46 |
| 36:BA:1204:A:C2 | 36:BA:1241:A:N1 | 2.84 | 0.46 |
| 36:BA:1373:A:H2' | 36:BA:1374:G:O4' | 2.16 | 0.46 |
| 36:BA:1517:G:H5' | 36:BA:1517:G:C8 | 2.51 | 0.46 |
| 36:BA:1543:C:C3' | 36:BA:1544:A:C5' | 2.87 | 0.46 |
| 36:BA:2287:A:C2 | 36:BA:2346:A:C2 | 3.04 | 0.46 |
| 36:BA:272(D):G:H1 | 36:BA:364:C:N4 | 2.13 | 0.46 |
| 36:BA:673:C:H6 | 36:BA:673:C:C5' | 2.20 | 0.46 |
| 36:BA:947:G:H2' | 36:BA:948:G:H8 | 1.81 | 0.46 |
| 36:BA:1820:U:C2 | 39:BD:202:LYS:HB3 | 2.51 | 0.46 |
| 39:BD:224:ALA:O | 39:BD:225:ALA:CB | 2.63 | 0.46 |
| 39:BD:26:LYS:O | 39:BD:27:THR:CG2 | 2.63 | 0.46 |
| 39:BD:30:GLU:HG3 | 39:BD:63:ARG:HH21 | 1.81 | 0.46 |
| 40:BE:44:TYR:CD2 | 40:BE:45:THR:O | 2.69 | 0.46 |
| 41:BF:118:ALA:O | 41:BF:121:GLY:N | 2.36 | 0.46 |
| 41:BF:132:VAL:O | 41:BF:134:GLY:N | 2.48 | 0.46 |
| 42:BG:16:ARG:HE | 42:BG:31:VAL:HG11 | 1.81 | 0.46 |
| 43:BH:85:LYS:CE | 43:BH:133:VAL:H | 2.29 | 0.46 |
| 43:BH:23:ARG:O | 43:BH:24:VAL:HG23 | 2.16 | 0.46 |
| 43:BH:42:ARG:HG2 | 43:BH:43:VAL:N | 2.31 | 0.46 |
| 46:BN:55:VAL:HG21 | 46:BN:127:ASP:N | 2.31 | 0.46 |
| 48:BP:122:PRO:HB3 | 48:BP:141:ALA:HB3 | 1.98 | 0.46 |
| 48:BP:147:LEU:HG | 48:BP:148:LEU:H | 1.80 | 0.46 |
| 52:BT:13:ARG:NE | 52:BT:13:ARG:HA | 2.29 | 0.46 |
| 53:BU:95:LEU:HD12 | 54:BV:11:GLN:HG3 | 1.96 | 0.46 |
| 57:BY:13:VAL:CG1 | 57:BY:28:LYS:HZ3 | 2.27 | 0.46 |
| 57:BY:95:LYS:HG3 | 57:BY:100:ALA:CA | 2.35 | 0.46 |
| 1:AA:1286:A:O2' | 1:AA:1287:A:P | 2.74 | 0.46 |
| 1:AA:147:G:N3 | 1:AA:147:G:H2' | 2.30 | 0.46 |
| 1:AA:262:A:C6 | 1:AA:263:A:C6 | 3.03 | 0.46 |
| 1:AA:390:C:H2' | 1:AA:391:G:H8 | 1.79 | 0.46 |
| 1:AA:805:C:O2' | 1:AA:806:C:H5' | 2.15 | 0.46 |
| 1:AA:76:C:H42 | 1:AA:93:G:H1 | 1.63 | 0.46 |
| 2:AB:221:LEU:O | 2:AB:221:LEU:HD13 | 2.15 | 0.46 |
| 4:AD:157:LEU:N | 4:AD:157:LEU:HD12 | 2.31 | 0.46 |
| 7:AG:45:ASP:O | 7:AG:48:LYS:HB2 | 2.16 | 0.46 |
| 9:AI:65:VAL:HG22 | 9:AI:66:ARG:N | 2.31 | 0.46 |
| 12:AL:87:GLY:HA2 | 12:AL:98:TYR:HA | 1.97 | 0.46 |
| 13:AM:32:GLU:O | 13:AM:34:LEU:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:AQ:91:ARG:NH1 | 17:AQ:91:ARG:CB | 2.79 | 0.46 |
| 19:AS:60:VAL:HG13 | 19:AS:60:VAL:O | 2.15 | 0.46 |
| 23:AX:14:A:H2' | 23:AX:15:A:O4' | 2.16 | 0.46 |
| 26:B0:20:ARG:CD | 26:B0:20:ARG:H | 2.27 | 0.46 |
| 26:B0:23:VAL:HG22 | 26:B0:38:VAL:HG22 | 1.98 | 0.46 |
| 28:B2:68:ARG:C | 28:B2:69:ARG:HG3 | 2.37 | 0.46 |
| 30:B4:28:LYS:HE2 | 30:B4:29:PRO:HD2 | 1.98 | 0.46 |
| 30:B4:12:ALA:HB2 | 30:B4:29:PRO:HA | 1.98 | 0.46 |
| 31:B5:40:LYS:HE2 | 31:B5:46:CYS:CB | 2.46 | 0.46 |
| 32:B6:15:GLU:OE2 | 32:B6:18:ARG:NH2 | 2.49 | 0.46 |
| 34:B8:47:LYS:CB | 34:B8:47:LYS:NZ | 2.72 | 0.46 |
| 36:BA:1109:C:C2' | 36:BA:1110:G:H5' | 2.46 | 0.46 |
| 36:BA:1742:G:N7 | 36:BA:1743:C:C4 | 2.84 | 0.46 |
| 36:BA:2312:U:H4' | 42:BG:71:THR:HG22 | 1.98 | 0.46 |
| 36:BA:497:A:H2' | 36:BA:498:G:C8 | 2.51 | 0.46 |
| 36:BA:673:C:H2' | 36:BA:674:G:H5' | 1.98 | 0.46 |
| 36:BA:69:C:H2' | 36:BA:69:C:O2 | 2.16 | 0.46 |
| 36:BA:733:G:N7 | 36:BA:761:A:C5 | 2.83 | 0.46 |
| 36:BA:943:U:OP2 | 48:BP:38:GLN:CG | 2.64 | 0.46 |
| 37:BB:75:G:H5' | 37:BB:76:G:OP2 | 2.16 | 0.46 |
| 38:BC:21:THR:O | 38:BC:25:ALA:HB3 | 2.16 | 0.46 |
| 38:BC:72:VAL:HG11 | 38:BC:156:ILE:O | 2.16 | 0.46 |
| 39:BD:132:PRO:O | 39:BD:136:ILE:HD12 | 2.16 | 0.46 |
| 39:BD:97:TYR:C | 39:BD:99:ASP:N | 2.67 | 0.46 |
| 40:BE:200:GLU:H | 40:BE:200:GLU:CD | 2.18 | 0.46 |
| 41:BF:152:GLU:OE1 | 41:BF:191:ARG:HD2 | 2.16 | 0.46 |
| 42:BG:171:ALA:O | 42:BG:172:LEU:C | 2.54 | 0.46 |
| 42:BG:64:THR:HG1 | 42:BG:94:LEU:HD11 | 1.81 | 0.46 |
| 46:BN:51:PHE:CE1 | 46:BN:119:ARG:HD2 | 2.51 | 0.46 |
| 46:BN:123:TYR:CD1 | 46:BN:123:TYR:N | 2.84 | 0.46 |
| 48:BP:97:PRO:HD3 | 48:BP:126:VAL:O | 2.15 | 0.46 |
| 36:BA:807:U:H5 | 48:BP:39:LYS:HZ1 | 1.64 | 0.46 |
| 48:BP:77:ARG:HH11 | 48:BP:77:ARG:CG | 2.29 | 0.46 |
| 54:BV:70:ILE:HG22 | 54:BV:71:LEU:N | 2.31 | 0.46 |
| 57:BY:38:ILE:CD1 | 57:BY:66:PRO:HG3 | 2.46 | 0.46 |
| 58:BZ:162:GLU:O | 58:BZ:163:LEU:O | 2.34 | 0.46 |
| 58:BZ:70:LEU:N | 58:BZ:70:LEU:CD2 | 2.79 | 0.46 |
| 1:AA:1195:C:H5'' | 1:AA:1196:U:OP2 | 2.15 | 0.46 |
| 1:AA:274:A:O2' | 1:AA:275:G:C8 | 2.64 | 0.46 |
| 1:AA:324:G:N2 | 1:AA:326:G:H3' | 2.32 | 0.46 |
| 1:AA:911:U:H2' | 1:AA:912:C:C6 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:936:C:H2' | 1:AA:937:A:O4' | 2.16 | 0.46 |
| 2:AB:41:ILE:O | 2:AB:41:ILE:HG22 | 2.15 | 0.46 |
| 5:AE:20:GLN:HE21 | 5:AE:25:ARG:NE | 2.13 | 0.46 |
| 7:AG:79:ARG:HA | 7:AG:84:ASN:HA | 1.98 | 0.46 |
| 8:AH:17:THR:HB | 8:AH:78:GLN:OE1 | 2.16 | 0.46 |
| 11:AK:13:GLN:HG2 | 11:AK:75:TYR:O | 2.15 | 0.46 |
| 11:AK:69:ALA:O | 11:AK:73:MET:HG3 | 2.15 | 0.46 |
| 13:AM:19:LEU:HB3 | 13:AM:25:ILE:HG21 | 1.98 | 0.46 |
| 13:AM:29:ARG:O | 13:AM:32:GLU:N | 2.48 | 0.46 |
| 19:AS:46:GLY:N | 19:AS:62:ILE:CG2 | 2.74 | 0.46 |
| 20:AT:29:LYS:O | 20:AT:33:ILE:HG13 | 2.16 | 0.46 |
| 24:AY:28:C:O2' | 24:AY:29:G:H5' | 2.16 | 0.46 |
| 24:AY:7:G:H3' | 24:AY:8:4SU:C5' | 2.46 | 0.46 |
| 25:AZ:324:LYS:HE3 | 25:AZ:364:PRO:CB | 2.46 | 0.46 |
| 30:B4:20:ASN:C | 30:B4:20:ASN:ND2 | 2.69 | 0.46 |
| 36:BA:1375:C:O2' | 36:BA:1376:C:H5' | 2.16 | 0.46 |
| 36:BA:1398:C:H2' | 36:BA:1399:C:C6 | 2.50 | 0.46 |
| 36:BA:1788:C:H2' | 36:BA:1789:A:H8 | 1.81 | 0.46 |
| 36:BA:2223:G:H2' | 36:BA:2224:G:C5' | 2.45 | 0.46 |
| 36:BA:2641:G:H2' | 36:BA:2642:G:O4' | 2.16 | 0.46 |
| 36:BA:2870:C:H2' | 36:BA:2871:C:H5' | 1.97 | 0.46 |
| 36:BA:491:G:H2' | 36:BA:492:A:H8 | 1.79 | 0.46 |
| 36:BA:510:C:H2' | 36:BA:511:U:O4' | 2.15 | 0.46 |
| 36:BA:615:G:H2' | 36:BA:616:G:O4' | 2.16 | 0.46 |
| 34:B8:48:PHE:CZ | 36:BA:650:C:OP1 | 2.69 | 0.46 |
| 36:BA:738:G:C6 | 36:BA:739:G:C6 | 3.03 | 0.46 |
| 36:BA:880:G:H2' | 36:BA:881:G:H8 | 1.81 | 0.46 |
| 37:BB:71:C:H42 | 37:BB:106:G:H1 | 1.64 | 0.46 |
| 38:BC:14:VAL:HG11 | 38:BC:222:VAL:HG13 | 1.98 | 0.46 |
| 39:BD:35:LYS:O | 39:BD:36:PRO:C | 2.54 | 0.46 |
| 40:BE:188:VAL:O | 40:BE:188:VAL:HG13 | 2.16 | 0.46 |
| 41:BF:139:PHE:HB2 | 41:BF:166:ALA:HB1 | 1.98 | 0.46 |
| 48:BP:106:LEU:O | 48:BP:107:LYS:CG | 2.64 | 0.46 |
| 52:BT:56:GLY:O | 52:BT:57:PHE:C | 2.54 | 0.46 |
| 54:BV:37:VAL:HG23 | 54:BV:37:VAL:O | 2.16 | 0.46 |
| 54:BV:40:LEU:HD13 | 54:BV:46:VAL:HA | 1.96 | 0.46 |
| 58:BZ:103:ARG:O | 58:BZ:103:ARG:HG2 | 2.16 | 0.46 |
| 1:AA:1030:C:H2' | 1:AA:1030(A):G:H5' | 1.97 | 0.45 |
| 1:AA:1259:C:O5' | 1:AA:1259:C:H6 | 1.99 | 0.45 |
| 1:AA:1343:G:H2' | 1:AA:1344:C:C6 | 2.51 | 0.45 |
| 1:AA:1499:A:C1' | 1:AA:1520:G:H5' | 2.43 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:198:G:O2' | 1:AA:199:G:O5' | 2.34 | 0.45 |
| 1:AA:358:U:H2' | 1:AA:359:U:C6 | 2.51 | 0.45 |
| 1:AA:790:A:N1 | 1:AA:1497:G:H5'' | 2.31 | 0.45 |
| 1:AA:811:C:H4' | 1:AA:900:A:N6 | 2.31 | 0.45 |
| 2:AB:131:PRO:O | 2:AB:135:GLN:HG3 | 2.15 | 0.45 |
| 2:AB:69:LEU:HD23 | 2:AB:155:LEU:HG | 1.97 | 0.45 |
| 6:AF:22:GLU:O | 6:AF:24:GLU:N | 2.49 | 0.45 |
| 11:AK:57:THR:HG23 | 11:AK:59:TYR:N | 2.31 | 0.45 |
| 12:AL:50:SER:O | 12:AL:51:ALA:HB2 | 2.15 | 0.45 |
| 20:AT:27:LYS:O | 20:AT:27:LYS:HD3 | 2.16 | 0.45 |
| 20:AT:59:ALA:C | 20:AT:61:SER:N | 2.68 | 0.45 |
| 22:AV:44:G:N3 | 22:AV:44:G:H2' | 2.31 | 0.45 |
| 23:AX:26:A:O2' | 23:AX:27:A:P | 2.74 | 0.45 |
| 24:AY:5:G:O2' | 24:AY:6:C:H5' | 2.16 | 0.45 |
| 25:AZ:93:ILE:HG12 | 25:AZ:122:LEU:HD13 | 1.97 | 0.45 |
| 25:AZ:222:LEU:HB3 | 25:AZ:243:GLU:HB3 | 1.98 | 0.45 |
| 25:AZ:65:THR:HA | 25:AZ:81:ASP:O | 2.17 | 0.45 |
| 26:B0:56:ASP:O | 26:B0:57:PHE:HB2 | 2.15 | 0.45 |
| 27:B1:58:ILE:HD11 | 27:B1:91:LYS:HB2 | 1.99 | 0.45 |
| 34:B8:12:LYS:O | 48:BP:65:ARG:HB2 | 2.17 | 0.45 |
| 35:B9:2:LYS:HD3 | 35:B9:33:LYS:O | 2.16 | 0.45 |
| 36:BA:1069:A:H1' | 36:BA:1070:A:OP2 | 2.16 | 0.45 |
| 36:BA:1222:C:C3' | 36:BA:1223:G:H5'' | 2.45 | 0.45 |
| 36:BA:1517:G:C5' | 36:BA:1517:G:H8 | 2.29 | 0.45 |
| 36:BA:1717:G:H2' | 36:BA:1718:G:H5'' | 1.98 | 0.45 |
| 36:BA:196:A:O4' | 48:BP:46:LYS:HE2 | 2.17 | 0.45 |
| 26:B0:43:THR:HG22 | 36:BA:2331:G:O2' | 2.15 | 0.45 |
| 36:BA:2579:C:O3' | 40:BE:131:ALA:CB | 2.63 | 0.45 |
| 36:BA:299:A:N6 | 36:BA:339:U:H3 | 2.15 | 0.45 |
| 36:BA:729:G:C6 | 39:BD:208:LYS:HB2 | 2.51 | 0.45 |
| 36:BA:887:A:H2 | 36:BA:889:C:OP2 | 1.99 | 0.45 |
| 37:BB:68:C:H2' | 37:BB:69:G:H8 | 1.81 | 0.45 |
| 37:BB:78:A:C6 | 37:BB:100:A:C8 | 3.04 | 0.45 |
| 38:BC:99:ILE:CG2 | 38:BC:102:LYS:HD2 | 2.47 | 0.45 |
| 39:BD:224:ALA:HA | 39:BD:233:HIS:O | 2.16 | 0.45 |
| 39:BD:70:TRP:C | 39:BD:70:TRP:CD1 | 2.90 | 0.45 |
| 40:BE:34:VAL:HG12 | 40:BE:48:GLN:O | 2.16 | 0.45 |
| 41:BF:9:ILE:HG23 | 41:BF:13:SER:O | 2.16 | 0.45 |
| 41:BF:89:VAL:HG12 | 41:BF:90:PHE:CD2 | 2.51 | 0.45 |
| 48:BP:23:PRO:HD2 | 48:BP:33:ARG:HH21 | 1.80 | 0.45 |
| 52:BT:109:GLU:O | 52:BT:110:ILE:C | 2.53 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:BW:6:ILE:HG12 | 55:BW:104:THR:CG2 | 2.45 | 0.45 |
| 57:BY:86:ARG:HD2 | 57:BY:88:LYS:HE3 | 1.96 | 0.45 |
| 57:BY:88:LYS:N | 57:BY:88:LYS:HD2 | 2.31 | 0.45 |
| 58:BZ:19:ARG:HA | 58:BZ:23:LYS:O | 2.16 | 0.45 |
| 1:AA:1018:C:H2' | 1:AA:1019:C:C6 | 2.51 | 0.45 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:C4 | 2.51 | 0.45 |
| 1:AA:187:C:OP1 | 20:AT:82:SER:HB2 | 2.16 | 0.45 |
| 1:AA:338:A:H2' | 1:AA:339:C:O4' | 2.17 | 0.45 |
| 1:AA:575:G:H4' | 1:AA:576:G:O5' | 2.17 | 0.45 |
| 1:AA:662:G:H2' | 1:AA:663:A:C8 | 2.51 | 0.45 |
| 3:AC:181:ASN:ND2 | 3:AC:204:LEU:HB2 | 2.31 | 0.45 |
| 4:AD:126:ILE:HG22 | 4:AD:127:THR:N | 2.30 | 0.45 |
| 7:AG:144:MET:O | 7:AG:148:ASN:ND2 | 2.49 | 0.45 |
| 7:AG:23:VAL:CG1 | 7:AG:43:PHE:CE2 | 3.00 | 0.45 |
| 12:AL:6:THR:O | 12:AL:7:ILE:C | 2.54 | 0.45 |
| 16:AP:39:TYR:CD2 | 16:AP:73:LEU:HD11 | 2.52 | 0.45 |
| 1:AA:194:C:O3' | 20:AT:68:LYS:HD3 | 2.16 | 0.45 |
| 25:AZ:34:VAL:CG2 | 25:AZ:199:ILE:HG21 | 2.43 | 0.45 |
| 25:AZ:96:ALA:C | 25:AZ:98:GLN:N | 2.68 | 0.45 |
| 31:B5:12:SER:HB3 | 36:BA:2020:A:H5' | 1.98 | 0.45 |
| 36:BA:1056:G:C4 | 36:BA:1102:C:H5 | 2.34 | 0.45 |
| 36:BA:1210:A:H4' | 36:BA:1211:U:O5' | 2.17 | 0.45 |
| 36:BA:1537:G:H2' | 36:BA:1538:G:H8 | 1.80 | 0.45 |
| 36:BA:1980:G:O2' | 36:BA:1982:C:OP2 | 2.27 | 0.45 |
| 36:BA:2131:G:C4' | 36:BA:2133:G:H21 | 2.28 | 0.45 |
| 36:BA:2023:G:H4' | 36:BA:2617:C:O3' | 2.16 | 0.45 |
| 36:BA:2691:C:C4 | 36:BA:2719:G:N2 | 2.85 | 0.45 |
| 36:BA:83:G:H22 | 36:BA:102:G:C2' | 2.24 | 0.45 |
| 38:BC:155:GLU:HG3 | 38:BC:160:ARG:HD3 | 1.96 | 0.45 |
| 38:BC:163:PHE:CD2 | 38:BC:192:PHE:CE1 | 3.03 | 0.45 |
| 38:BC:62:VAL:HG22 | 38:BC:63:SER:N | 2.31 | 0.45 |
| 39:BD:142:VAL:HG22 | 39:BD:143:HIS:N | 2.31 | 0.45 |
| 41:BF:132:VAL:CG2 | 41:BF:133:ASN:H | 2.09 | 0.45 |
| 42:BG:7:LEU:HD22 | 42:BG:176:LEU:CD2 | 2.47 | 0.45 |
| 43:BH:20:ALA:CB | 43:BH:21:PRO:CD | 2.87 | 0.45 |
| 46:BN:67:LEU:O | 46:BN:68:GLU:CB | 2.64 | 0.45 |
| 46:BN:73:THR:HG23 | 46:BN:82:LEU:CD1 | 2.26 | 0.45 |
| 46:BN:67:LEU:HD22 | 46:BN:88:GLU:HG2 | 1.97 | 0.45 |
| 48:BP:107:LYS:HE3 | 48:BP:107:LYS:HB2 | 1.76 | 0.45 |
| 48:BP:125:VAL:CG1 | 48:BP:138:LEU:HD21 | 2.46 | 0.45 |
| 52:BT:7:ILE:O | 52:BT:11:GLU:OE2 | 2.33 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:445:C:O3' | 53:BU:3:ARG:HD3 | 2.17 | 0.45 |
| 58:BZ:69:THR:HG22 | 58:BZ:90:VAL:CA | 2.31 | 0.45 |
| 58:BZ:99:TYR:HA | 58:BZ:124:ILE:O | 2.16 | 0.45 |
| 1:AA:1004:A:N6 | 1:AA:1035:A:N7 | 2.64 | 0.45 |
| 1:AA:1134:G:C2 | 1:AA:1142:G:N1 | 2.83 | 0.45 |
| 1:AA:1486:G:H2' | 1:AA:1487:G:O4' | 2.15 | 0.45 |
| 1:AA:333:G:H2' | 1:AA:334:C:C6 | 2.51 | 0.45 |
| 1:AA:640:A:O2' | 1:AA:641:U:H5' | 2.17 | 0.45 |
| 2:AB:132:LYS:O | 2:AB:136:VAL:HG23 | 2.16 | 0.45 |
| 2:AB:233:SER:O | 2:AB:235:SER:N | 2.50 | 0.45 |
| 3:AC:72:LYS:HD3 | 3:AC:75:VAL:HG21 | 1.96 | 0.45 |
| 4:AD:78:LEU:HD21 | 4:AD:96:LEU:HB3 | 1.97 | 0.45 |
| 5:AE:78:HIS:CD2 | 8:AH:107:LEU:HD12 | 2.51 | 0.45 |
| 9:AI:114:TYR:HD2 | 9:AI:114:TYR:O | 2.00 | 0.45 |
| 9:AI:34:ASN:O | 9:AI:38:GLN:HB2 | 2.16 | 0.45 |
| 9:AI:4:TYR:CE2 | 9:AI:88:TYR:CB | 3.00 | 0.45 |
| 15:AO:32:LEU:O | 15:AO:35:ARG:N | 2.49 | 0.45 |
| 6:AF:7:ASN:ND2 | 18:AR:34:TYR:OH | 2.43 | 0.45 |
| 18:AR:50:ILE:HD13 | 18:AR:70:ILE:HG21 | 1.97 | 0.45 |
| 25:AZ:281:ILE:HG12 | 25:AZ:284:ASP:OD1 | 2.15 | 0.45 |
| 25:AZ:340:PRO:O | 25:AZ:350:THR:HG23 | 2.16 | 0.45 |
| 25:AZ:371:THR:CG2 | 25:AZ:372:VAL:H | 2.27 | 0.45 |
| 30:B4:14:ILE:HG13 | 30:B4:31:ILE:HB | 1.99 | 0.45 |
| 36:BA:1578:U:H2' | 36:BA:1579:A:C5' | 2.46 | 0.45 |
| 36:BA:1999:C:O2' | 36:BA:2000:G:H5' | 2.17 | 0.45 |
| 26:B0:20:ARG:HH12 | 36:BA:2271:G:H4' | 1.81 | 0.45 |
| 36:BA:471:A:C2' | 36:BA:472:A:C5' | 2.93 | 0.45 |
| 36:BA:483:A:H5'' | 57:BY:49:VAL:CG2 | 2.46 | 0.45 |
| 36:BA:673:C:C2' | 36:BA:674:G:H5' | 2.46 | 0.45 |
| 36:BA:925:C:C3' | 36:BA:926:A:H5'' | 2.47 | 0.45 |
| 36:BA:99:U:C6 | 36:BA:102:G:C2 | 3.04 | 0.45 |
| 37:BB:20:C:C3' | 37:BB:21:G:H5'' | 2.47 | 0.45 |
| 38:BC:67:GLY:CA | 38:BC:159:GLY:HA3 | 2.46 | 0.45 |
| 40:BE:197:ILE:HG13 | 40:BE:197:ILE:O | 2.17 | 0.45 |
| 41:BF:20:LEU:H | 41:BF:24:LEU:HD21 | 1.82 | 0.45 |
| 42:BG:133:LEU:HD13 | 42:BG:135:LEU:CD1 | 2.47 | 0.45 |
| 47:BO:68:GLU:HB3 | 47:BO:78:ARG:HB2 | 1.98 | 0.45 |
| 48:BP:147:LEU:HG | 48:BP:148:LEU:N | 2.30 | 0.45 |
| 48:BP:30:THR:HG22 | 48:BP:31:ALA:H | 1.81 | 0.45 |
| 48:BP:23:PRO:O | 48:BP:33:ARG:CD | 2.65 | 0.45 |
| 36:BA:1654:A:P | 50:BR:3:HIS:HB2 | 2.56 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:BS:89:ARG:CB | 51:BS:92:TYR:HB3 | 2.46 | 0.45 |
| 52:BT:134:GLU:O | 52:BT:135:ALA:CB | 2.64 | 0.45 |
| 54:BV:18:LEU:CD2 | 54:BV:19:LYS:N | 2.75 | 0.45 |
| 56:BX:23:GLU:N | 56:BX:23:GLU:CD | 2.70 | 0.45 |
| 57:BY:28:LYS:CA | 57:BY:38:ILE:HG22 | 2.46 | 0.45 |
| 57:BY:7:VAL:HB | 57:BY:8:LYS:H | 1.53 | 0.45 |
| 1:AA:1063:C:H2' | 1:AA:1064:G:C8 | 2.52 | 0.45 |
| 1:AA:436:C:H2' | 1:AA:437:U:C6 | 2.51 | 0.45 |
| 1:AA:453:A:O2' | 1:AA:454:C:C5' | 2.65 | 0.45 |
| 1:AA:479:C:O2' | 1:AA:480:U:H5' | 2.16 | 0.45 |
| 1:AA:518:C:H2' | 1:AA:530:G:C2 | 2.51 | 0.45 |
| 1:AA:849:C:H2' | 1:AA:850:U:C6 | 2.51 | 0.45 |
| 1:AA:858:G:C5 | 1:AA:869:G:N7 | 2.83 | 0.45 |
| 2:AB:138:LEU:O | 2:AB:140:HIS:N | 2.49 | 0.45 |
| 9:AI:29:ASN:OD1 | 9:AI:64:THR:HA | 2.16 | 0.45 |
| 14:AN:40:CYS:O | 14:AN:41:ARG:C | 2.53 | 0.45 |
| 16:AP:53:VAL:CG2 | 16:AP:54:GLU:N | 2.74 | 0.45 |
| 18:AR:25:THR:O | 18:AR:25:THR:HG22 | 2.16 | 0.45 |
| 19:AS:52:TYR:CE2 | 19:AS:54:GLY:HA2 | 2.52 | 0.45 |
| 20:AT:100:ILE:CD1 | 20:AT:100:ILE:N | 2.78 | 0.45 |
| 25:AZ:294:SER:C | 25:AZ:296:GLU:H | 2.20 | 0.45 |
| 31:B5:50:GLY:HA3 | 31:B5:56:LYS:CB | 2.45 | 0.45 |
| 32:B6:16:CYS:SG | 32:B6:48:VAL:O | 2.75 | 0.45 |
| 32:B6:17:LYS:CB | 32:B6:18:ARG:HH12 | 2.29 | 0.45 |
| 32:B6:20:ASN:C | 32:B6:21:TYR:CG | 2.90 | 0.45 |
| 35:B9:1:MET:N | 35:B9:1:MET:SD | 2.87 | 0.45 |
| 36:BA:1257:C:H4' | 41:BF:83:PHE:CE2 | 2.52 | 0.45 |
| 36:BA:1403:C:H2' | 36:BA:1404:C:O5' | 2.16 | 0.45 |
| 36:BA:1658:C:H2' | 36:BA:1659:U:H6 | 1.81 | 0.45 |
| 36:BA:2128:C:OP2 | 36:BA:2128:C:H6 | 1.99 | 0.45 |
| 36:BA:2396:G:O2' | 36:BA:2397:G:H5' | 2.16 | 0.45 |
| 36:BA:2508:G:O3' | 36:BA:2555:U:H5' | 2.16 | 0.45 |
| 36:BA:297:C:N4 | 36:BA:298:G:C2 | 2.85 | 0.45 |
| 36:BA:491:G:H2' | 36:BA:492:A:O4' | 2.16 | 0.45 |
| 37:BB:19:G:H2' | 37:BB:19:G:N3 | 2.31 | 0.45 |
| 37:BB:86:G:H2' | 37:BB:87:G:C8 | 2.49 | 0.45 |
| 39:BD:97:TYR:C | 39:BD:99:ASP:H | 2.19 | 0.45 |
| 40:BE:34:VAL:O | 40:BE:35:GLN:CB | 2.62 | 0.45 |
| 41:BF:206:ILE:HG22 | 41:BF:207:GLY:N | 2.21 | 0.45 |
| 42:BG:16:ARG:HE | 42:BG:31:VAL:CG1 | 2.30 | 0.45 |
| 43:BH:103:LEU:HB2 | 43:BH:123:PHE:HD2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:BH:54:ARG:HD3 | 43:BH:56:SER:O | 2.16 | 0.45 |
| 44:BJ:27:UNK:O | 44:BJ:83:UNK:N | 2.49 | 0.45 |
| 48:BP:6:LEU:H | 48:BP:6:LEU:CD2 | 2.13 | 0.45 |
| 50:BR:33:ARG:O | 50:BR:34:ILE:HG12 | 2.17 | 0.45 |
| 52:BT:65:LYS:HE3 | 52:BT:66:VAL:N | 2.07 | 0.45 |
| 52:BT:92:GLY:C | 52:BT:94:ALA:N | 2.69 | 0.45 |
| 53:BU:83:LEU:N | 53:BU:83:LEU:HD12 | 2.31 | 0.45 |
| 55:BW:29:LEU:CD2 | 55:BW:33:ARG:HD2 | 2.46 | 0.45 |
| 58:BZ:35:ARG:HH11 | 58:BZ:35:ARG:HG3 | 1.81 | 0.45 |
| 58:BZ:8:TYR:HD2 | 58:BZ:38:TYR:OH | 1.99 | 0.45 |
| 58:BZ:99:TYR:HD2 | 58:BZ:99:TYR:N | 2.14 | 0.45 |
| 1:AA:1050:G:O2' | 1:AA:1051:C:O5' | 2.34 | 0.45 |
| 1:AA:1245:A:H2' | 1:AA:1246:C:O4' | 2.17 | 0.45 |
| 1:AA:226:G:O2' | 1:AA:227:G:H5' | 2.16 | 0.45 |
| 1:AA:62:U:O2' | 1:AA:379:C:H1' | 2.16 | 0.45 |
| 1:AA:404:U:H2' | 1:AA:405:U:H6 | 1.79 | 0.45 |
| 1:AA:742:G:O2' | 1:AA:743:U:H5' | 2.17 | 0.45 |
| 1:AA:652:U:C2 | 1:AA:752:G:N2 | 2.84 | 0.45 |
| 1:AA:765:G:C6 | 1:AA:812:C:C2 | 3.05 | 0.45 |
| 4:AD:199:ASN:OD1 | 4:AD:199:ASN:C | 2.54 | 0.45 |
| 4:AD:3:ARG:O | 4:AD:4:TYR:C | 2.54 | 0.45 |
| 7:AG:92:SER:HB3 | 7:AG:95:ARG:CB | 2.47 | 0.45 |
| 7:AG:95:ARG:HH11 | 7:AG:95:ARG:HG3 | 1.82 | 0.45 |
| 8:AH:37:ARG:CZ | 8:AH:41:ARG:HH22 | 2.29 | 0.45 |
| 9:AI:95:LYS:HZ3 | 9:AI:96:LEU:HD13 | 1.81 | 0.45 |
| 11:AK:108:ILE:O | 18:AR:87:ARG:N | 2.46 | 0.45 |
| 18:AR:84:LYS:HZ3 | 18:AR:84:LYS:H | 1.65 | 0.45 |
| 24:AY:62:U:H5' | 24:AY:62:U:C6 | 2.42 | 0.45 |
| 25:AZ:98:GLN:O | 25:AZ:99:MET:C | 2.54 | 0.45 |
| 26:B0:45:PHE:CE2 | 26:B0:77:ARG:NH2 | 2.85 | 0.45 |
| 31:B5:4:HIS:CB | 31:B5:5:PRO:CD | 2.81 | 0.45 |
| 36:BA:1139:G:H5'' | 46:BN:70:LYS:HZ1 | 1.78 | 0.45 |
| 36:BA:1141:U:H4' | 36:BA:1142(A):A:C8 | 2.50 | 0.45 |
| 36:BA:142:A:H5'' | 36:BA:142(A):C:H5 | 1.82 | 0.45 |
| 36:BA:1484:G:C3' | 36:BA:1485:G:H5'' | 2.46 | 0.45 |
| 36:BA:2110:G:N2 | 36:BA:2178:C:H5 | 2.14 | 0.45 |
| 36:BA:2131:G:H4' | 36:BA:2132:U:OP2 | 2.16 | 0.45 |
| 26:B0:17:GLN:HB3 | 36:BA:2261:C:OP1 | 2.16 | 0.45 |
| 36:BA:2450:A:O2' | 36:BA:2451:A:H5' | 2.16 | 0.45 |
| 36:BA:2491:U:C5' | 36:BA:2570:G:H5'' | 2.22 | 0.45 |
| 36:BA:2584:U:C2' | 36:BA:2585:U:H5' | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:29:U:H2' | 36:BA:30:G:C8 | 2.52 | 0.45 |
| 36:BA:782:A:N1 | 39:BD:226:MET:HE3 | 2.32 | 0.45 |
| 36:BA:941:A:H4' | 48:BP:35:HIS:HE1 | 1.78 | 0.45 |
| 40:BE:35:GLN:O | 40:BE:36:ARG:HD2 | 2.16 | 0.45 |
| 42:BG:111:LEU:HB3 | 42:BG:112:PRO:HD3 | 1.97 | 0.45 |
| 42:BG:7:LEU:O | 42:BG:8:LYS:C | 2.54 | 0.45 |
| 43:BH:143:GLN:CA | 43:BH:143:GLN:NE2 | 2.78 | 0.45 |
| 43:BH:76:VAL:O | 43:BH:78:GLY:N | 2.49 | 0.45 |
| 46:BN:120:LEU:HD13 | 46:BN:122:VAL:HG23 | 1.97 | 0.45 |
| 46:BN:9:VAL:HG11 | 46:BN:39:ARG:NH1 | 2.32 | 0.45 |
| 48:BP:71:VAL:O | 48:BP:72:PRO:C | 2.55 | 0.45 |
| 48:BP:85:LEU:HA | 48:BP:88:LEU:HB2 | 1.99 | 0.45 |
| 50:BR:72:ASP:OD1 | 50:BR:75:LEU:HB2 | 2.17 | 0.45 |
| 52:BT:57:PHE:CD2 | 52:BT:57:PHE:C | 2.89 | 0.45 |
| 54:BV:40:LEU:CD2 | 54:BV:40:LEU:N | 2.80 | 0.45 |
| 55:BW:74:ALA:HB2 | 55:BW:105:VAL:HG13 | 1.97 | 0.45 |
| 56:BX:5:TYR:HE2 | 56:BX:46:ALA:HA | 1.81 | 0.45 |
| 58:BZ:44:PHE:CE1 | 58:BZ:48:PHE:CD1 | 3.05 | 0.45 |
| 1:AA:1401:G:C2 | 1:AA:1402:C:H1' | 2.52 | 0.45 |
| 1:AA:415:A:H2' | 1:AA:416:G:H8 | 1.82 | 0.45 |
| 1:AA:78:G:H2' | 1:AA:79:G:C4' | 2.47 | 0.45 |
| 2:AB:222:ILE:O | 2:AB:223:ILE:C | 2.55 | 0.45 |
| 2:AB:17:PHE:HD1 | 2:AB:44:LEU:HD11 | 1.82 | 0.45 |
| 1:AA:1350:A:N7 | 9:AI:118:LYS:NZ | 2.65 | 0.45 |
| 9:AI:14:VAL:HG12 | 9:AI:15:ALA:N | 2.31 | 0.45 |
| 10:AJ:29:ARG:O | 10:AJ:29:ARG:HG2 | 2.16 | 0.45 |
| 12:AL:119:LYS:O | 12:AL:120:TYR:CG | 2.70 | 0.45 |
| 14:AN:59:ALA:O | 14:AN:60:SER:HB3 | 2.16 | 0.45 |
| 15:AO:82:ILE:HD13 | 15:AO:82:ILE:O | 2.17 | 0.45 |
| 16:AP:21:VAL:HG12 | 16:AP:34:GLU:O | 2.17 | 0.45 |
| 16:AP:74:LEU:C | 16:AP:79:VAL:HG23 | 2.37 | 0.45 |
| 19:AS:12:ASP:H | 19:AS:38:SER:HB3 | 1.82 | 0.45 |
| 1:AA:1196:U:C5 | 23:AX:26:A:H1' | 2.51 | 0.45 |
| 25:AZ:234:ARG:HA | 25:AZ:234:ARG:NE | 2.21 | 0.45 |
| 26:B0:52:GLY:N | 26:B0:62:LEU:CD2 | 2.80 | 0.45 |
| 28:B2:8:LYS:O | 28:B2:11:GLU:HB2 | 2.16 | 0.45 |
| 29:B3:23:LEU:HD21 | 29:B3:50:VAL:HG11 | 1.97 | 0.45 |
| 30:B4:20:ASN:ND2 | 30:B4:21:VAL:N | 2.63 | 0.45 |
| 34:B8:28:GLY:C | 34:B8:32:LEU:HG | 2.37 | 0.45 |
| 34:B8:52:LYS:H | 34:B8:53:PRO:HD2 | 1.79 | 0.45 |
| 36:BA:1011:G:O2' | 36:BA:1013:C:C5' | 2.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BA:1299:G:C5 | 36:BA:1639:U:C5 | 3.05 | 0.45 |
| 36:BA:1498:C:H2' | 36:BA:1499:C:H5'' | 1.98 | 0.45 |
| 36:BA:2179:C:C5' | 36:BA:2180:U:OP1 | 2.64 | 0.45 |
| 36:BA:225:A:H2' | 36:BA:226:G:H5' | 1.98 | 0.45 |
| 36:BA:2502:G:H5'' | 36:BA:2503:A:C5' | 2.47 | 0.45 |
| 36:BA:2777:G:H5'' | 36:BA:2778:A:H5'' | 1.99 | 0.45 |
| 36:BA:845:G:HO2' | 36:BA:846:C:H5 | 1.64 | 0.45 |
| 40:BE:132:HIS:CD2 | 40:BE:135:HIS:NE2 | 2.84 | 0.45 |
| 40:BE:33:VAL:HG23 | 40:BE:47:VAL:HG13 | 1.98 | 0.45 |
| 41:BF:116:ASP:OD2 | 48:BP:5:ASP:HB2 | 2.16 | 0.45 |
| 46:BN:24:GLY:C | 46:BN:26:LEU:N | 2.70 | 0.45 |
| 48:BP:75:ILE:N | 48:BP:75:ILE:HD12 | 2.17 | 0.45 |
| 26:B0:7:LEU:HD22 | 49:BQ:85:LYS:CG | 2.45 | 0.45 |
| 49:BQ:21:THR:OG1 | 49:BQ:99:PRO:O | 2.34 | 0.45 |
| 51:BS:99:LYS:C | 51:BS:101:LEU:H | 2.19 | 0.45 |
| 1:AA:1442(B):A:C2 | 52:BT:118:ARG:CZ | 3.00 | 0.45 |
| 52:BT:129:ARG:HD2 | 52:BT:129:ARG:C | 2.36 | 0.45 |
| 52:BT:50:ILE:H | 52:BT:50:ILE:HD12 | 1.80 | 0.45 |
| 53:BU:35:ALA:O | 53:BU:36:ARG:C | 2.54 | 0.45 |
| 36:BA:1224:C:O2' | 54:BV:85:LYS:HA | 2.15 | 0.45 |
| 57:BY:27:VAL:HG12 | 57:BY:29:GLU:H | 1.80 | 0.45 |
| 36:BA:483:A:H5'' | 57:BY:49:VAL:HG22 | 1.98 | 0.45 |
| 57:BY:17:SER:CB | 57:BY:71:LYS:HB3 | 2.47 | 0.45 |
| 1:AA:1152:A:C6 | 1:AA:1153:C:N4 | 2.85 | 0.45 |
| 1:AA:1216:G:H2' | 1:AA:1217:C:C6 | 2.51 | 0.45 |
| 1:AA:1270:C:C6 | 1:AA:1270:C:H3' | 2.52 | 0.45 |
| 1:AA:1410:G:H2' | 1:AA:1411:C:H6 | 1.82 | 0.45 |
| 1:AA:1496:C:H2' | 1:AA:1497:G:O4' | 2.17 | 0.45 |
| 1:AA:80:G:C3' | 1:AA:81:U:C5' | 2.94 | 0.45 |
| 2:AB:22:LYS:NZ | 2:AB:40:HIS:CE1 | 2.84 | 0.45 |
| 7:AG:69:VAL:HG13 | 7:AG:100:ALA:HA | 1.98 | 0.45 |
| 12:AL:87:GLY:HA2 | 12:AL:98:TYR:HD2 | 1.82 | 0.45 |
| 13:AM:96:LEU:HB3 | 13:AM:97:PRO:HD2 | 1.97 | 0.45 |
| 20:AT:10:LEU:HD12 | 20:AT:11:SER:N | 2.32 | 0.45 |
| 20:AT:50:GLU:C | 20:AT:52:ALA:H | 2.20 | 0.45 |
| 22:AW:31:A:O2' | 22:AW:32:U:H5' | 2.16 | 0.45 |
| 22:AW:43:C:C3' | 22:AW:44:G:O4' | 2.64 | 0.45 |
| 22:AW:7:A:C5 | 22:AW:49:C:H5 | 2.34 | 0.45 |
| 25:AZ:96:ALA:O | 25:AZ:98:GLN:N | 2.50 | 0.45 |
| 26:B0:26:TYR:HA | 26:B0:69:PHE:HE1 | 1.82 | 0.45 |
| 29:B3:5:LYS:HD2 | 29:B3:57:GLU:CB | 2.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:B6:15:GLU:HG2 | 32:B6:15:GLU:O | 2.17 | 0.45 |
| 32:B6:6:ARG:HB3 | 32:B6:6:ARG:CZ | 2.42 | 0.45 |
| 36:BA:1243:G:C3' | 36:BA:1244:G:H5'' | 2.46 | 0.45 |
| 36:BA:2238:G:N3 | 36:BA:2238:G:H5' | 2.31 | 0.45 |
| 36:BA:236:C:H2' | 36:BA:237:C:H6 | 1.82 | 0.45 |
| 36:BA:271(H):G:H21 | 36:BA:271(I):G:H1' | 1.82 | 0.45 |
| 36:BA:302:C:H2' | 36:BA:303:U:C6 | 2.52 | 0.45 |
| 36:BA:654(S):G:H2' | 36:BA:654(T):C:C1' | 2.47 | 0.45 |
| 36:BA:943:U:OP2 | 48:BP:38:GLN:OE1 | 2.35 | 0.45 |
| 36:BA:944:G:H5' | 36:BA:945:A:C5' | 2.47 | 0.45 |
| 37:BB:65:C:H2' | 37:BB:109:C:H41 | 1.81 | 0.45 |
| 42:BG:9:ARG:HB3 | 42:BG:9:ARG:HH11 | 1.81 | 0.45 |
| 43:BH:30:LYS:HG2 | 43:BH:79:VAL:O | 2.16 | 0.45 |
| 48:BP:96:THR:HG22 | 48:BP:126:VAL:HG23 | 1.99 | 0.45 |
| 49:BQ:141:GLN:H | 58:BZ:53:ILE:CD1 | 2.25 | 0.45 |
| 51:BS:12:PHE:O | 51:BS:13:ARG:C | 2.54 | 0.45 |
| 51:BS:52:SER:CB | 51:BS:55:ALA:HB3 | 2.46 | 0.45 |
| 51:BS:64:GLU:HA | 51:BS:67:ARG:HG3 | 1.98 | 0.45 |
| 52:BT:39:ARG:CD | 52:BT:39:ARG:H | 2.16 | 0.45 |
| 47:BO:76:ALA:HB3 | 52:BT:75:ILE:HB | 1.97 | 0.45 |
| 53:BU:95:LEU:O | 53:BU:98:LEU:HG | 2.15 | 0.45 |
| 55:BW:52:GLU:OE2 | 55:BW:52:GLU:N | 2.49 | 0.45 |
| 56:BX:14:SER:O | 56:BX:17:ALA:HB3 | 2.17 | 0.45 |
| 57:BY:12:THR:HG22 | 57:BY:13:VAL:N | 2.32 | 0.45 |
| 57:BY:50:ARG:HB3 | 57:BY:53:PRO:CG | 2.43 | 0.45 |
| 58:BZ:129:SER:O | 58:BZ:132:ASN:N | 2.50 | 0.45 |
| 58:BZ:96:VAL:HG22 | 58:BZ:97:GLU:N | 2.30 | 0.45 |
| 1:AA:376:G:H4' | 16:AP:5:ARG:HH11 | 1.81 | 0.45 |
| 1:AA:624:C:H2' | 1:AA:625:G:H8 | 1.81 | 0.45 |
| 2:AB:97:TRP:CH2 | 2:AB:176:GLU:OE2 | 2.69 | 0.45 |
| 3:AC:78:GLY:HA3 | 3:AC:82:GLU:OE2 | 2.17 | 0.45 |
| 4:AD:12:CYS:SG | 4:AD:19:LEU:O | 2.74 | 0.45 |
| 4:AD:67:ILE:O | 4:AD:67:ILE:CG2 | 2.65 | 0.45 |
| 10:AJ:85:LEU:O | 10:AJ:87:THR:N | 2.50 | 0.45 |
| 11:AK:38:ASN:N | 11:AK:38:ASN:ND2 | 2.64 | 0.45 |
| 1:AA:1216:G:P | 14:AN:2:ALA:HB2 | 2.56 | 0.45 |
| 19:AS:45:VAL:O | 19:AS:45:VAL:HG23 | 2.15 | 0.45 |
| 24:AY:18:G:N2 | 24:AY:58:A:O4' | 2.49 | 0.45 |
| 25:AZ:158:LEU:C | 25:AZ:160:GLN:H | 2.18 | 0.45 |
| 25:AZ:315:LYS:HG2 | 25:AZ:373:GLU:CG | 2.34 | 0.45 |
| 25:AZ:324:LYS:CD | 25:AZ:325:LYS:H | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:374:LEU:HD13 | 25:AZ:378:VAL:CG1 | 2.47 | 0.45 |
| 31:B5:57:VAL:HG12 | 31:B5:58:LEU:N | 2.32 | 0.45 |
| 32:B6:40:CYS:HA | 32:B6:41:PRO:HD3 | 1.77 | 0.45 |
| 36:BA:1053:C:O2' | 36:BA:1054:A:H5' | 2.17 | 0.45 |
| 36:BA:1296:G:H2' | 36:BA:1297:C:H6 | 1.82 | 0.45 |
| 36:BA:1639:U:H2' | 36:BA:1640:C:C5' | 2.42 | 0.45 |
| 36:BA:1668:A:H4' | 36:BA:1669:A:O5' | 2.17 | 0.45 |
| 36:BA:1268:A:C6 | 36:BA:2013:A:C8 | 3.05 | 0.45 |
| 36:BA:2106:G:O6 | 36:BA:2183:C:N3 | 2.50 | 0.45 |
| 36:BA:2665:A:OP1 | 36:BA:2665:A:H4' | 2.17 | 0.45 |
| 36:BA:271(L):U:H4' | 36:BA:271(M):G:N7 | 2.31 | 0.45 |
| 36:BA:2006:C:O2' | 36:BA:2823:A:N3 | 2.44 | 0.45 |
| 36:BA:563:G:OP2 | 36:BA:572:A:H5' | 2.17 | 0.45 |
| 38:BC:76:ALA:O | 38:BC:94:VAL:HA | 2.16 | 0.45 |
| 38:BC:7:TYR:O | 38:BC:10:LEU:HB2 | 2.16 | 0.45 |
| 39:BD:263:ARG:O | 39:BD:264:LYS:C | 2.55 | 0.45 |
| 41:BF:119:ARG:O | 41:BF:119:ARG:HG2 | 2.17 | 0.45 |
| 41:BF:20:LEU:H | 41:BF:24:LEU:CD2 | 2.29 | 0.45 |
| 47:BO:107:ARG:O | 47:BO:112:MET:CE | 2.64 | 0.45 |
| 47:BO:67:LYS:O | 47:BO:67:LYS:HG3 | 2.16 | 0.45 |
| 47:BO:87:ILE:HG22 | 47:BO:88:ASN:H | 1.81 | 0.45 |
| 47:BO:11:ALA:O | 47:BO:98:VAL:HG23 | 2.16 | 0.45 |
| 50:BR:97:VAL:HG13 | 50:BR:114:VAL:HG12 | 1.98 | 0.45 |
| 52:BT:82:LEU:O | 52:BT:83:ILE:O | 2.34 | 0.45 |
| 53:BU:59:ARG:O | 53:BU:61:TRP:N | 2.50 | 0.45 |
| 56:BX:10:ALA:O | 56:BX:28:PHE:HB2 | 2.16 | 0.45 |
| 57:BY:96:ILE:HD12 | 57:BY:99:CYS:SG | 2.57 | 0.45 |
| 1:AA:1097:C:O2' | 1:AA:1098:C:H5' | 2.17 | 0.45 |
| 1:AA:134:A:H1' | 1:AA:325:A:C5 | 2.51 | 0.45 |
| 1:AA:1431:C:C2' | 1:AA:1432:G:H5' | 2.47 | 0.45 |
| 1:AA:346:G:N3 | 1:AA:346:G:C2' | 2.80 | 0.45 |
| 1:AA:754:C:O2 | 1:AA:754:C:H3' | 2.17 | 0.45 |
| 1:AA:849:C:H2' | 1:AA:850:U:O4' | 2.17 | 0.45 |
| 1:AA:992:U:O2' | 1:AA:993:G:P | 2.75 | 0.45 |
| 2:AB:212:GLN:O | 2:AB:216:SER:CB | 2.64 | 0.45 |
| 4:AD:3:ARG:HG2 | 4:AD:118:ARG:NE | 2.31 | 0.45 |
| 4:AD:170:VAL:HG12 | 4:AD:171:GLY:N | 2.31 | 0.45 |
| 5:AE:41:VAL:HG13 | 5:AE:113:ALA:CA | 2.46 | 0.45 |
| 8:AH:6:ILE:HD11 | 8:AH:31:PHE:CD2 | 2.52 | 0.45 |
| 10:AJ:16:LEU:CD1 | 10:AJ:70:ARG:CG | 2.94 | 0.45 |
| 12:AL:91:LYS:O | 12:AL:92:ASP:CB | 2.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:AM:66:LEU:CD1 | 13:AM:66:LEU:N | 2.77 | 0.45 |
| 15:AO:56:LEU:O | 15:AO:60:VAL:HG23 | 2.17 | 0.45 |
| 16:AP:8:ARG:HB3 | 16:AP:28:ARG:HH22 | 1.81 | 0.45 |
| 17:AQ:78:GLU:O | 17:AQ:78:GLU:HG3 | 2.17 | 0.45 |
| 22:AW:56:C:C5' | 38:BC:132:GLY:HA3 | 2.47 | 0.45 |
| 28:B2:68:ARG:HA | 28:B2:71:ASN:O | 2.17 | 0.45 |
| 31:B5:33:CYS:HG | 31:B5:49:CYS:HG | 1.59 | 0.45 |
| 31:B5:57:VAL:HG12 | 31:B5:58:LEU:H | 1.82 | 0.45 |
| 36:BA:1331:A:H2' | 36:BA:1332:G:H5'' | 1.98 | 0.45 |
| 36:BA:1336:A:O2' | 36:BA:1337:G:H5' | 2.17 | 0.45 |
| 36:BA:1486:A:C2 | 36:BA:1504:C:N3 | 2.85 | 0.45 |
| 36:BA:2533:A:H2' | 36:BA:2534:A:H5' | 1.99 | 0.45 |
| 36:BA:36:G:O2' | 36:BA:37:C:H5' | 2.16 | 0.45 |
| 36:BA:768:G:H2' | 36:BA:769:G:C8 | 2.52 | 0.45 |
| 40:BE:8:LYS:HD2 | 40:BE:188:VAL:HG13 | 1.98 | 0.45 |
| 42:BG:128:ARG:HD3 | 42:BG:128:ARG:HA | 1.67 | 0.45 |
| 42:BG:141:PHE:C | 42:BG:143:GLU:H | 2.20 | 0.45 |
| 42:BG:41:GLN:O | 42:BG:43:LEU:N | 2.49 | 0.45 |
| 42:BG:53:LEU:HD22 | 42:BG:53:LEU:N | 2.32 | 0.45 |
| 48:BP:143:GLY:C | 48:BP:145:PRO:HD3 | 2.37 | 0.45 |
| 48:BP:17:LYS:C | 48:BP:19:VAL:H | 2.19 | 0.45 |
| 49:BQ:54:MET:HE2 | 49:BQ:64:ILE:HD13 | 1.98 | 0.45 |
| 51:BS:39:ILE:HD12 | 51:BS:73:LEU:HD21 | 1.98 | 0.45 |
| 53:BU:10:ARG:O | 53:BU:11:ARG:C | 2.54 | 0.45 |
| 56:BX:18:TYR:C | 56:BX:20:GLY:N | 2.70 | 0.45 |
| 58:BZ:5:LEU:O | 58:BZ:59:LEU:HA | 2.17 | 0.45 |
| 1:AA:1031:G:O2' | 1:AA:1032:G:H5' | 2.17 | 0.45 |
| 1:AA:1200:C:O2' | 1:AA:1201:A:OP2 | 2.32 | 0.45 |
| 1:AA:1286:A:H2 | 21:AU:18:TYR:HH | 1.62 | 0.45 |
| 1:AA:425:G:O2' | 1:AA:426:G:H5' | 2.16 | 0.45 |
| 2:AB:138:LEU:C | 2:AB:140:HIS:N | 2.69 | 0.45 |
| 2:AB:54:THR:O | 2:AB:57:PHE:HB3 | 2.17 | 0.45 |
| 5:AE:36:ASP:O | 5:AE:37:ARG:HB2 | 2.17 | 0.45 |
| 1:AA:738:C:OP1 | 6:AF:92:LYS:HE3 | 2.17 | 0.45 |
| 8:AH:33:GLU:HG2 | 8:AH:48:TYR:CZ | 2.52 | 0.45 |
| 9:AI:44:VAL:HB | 9:AI:51:ARG:HH22 | 1.81 | 0.45 |
| 12:AL:67:THR:HG22 | 12:AL:96:VAL:HG13 | 1.98 | 0.45 |
| 13:AM:25:ILE:HD11 | 13:AM:60:VAL:CG1 | 2.46 | 0.45 |
| 13:AM:45:VAL:HG12 | 13:AM:45:VAL:O | 2.17 | 0.45 |
| 15:AO:8:LYS:HE3 | 15:AO:31:LEU:HD11 | 1.98 | 0.45 |
| 19:AS:27:GLU:HB3 | 19:AS:28:LYS:H | 1.59 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AV:47:U:H3' | 22:AV:48:C:H5' | 1.99 | 0.45 |
| 25:AZ:113:MET:O | 25:AZ:116:THR:HB | 2.17 | 0.45 |
| 25:AZ:68:VAL:CG2 | 25:AZ:79:HIS:HB3 | 2.22 | 0.45 |
| 27:B1:80:LEU:CD2 | 27:B1:81:LYS:N | 2.78 | 0.45 |
| 31:B5:12:SER:OG | 31:B5:14:ALA:HB3 | 2.17 | 0.45 |
| 31:B5:6:VAL:CG2 | 31:B5:7:PRO:HD2 | 2.47 | 0.45 |
| 36:BA:1109:C:H2' | 36:BA:1110:G:O4' | 2.17 | 0.45 |
| 36:BA:187:G:N3 | 36:BA:1365:A:H2 | 2.15 | 0.45 |
| 36:BA:1400:G:O2' | 36:BA:1401:G:H5' | 2.17 | 0.45 |
| 36:BA:1498:C:C2' | 36:BA:1499:C:C5' | 2.94 | 0.45 |
| 36:BA:21:A:O2' | 36:BA:22:C:H5' | 2.16 | 0.45 |
| 36:BA:440:G:H2' | 36:BA:441:U:C6 | 2.52 | 0.45 |
| 36:BA:449:A:O2' | 53:BU:3:ARG:NE | 2.49 | 0.45 |
| 36:BA:481:G:C2' | 36:BA:482:A:OP2 | 2.65 | 0.45 |
| 36:BA:556:G:H2' | 36:BA:557:U:H6 | 1.81 | 0.45 |
| 36:BA:654(N):G:O2' | 36:BA:654(O):G:H5' | 2.16 | 0.45 |
| 36:BA:2170:A:C5' | 38:BC:133:PRO:HG2 | 2.44 | 0.45 |
| 38:BC:66:HIS:H | 38:BC:188:ASN:ND2 | 2.15 | 0.45 |
| 39:BD:120:GLY:O | 39:BD:123:ALA:HB3 | 2.17 | 0.45 |
| 39:BD:170:GLY:C | 39:BD:172:TYR:H | 2.20 | 0.45 |
| 40:BE:145:LYS:HD3 | 40:BE:145:LYS:HA | 1.73 | 0.45 |
| 41:BF:158:THR:O | 41:BF:158:THR:HG23 | 2.17 | 0.45 |
| 41:BF:62:ARG:HH11 | 41:BF:62:ARG:CG | 2.29 | 0.45 |
| 41:BF:81:PRO:C | 41:BF:82:ILE:O | 2.48 | 0.45 |
| 46:BN:65:LYS:O | 46:BN:69:GLN:HG3 | 2.16 | 0.45 |
| 46:BN:41:ASP:C | 53:BU:64:ARG:HH22 | 2.20 | 0.45 |
| 55:BW:44:ALA:O | 55:BW:45:TYR:C | 2.55 | 0.45 |
| 58:BZ:151:HIS:O | 58:BZ:152:ALA:C | 2.54 | 0.45 |
| 1:AA:1020:U:O2' | 1:AA:1021:G:H5' | 2.18 | 0.44 |
| 1:AA:1128:C:C5 | 1:AA:1139:G:H2' | 2.52 | 0.44 |
| 1:AA:22:G:H2' | 1:AA:23:C:C6 | 2.52 | 0.44 |
| 1:AA:80:G:O2' | 1:AA:81:U:H5' | 2.17 | 0.44 |
| 4:AD:155:LEU:HB2 | 4:AD:158:ILE:CG1 | 2.46 | 0.44 |
| 6:AF:3:ARG:CG | 6:AF:3:ARG:HH11 | 2.28 | 0.44 |
| 9:AI:10:ARG:HD2 | 9:AI:75:ASP:HB2 | 1.99 | 0.44 |
| 12:AL:8:ASN:O | 12:AL:12:ARG:HG3 | 2.17 | 0.44 |
| 1:AA:1321:C:H5' | 13:AM:87:TYR:CE2 | 2.52 | 0.44 |
| 17:AQ:66:SER:C | 17:AQ:67:LYS:O | 2.53 | 0.44 |
| 19:AS:9:VAL:O | 19:AS:11:VAL:HG12 | 2.17 | 0.44 |
| 20:AT:72:LEU:CD1 | 20:AT:80:ARG:HE | 2.30 | 0.44 |
| 25:AZ:130:TYR:CD2 | 25:AZ:210:ILE:HA | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:B4:20:ASN:HD22 | 30:B4:20:ASN:C | 2.20 | 0.44 |
| 36:BA:1090:U:H2' | 36:BA:1091:G:O4' | 2.18 | 0.44 |
| 36:BA:1121:C:H2' | 36:BA:1122:G:O4' | 2.17 | 0.44 |
| 36:BA:1144:G:H2' | 36:BA:1145:C:C6 | 2.52 | 0.44 |
| 36:BA:1192:G:N7 | 48:BP:29:LYS:NZ | 2.55 | 0.44 |
| 36:BA:1590:U:C2' | 36:BA:1591:G:C5' | 2.92 | 0.44 |
| 36:BA:2733:A:O2' | 36:BA:2734:A:H5' | 2.17 | 0.44 |
| 36:BA:2758:A:C2 | 36:BA:2759:G:H1' | 2.52 | 0.44 |
| 36:BA:981:A:H1' | 36:BA:2037:G:H1' | 1.99 | 0.44 |
| 37:BB:16:G:O2' | 37:BB:17:C:O5' | 2.35 | 0.44 |
| 37:BB:48:A:H2' | 37:BB:49:C:C6 | 2.52 | 0.44 |
| 36:BA:2176:A:H1' | 38:BC:44:HIS:CG | 2.52 | 0.44 |
| 39:BD:11:PRO:C | 39:BD:13:ARG:H | 2.21 | 0.44 |
| 40:BE:35:GLN:CG | 40:BE:36:ARG:N | 2.73 | 0.44 |
| 41:BF:162:LEU:H | 41:BF:162:LEU:CD1 | 2.30 | 0.44 |
| 41:BF:80:ALA:HB1 | 41:BF:81:PRO:HD2 | 1.98 | 0.44 |
| 43:BH:41:MET:HA | 43:BH:41:MET:HE3 | 1.99 | 0.44 |
| 47:BO:107:ARG:HH21 | 47:BO:115:VAL:CG1 | 2.26 | 0.44 |
| 48:BP:108:LYS:C | 48:BP:110:TYR:N | 2.67 | 0.44 |
| 36:BA:811:U:H3' | 48:BP:25:SER:HA | 1.99 | 0.44 |
| 50:BR:59:ASP:O | 50:BR:60:LEU:C | 2.56 | 0.44 |
| 51:BS:16:ASN:OD1 | 51:BS:17:ARG:N | 2.50 | 0.44 |
| 52:BT:27:THR:O | 52:BT:28:VAL:CG2 | 2.66 | 0.44 |
| 53:BU:47:TYR:CD1 | 53:BU:47:TYR:C | 2.88 | 0.44 |
| 55:BW:62:HIS:O | 55:BW:63:ASP:C | 2.55 | 0.44 |
| 56:BX:18:TYR:O | 56:BX:21:PHE:HD1 | 2.00 | 0.44 |
| 56:BX:26:TYR:CD2 | 56:BX:92:LEU:HD12 | 2.49 | 0.44 |
| 36:BA:81:G:N2 | 57:BY:2:ARG:NH1 | 2.59 | 0.44 |
| 1:AA:1503:A:C2 | 23:AX:16:A:C5 | 3.04 | 0.44 |
| 1:AA:405:U:OP2 | 4:AD:3:ARG:HD2 | 2.17 | 0.44 |
| 2:AB:224:GLN:O | 2:AB:226:ARG:N | 2.50 | 0.44 |
| 2:AB:79:ASP:HA | 2:AB:82:ARG:HB2 | 1.98 | 0.44 |
| 3:AC:10:PHE:HD2 | 3:AC:11:ARG:NH1 | 2.16 | 0.44 |
| 3:AC:134:ILE:CG2 | 3:AC:151:VAL:HB | 2.47 | 0.44 |
| 3:AC:150:LYS:HE2 | 3:AC:152:ILE:HD11 | 1.99 | 0.44 |
| 3:AC:19:GLU:O | 3:AC:56:ASP:HA | 2.18 | 0.44 |
| 4:AD:118:ARG:O | 4:AD:121:VAL:N | 2.51 | 0.44 |
| 9:AI:118:LYS:O | 9:AI:119:ALA:HB3 | 2.17 | 0.44 |
| 9:AI:70:LYS:O | 9:AI:73:GLN:HB2 | 2.17 | 0.44 |
| 11:AK:103:LEU:N | 11:AK:103:LEU:HD22 | 2.33 | 0.44 |
| 12:AL:41:ARG:NH1 | 12:AL:57:LYS:NZ | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:221:PHE:CZ | 25:AZ:247:VAL:HG11 | 2.52 | 0.44 |
| 25:AZ:363:MET:HB3 | 25:AZ:364:PRO:CD | 2.43 | 0.44 |
| 25:AZ:341:GLN:NE2 | 25:AZ:390:GLU:HB2 | 2.30 | 0.44 |
| 31:B5:40:LYS:CE | 31:B5:46:CYS:SG | 3.05 | 0.44 |
| 32:B6:16:CYS:SG | 32:B6:48:VAL:HG23 | 2.58 | 0.44 |
| 36:BA:1285:G:C6 | 36:BA:1329:U:C5 | 3.06 | 0.44 |
| 36:BA:2627:G:N3 | 36:BA:2781:A:H2 | 2.15 | 0.44 |
| 36:BA:2720:U:H5' | 36:BA:2721:A:OP2 | 2.17 | 0.44 |
| 36:BA:2774:C:H2' | 36:BA:2775:A:O4' | 2.16 | 0.44 |
| 36:BA:478:A:C6 | 36:BA:480:A:C6 | 3.05 | 0.44 |
| 36:BA:654(E):G:H2' | 36:BA:654(F):C:C6 | 2.52 | 0.44 |
| 36:BA:768:G:H2' | 36:BA:769:G:H8 | 1.81 | 0.44 |
| 36:BA:812:C:H2' | 36:BA:813:U:C6 | 2.47 | 0.44 |
| 36:BA:986:C:C2' | 36:BA:987:G:H5' | 2.46 | 0.44 |
| 36:BA:987:G:H2' | 36:BA:988:A:O4' | 2.16 | 0.44 |
| 36:BA:999:U:O2 | 36:BA:1157:G:C2 | 2.70 | 0.44 |
| 38:BC:110:PHE:O | 38:BC:111:ASP:CB | 2.64 | 0.44 |
| 38:BC:40:THR:HG22 | 38:BC:41:VAL:N | 2.32 | 0.44 |
| 38:BC:47:LEU:HB2 | 38:BC:169:GLY:O | 2.18 | 0.44 |
| 42:BG:111:LEU:HD21 | 42:BG:179:PRO:CG | 2.48 | 0.44 |
| 42:BG:143:GLU:O | 42:BG:144:ILE:C | 2.55 | 0.44 |
| 42:BG:144:ILE:O | 42:BG:144:ILE:HG23 | 2.16 | 0.44 |
| 43:BH:85:LYS:CD | 43:BH:133:VAL:HB | 2.47 | 0.44 |
| 46:BN:10:GLU:OE2 | 46:BN:11:PRO:HD2 | 2.17 | 0.44 |
| 46:BN:74:ARG:HH22 | 46:BN:85:ILE:HD11 | 1.83 | 0.44 |
| 49:BQ:67:ARG:HD3 | 49:BQ:102:VAL:CG1 | 2.47 | 0.44 |
| 49:BQ:108:GLY:HA3 | 58:BZ:116:VAL:HG13 | 1.97 | 0.44 |
| 36:BA:2850:A:C2 | 50:BR:61:HIS:CD2 | 3.05 | 0.44 |
| 52:BT:128:GLU:CD | 52:BT:129:ARG:N | 2.70 | 0.44 |
| 52:BT:58:ASN:HD22 | 52:BT:58:ASN:N | 2.15 | 0.44 |
| 53:BU:79:PHE:HE1 | 53:BU:83:LEU:HD21 | 1.83 | 0.44 |
| 58:BZ:130:PRO:CA | 58:BZ:133:ILE:HD11 | 2.43 | 0.44 |
| 58:BZ:144:LEU:HA | 58:BZ:144:LEU:HD13 | 1.83 | 0.44 |
| 58:BZ:166:SER:HB2 | 58:BZ:167:PRO:HA | 1.98 | 0.44 |
| 1:AA:1410:G:H2' | 1:AA:1411:C:C6 | 2.52 | 0.44 |
| 1:AA:105:G:N2 | 1:AA:379:C:O3' | 2.50 | 0.44 |
| 1:AA:520:A:N1 | 1:AA:536:C:H1' | 2.32 | 0.44 |
| 3:AC:94:LEU:HD12 | 3:AC:94:LEU:C | 2.37 | 0.44 |
| 5:AE:67:VAL:CG2 | 5:AE:140:ARG:HG3 | 2.47 | 0.44 |
| 7:AG:149:ARG:NH1 | 7:AG:149:ARG:HG2 | 2.31 | 0.44 |
| 8:AH:6:ILE:HD11 | 8:AH:31:PHE:HD2 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:AI:10:ARG:O | 9:AI:11:LYS:CB | 2.65 | 0.44 |
| 9:AI:88:TYR:O | 9:AI:89:ASN:CG | 2.56 | 0.44 |
| 12:AL:110:VAL:H | 12:AL:122:THR:HG22 | 1.82 | 0.44 |
| 20:AT:48:LYS:HB3 | 20:AT:51:GLU:HG2 | 1.99 | 0.44 |
| 22:AW:40:C:H2' | 22:AW:41:C:C6 | 2.49 | 0.44 |
| 22:AW:54:U:C4 | 22:AW:55:U:C5 | 3.06 | 0.44 |
| 22:AW:56:C:C5' | 38:BC:137:LEU:CB | 2.95 | 0.44 |
| 25:AZ:15:GLY:HA3 | 25:AZ:99:MET:SD | 2.57 | 0.44 |
| 25:AZ:241:ARG:HB3 | 25:AZ:241:ARG:NH1 | 2.29 | 0.44 |
| 25:AZ:252:GLU:HB3 | 25:AZ:307:PRO:HG2 | 2.00 | 0.44 |
| 26:B0:28:GLY:O | 36:BA:923:C:O2' | 2.36 | 0.44 |
| 29:B3:17:LYS:HG2 | 36:BA:969:U:P | 2.57 | 0.44 |
| 36:BA:1217:C:C2 | 36:BA:1218:C:C5 | 3.05 | 0.44 |
| 36:BA:1369:G:H1' | 36:BA:1809:A:N1 | 2.33 | 0.44 |
| 36:BA:1551:C:O2' | 36:BA:1552:G:H5' | 2.16 | 0.44 |
| 26:B0:10:THR:CG2 | 36:BA:2277:G:OP2 | 2.66 | 0.44 |
| 36:BA:2450:A:C2' | 36:BA:2451:A:H5' | 2.48 | 0.44 |
| 36:BA:2447:G:O6 | 36:BA:2504:U:O4 | 2.35 | 0.44 |
| 36:BA:271(J):C:C2' | 36:BA:271(K):U:H5'' | 2.47 | 0.44 |
| 36:BA:2791:C:H41 | 36:BA:2801(A):A:N6 | 2.15 | 0.44 |
| 36:BA:502:A:H2' | 36:BA:503:A:H5' | 1.98 | 0.44 |
| 36:BA:848:G:O2' | 36:BA:849:A:H5' | 2.17 | 0.44 |
| 38:BC:107:TRP:H | 38:BC:108:MET:HE3 | 1.82 | 0.44 |
| 38:BC:210:ARG:HD3 | 38:BC:210:ARG:HA | 1.74 | 0.44 |
| 38:BC:67:GLY:HA2 | 38:BC:159:GLY:HA3 | 2.00 | 0.44 |
| 39:BD:64:ILE:C | 39:BD:64:ILE:HD12 | 2.38 | 0.44 |
| 40:BE:103:ASP:OD1 | 40:BE:201:THR:HA | 2.15 | 0.44 |
| 40:BE:44:TYR:O | 40:BE:45:THR:OG1 | 2.28 | 0.44 |
| 42:BG:129:GLY:O | 42:BG:130:ASN:CB | 2.65 | 0.44 |
| 42:BG:21:ARG:CZ | 42:BG:22:ARG:HA | 2.47 | 0.44 |
| 42:BG:96:ARG:O | 42:BG:97:ASP:CB | 2.62 | 0.44 |
| 43:BH:105:LEU:HD23 | 43:BH:105:LEU:N | 2.28 | 0.44 |
| 36:BA:1285:G:O3' | 50:BR:105:ARG:NH1 | 2.51 | 0.44 |
| 50:BR:117:VAL:HG22 | 50:BR:118:GLU:N | 2.28 | 0.44 |
| 50:BR:44:LEU:HD13 | 50:BR:44:LEU:C | 2.36 | 0.44 |
| 36:BA:1252:G:N2 | 53:BU:37:GLU:OE2 | 2.42 | 0.44 |
| 54:BV:18:LEU:CD2 | 54:BV:19:LYS:H | 2.30 | 0.44 |
| 55:BW:65:LEU:HD23 | 55:BW:68:ARG:CD | 2.47 | 0.44 |
| 1:AA:499:A:C6 | 1:AA:547:A:C8 | 3.06 | 0.44 |
| 4:AD:127:THR:HB | 4:AD:147:ALA:O | 2.18 | 0.44 |
| 5:AE:98:THR:HB | 5:AE:117:ASP:HB3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AI:100:GLY:O | 9:AI:103:THR:N | 2.43 | 0.44 |
| 12:AL:31:PRO:HB2 | 12:AL:32:PHE:CD2 | 2.52 | 0.44 |
| 13:AM:107:ALA:O | 13:AM:111:LYS:HG3 | 2.17 | 0.44 |
| 13:AM:73:GLU:O | 13:AM:76:ALA:HB3 | 2.17 | 0.44 |
| 13:AM:81:LEU:HD22 | 13:AM:86:CYS:SG | 2.58 | 0.44 |
| 15:AO:56:LEU:HD12 | 15:AO:56:LEU:O | 2.17 | 0.44 |
| 22:AV:19:G:C2 | 22:AV:57:G:C2 | 3.06 | 0.44 |
| 25:AZ:171:ILE:CG2 | 25:AZ:172:ARG:N | 2.81 | 0.44 |
| 1:AA:55:A:C5 | 25:AZ:233:GLY:HA3 | 2.53 | 0.44 |
| 25:AZ:317:GLU:HA | 25:AZ:371:THR:HA | 1.99 | 0.44 |
| 26:B0:10:THR:HG21 | 36:BA:2277:G:OP2 | 2.18 | 0.44 |
| 26:B0:24:LYS:O | 26:B0:25:ARG:HD3 | 2.18 | 0.44 |
| 27:B1:30:VAL:HG23 | 27:B1:31:GLY:N | 2.32 | 0.44 |
| 29:B3:27:GLY:O | 29:B3:29:ARG:NH1 | 2.50 | 0.44 |
| 36:BA:1504:C:O2' | 36:BA:1505:C:C5' | 2.66 | 0.44 |
| 36:BA:1353:A:O4' | 36:BA:1569:A:H2 | 1.99 | 0.44 |
| 36:BA:1678:G:H22 | 36:BA:1989:G:N2 | 2.00 | 0.44 |
| 36:BA:1991:U:C2' | 36:BA:1992:G:H5'' | 2.43 | 0.44 |
| 36:BA:2197:U:O2' | 36:BA:2198:A:H2' | 2.18 | 0.44 |
| 36:BA:2580:U:H5'' | 40:BE:131:ALA:N | 2.31 | 0.44 |
| 36:BA:2624:G:O2' | 36:BA:2625:G:H5' | 2.17 | 0.44 |
| 36:BA:2643:G:H2' | 36:BA:2644:G:C8 | 2.52 | 0.44 |
| 36:BA:381:G:O2' | 36:BA:382:G:H5' | 2.17 | 0.44 |
| 37:BB:104:U:C2' | 37:BB:105:A:H5' | 2.47 | 0.44 |
| 36:BA:2572:A:N3 | 40:BE:144:ARG:NH1 | 2.65 | 0.44 |
| 40:BE:176:ILE:CG2 | 40:BE:178:GLU:HB3 | 2.48 | 0.44 |
| 42:BG:121:ASN:ND2 | 42:BG:123:ASN:H | 2.16 | 0.44 |
| 46:BN:120:LEU:HD13 | 46:BN:120:LEU:C | 2.37 | 0.44 |
| 46:BN:93:THR:O | 46:BN:94:HIS:HB2 | 2.18 | 0.44 |
| 48:BP:107:LYS:O | 48:BP:107:LYS:HG3 | 2.18 | 0.44 |
| 52:BT:106:SER:O | 52:BT:107:ASP:HB3 | 2.17 | 0.44 |
| 36:BA:18:C:O2' | 53:BU:23:GLY:HA2 | 2.17 | 0.44 |
| 54:BV:21:ARG:HB3 | 54:BV:91:TYR:CB | 2.40 | 0.44 |
| 54:BV:35:LEU:C | 54:BV:37:VAL:N | 2.71 | 0.44 |
| 53:BU:112:ARG:CZ | 54:BV:46:VAL:HG21 | 2.47 | 0.44 |
| 55:BW:6:ILE:HA | 55:BW:104:THR:HA | 1.99 | 0.44 |
| 57:BY:39:VAL:CG1 | 57:BY:40:GLU:H | 2.28 | 0.44 |
| 49:BQ:134:ARG:CZ | 58:BZ:122:ARG:HH21 | 2.30 | 0.44 |
| 1:AA:1030:C:N4 | 1:AA:1032:G:C2 | 2.85 | 0.44 |
| 1:AA:489:C:H2' | 1:AA:490:G:H8 | 1.83 | 0.44 |
| 1:AA:748:C:O2' | 1:AA:749:C:P | 2.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:761:G:H2' | 1:AA:762:C:C6 | 2.52 | 0.44 |
| 1:AA:939:G:H5'' | 7:AG:102:ARG:CZ | 2.46 | 0.44 |
| 2:AB:58:ILE:O | 2:AB:61:LEU:HB3 | 2.17 | 0.44 |
| 2:AB:7:VAL:HA | 2:AB:11:LEU:CG | 2.48 | 0.44 |
| 4:AD:102:ASP:O | 4:AD:117:ALA:HB1 | 2.18 | 0.44 |
| 1:AA:495:A:N6 | 4:AD:119:GLN:HE22 | 2.16 | 0.44 |
| 7:AG:15:ASP:HB3 | 7:AG:19:GLY:N | 2.32 | 0.44 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:HD1 | 1.82 | 0.44 |
| 13:AM:81:LEU:O | 13:AM:89:GLY:HA3 | 2.17 | 0.44 |
| 17:AQ:27:PHE:C | 17:AQ:27:PHE:CD1 | 2.91 | 0.44 |
| 19:AS:11:VAL:O | 19:AS:11:VAL:HG13 | 2.18 | 0.44 |
| 25:AZ:122:LEU:O | 25:AZ:126:VAL:N | 2.48 | 0.44 |
| 25:AZ:389:ARG:O | 25:AZ:390:GLU:HB2 | 2.17 | 0.44 |
| 24:AY:2:G:P | 25:AZ:90:LYS:HZ1 | 2.40 | 0.44 |
| 26:B0:27:GLU:CD | 26:B0:27:GLU:N | 2.68 | 0.44 |
| 26:B0:41:ARG:HB3 | 26:B0:42:GLY:H | 1.58 | 0.44 |
| 30:B4:31:ILE:HG22 | 30:B4:31:ILE:O | 2.18 | 0.44 |
| 30:B4:9:LEU:O | 30:B4:10:VAL:CB | 2.66 | 0.44 |
| 32:B6:17:LYS:O | 32:B6:18:ARG:HB3 | 2.17 | 0.44 |
| 32:B6:18:ARG:CG | 32:B6:19:ARG:N | 2.77 | 0.44 |
| 34:B8:33:ASN:OD1 | 34:B8:35:GLN:N | 2.51 | 0.44 |
| 36:BA:1170:G:N2 | 36:BA:1180:C:N3 | 2.66 | 0.44 |
| 36:BA:1448:G:H5' | 36:BA:1449:A:OP1 | 2.17 | 0.44 |
| 36:BA:1551:C:C2' | 36:BA:1552:G:H5' | 2.48 | 0.44 |
| 36:BA:1651:G:H2' | 36:BA:1652:A:O4' | 2.17 | 0.44 |
| 36:BA:1658:C:H2' | 36:BA:1659:U:C6 | 2.53 | 0.44 |
| 36:BA:1847:A:H2' | 36:BA:1847:A:N3 | 2.32 | 0.44 |
| 36:BA:188:G:C2' | 36:BA:189:G:H5' | 2.47 | 0.44 |
| 36:BA:2243:U:H2' | 36:BA:2244:U:H6 | 1.74 | 0.44 |
| 36:BA:2319:G:OP2 | 36:BA:2319:G:H4' | 2.17 | 0.44 |
| 36:BA:2339:G:H2' | 36:BA:2340:G:H8 | 1.83 | 0.44 |
| 36:BA:343:C:O2 | 36:BA:343:C:H2' | 2.16 | 0.44 |
| 37:BB:91:C:H5' | 49:BQ:17:LEU:O | 2.17 | 0.44 |
| 39:BD:213:ARG:HA | 39:BD:213:ARG:HD2 | 1.63 | 0.44 |
| 39:BD:21:PHE:O | 39:BD:24:ILE:CG2 | 2.65 | 0.44 |
| 36:BA:2820:A:N6 | 40:BE:192:ASN:HB3 | 2.32 | 0.44 |
| 40:BE:60:ASN:O | 40:BE:61:ARG:C | 2.56 | 0.44 |
| 40:BE:74:PRO:CG | 40:BE:77:ILE:O | 2.66 | 0.44 |
| 41:BF:117:ARG:HA | 41:BF:117:ARG:HD3 | 1.74 | 0.44 |
| 41:BF:82:ILE:O | 41:BF:83:PHE:CB | 2.66 | 0.44 |
| 42:BG:43:LEU:CD1 | 42:BG:153:ARG:HG3 | 2.41 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:BG:87:PRO:O | 42:BG:88:ILE:HG12 | 2.17 | 0.44 |
| 44:BJ:109:UNK:C | 44:BJ:111:UNK:N | 2.79 | 0.44 |
| 46:BN:65:LYS:HZ2 | 46:BN:65:LYS:CB | 2.30 | 0.44 |
| 48:BP:102:ARG:O | 48:BP:103:ALA:HB2 | 2.17 | 0.44 |
| 34:B8:58:ILE:O | 48:BP:49:ARG:HD2 | 2.18 | 0.44 |
| 48:BP:46:LYS:CB | 48:BP:52:GLU:HG2 | 2.47 | 0.44 |
| 53:BU:17:ILE:HA | 53:BU:20:LEU:HB2 | 1.99 | 0.44 |
| 1:AA:1125:U:O4 | 10:AJ:5:ARG:NE | 2.31 | 0.44 |
| 1:AA:116:A:H8 | 1:AA:116:A:O5' | 2.00 | 0.44 |
| 1:AA:1332:A:O2' | 1:AA:1333:A:H5' | 2.17 | 0.44 |
| 1:AA:399:G:H2' | 1:AA:400:C:C6 | 2.52 | 0.44 |
| 1:AA:921:U:H2' | 1:AA:922:G:O4' | 2.18 | 0.44 |
| 1:AA:966:G:H2' | 1:AA:967:C:C6 | 2.53 | 0.44 |
| 3:AC:107:GLN:CD | 3:AC:108:ASN:H | 2.21 | 0.44 |
| 3:AC:188:LEU:HD11 | 3:AC:195:VAL:CG1 | 2.47 | 0.44 |
| 8:AH:36:LEU:O | 8:AH:39:LEU:HB2 | 2.18 | 0.44 |
| 8:AH:49:GLU:O | 8:AH:49:GLU:HG3 | 2.18 | 0.44 |
| 12:AL:86:ARG:HB2 | 12:AL:101:VAL:CG2 | 2.47 | 0.44 |
| 13:AM:97:PRO:HB2 | 13:AM:101:GLN:HE21 | 1.82 | 0.44 |
| 1:AA:186:C:O4' | 20:AT:81:LYS:HE2 | 2.17 | 0.44 |
| 22:AV:12:U:H3 | 22:AV:23:A:H61 | 1.64 | 0.44 |
| 25:AZ:158:LEU:HD13 | 25:AZ:168:VAL:HG21 | 1.99 | 0.44 |
| 32:B6:27:LYS:CG | 32:B6:30:THR:OG1 | 2.65 | 0.44 |
| 36:BA:1403:C:C2' | 36:BA:1404:C:O5' | 2.66 | 0.44 |
| 36:BA:1569:A:H2' | 36:BA:1570:A:O4' | 2.17 | 0.44 |
| 36:BA:2157:G:O2' | 36:BA:2158:A:H5' | 2.18 | 0.44 |
| 36:BA:2556:C:H2' | 36:BA:2557:G:O4' | 2.16 | 0.44 |
| 36:BA:2801(A):A:C5' | 36:BA:2802:G:H5' | 2.48 | 0.44 |
| 38:BC:31:GLU:O | 38:BC:32:LEU:HD23 | 2.18 | 0.44 |
| 39:BD:22:SER:O | 39:BD:25:THR:OG1 | 2.20 | 0.44 |
| 41:BF:65:TRP:CZ3 | 41:BF:72:ARG:HB2 | 2.52 | 0.44 |
| 42:BG:42:GLY:O | 42:BG:43:LEU:C | 2.56 | 0.44 |
| 43:BH:154:PRO:O | 43:BH:155:SER:HB3 | 2.18 | 0.44 |
| 43:BH:15:VAL:O | 43:BH:16:SER:OG | 2.34 | 0.44 |
| 51:BS:25:ARG:HA | 51:BS:86:ALA:O | 2.18 | 0.44 |
| 52:BT:63:VAL:O | 52:BT:73:GLU:HA | 2.17 | 0.44 |
| 1:AA:1230:C:H2' | 1:AA:1231:G:H8 | 1.82 | 0.44 |
| 1:AA:312:C:H2' | 1:AA:313:A:H8 | 1.79 | 0.44 |
| 2:AB:20:GLU:HG2 | 2:AB:189:ASP:OD1 | 2.17 | 0.44 |
| 3:AC:43:LEU:O | 3:AC:47:LEU:HB2 | 2.18 | 0.44 |
| 7:AG:113:GLU:HG3 | 7:AG:119:ARG:HA | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:50:ILE:HD12 | 7:AG:125:MET:HG2 | 1.99 | 0.44 |
| 8:AH:65:TYR:N | 8:AH:65:TYR:CD1 | 2.86 | 0.44 |
| 9:AI:4:TYR:CG | 9:AI:88:TYR:HB2 | 2.52 | 0.44 |
| 11:AK:69:ALA:CB | 11:AK:103:LEU:HD21 | 2.43 | 0.44 |
| 11:AK:15:ALA:HB1 | 11:AK:78:GLN:CB | 2.46 | 0.44 |
| 3:AC:13:GLY:HA3 | 14:AN:57:ARG:CZ | 2.48 | 0.44 |
| 19:AS:22:LEU:HD13 | 19:AS:22:LEU:O | 2.17 | 0.44 |
| 21:AU:20:LYS:HE3 | 21:AU:21:TYR:CZ | 2.53 | 0.44 |
| 25:AZ:221:PHE:HE1 | 25:AZ:242:ILE:HG23 | 1.82 | 0.44 |
| 27:B1:19:GLN:O | 27:B1:35:THR:HG22 | 2.16 | 0.44 |
| 29:B3:8:LEU:HD22 | 29:B3:31:LEU:CA | 2.28 | 0.44 |
| 30:B4:12:ALA:HB1 | 30:B4:29:PRO:O | 2.18 | 0.44 |
| 31:B5:33:CYS:HB3 | 31:B5:36:CYS:SG | 2.58 | 0.44 |
| 32:B6:5:VAL:O | 32:B6:6:ARG:CB | 2.66 | 0.44 |
| 36:BA:1494:A:C3' | 36:BA:1494:A:N3 | 2.80 | 0.44 |
| 36:BA:1520:G:C2' | 36:BA:1523:U:H5' | 2.46 | 0.44 |
| 36:BA:1805:U:O2 | 39:BD:50:THR:HB | 2.18 | 0.44 |
| 36:BA:1827:C:H2' | 36:BA:1828:G:H5' | 1.99 | 0.44 |
| 36:BA:1901:A:H4' | 36:BA:1901:A:OP2 | 2.18 | 0.44 |
| 36:BA:2313:C:O2' | 36:BA:2314:C:H5' | 2.18 | 0.44 |
| 36:BA:2461:C:H2' | 36:BA:2462:U:H6 | 1.82 | 0.44 |
| 36:BA:2464:C:O2' | 36:BA:2465:C:O5' | 2.36 | 0.44 |
| 36:BA:271(L):U:C5' | 36:BA:271(M):G:H5' | 2.31 | 0.44 |
| 36:BA:676:A:H8 | 36:BA:2069:G:N2 | 2.02 | 0.44 |
| 36:BA:802:A:C5 | 36:BA:803:U:C4 | 3.05 | 0.44 |
| 36:BA:812:C:H5' | 48:BP:25:SER:CB | 2.43 | 0.44 |
| 29:B3:52:HIS:CD2 | 37:BB:83:G:H4' | 2.53 | 0.44 |
| 39:BD:166:GLN:NE2 | 39:BD:166:GLN:HA | 2.31 | 0.44 |
| 40:BE:33:VAL:O | 40:BE:33:VAL:HG22 | 2.17 | 0.44 |
| 41:BF:158:THR:C | 41:BF:160:ASN:N | 2.71 | 0.44 |
| 41:BF:20:LEU:O | 41:BF:24:LEU:HD23 | 2.18 | 0.44 |
| 41:BF:3:GLU:O | 41:BF:19:GLU:HG3 | 2.17 | 0.44 |
| 41:BF:4:VAL:HG13 | 41:BF:19:GLU:OE1 | 2.18 | 0.44 |
| 43:BH:17:VAL:O | 43:BH:18:GLU:HG2 | 2.18 | 0.44 |
| 48:BP:102:ARG:HG2 | 48:BP:102:ARG:O | 2.17 | 0.44 |
| 36:BA:626:U:C2 | 48:BP:105:LEU:HG | 2.53 | 0.44 |
| 48:BP:33:ARG:O | 48:BP:35:HIS:O | 2.36 | 0.44 |
| 49:BQ:104:PHE:O | 49:BQ:105:GLU:HB3 | 2.17 | 0.44 |
| 49:BQ:109:VAL:CG1 | 49:BQ:113:GLN:OE1 | 2.66 | 0.44 |
| 49:BQ:140:ALA:HB3 | 58:BZ:53:ILE:CD1 | 2.45 | 0.44 |
| 50:BR:107:ASP:C | 50:BR:107:ASP:OD2 | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:BT:28:VAL:HG12 | 52:BT:29:ARG:NH1 | 2.33 | 0.44 |
| 53:BU:59:ARG:C | 53:BU:61:TRP:H | 2.21 | 0.44 |
| 54:BV:47:VAL:C | 54:BV:49:THR:N | 2.71 | 0.44 |
| 56:BX:12:VAL:CB | 56:BX:17:ALA:HB1 | 2.32 | 0.44 |
| 1:AA:1242:C:H6 | 1:AA:1242:C:O5' | 2.01 | 0.44 |
| 1:AA:1261:A:H2' | 1:AA:1262:C:H5' | 1.98 | 0.44 |
| 1:AA:1421:G:H2' | 1:AA:1422:G:O4' | 2.18 | 0.44 |
| 1:AA:1452:C:H4' | 1:AA:1456:G:O5' | 2.18 | 0.44 |
| 1:AA:1521:G:H2' | 1:AA:1522:U:C6 | 2.53 | 0.44 |
| 1:AA:68:G:H2' | 1:AA:69:G:O4' | 2.18 | 0.44 |
| 1:AA:664:G:N2 | 1:AA:741:G:H1 | 1.85 | 0.44 |
| 1:AA:828:A:H2' | 1:AA:829:G:O4' | 2.18 | 0.44 |
| 1:AA:833:U:H2' | 1:AA:834:C:C6 | 2.53 | 0.44 |
| 2:AB:84:GLU:OE1 | 2:AB:216:SER:HA | 2.18 | 0.44 |
| 3:AC:155:GLY:HA3 | 3:AC:196:LEU:HD13 | 1.99 | 0.44 |
| 7:AG:108:ALA:CB | 7:AG:120:ILE:HD13 | 2.48 | 0.44 |
| 7:AG:15:ASP:OD2 | 7:AG:44:TYR:OH | 2.32 | 0.44 |
| 9:AI:114:TYR:HE1 | 10:AJ:60:ARG:O | 2.01 | 0.44 |
| 9:AI:53:VAL:CG1 | 9:AI:95:LYS:HE3 | 2.39 | 0.44 |
| 12:AL:55:VAL:HG22 | 12:AL:56:ALA:N | 2.32 | 0.44 |
| 12:AL:89:ARG:HD3 | 12:AL:91:LYS:N | 2.33 | 0.44 |
| 13:AM:39:ILE:CD1 | 13:AM:56:LEU:HB2 | 2.48 | 0.44 |
| 15:AO:44:LYS:HB2 | 15:AO:44:LYS:HE3 | 1.74 | 0.44 |
| 18:AR:69:THR:O | 18:AR:72:ARG:HB2 | 2.17 | 0.44 |
| 19:AS:13:ASP:C | 19:AS:15:LEU:H | 2.21 | 0.44 |
| 19:AS:72:GLY:C | 19:AS:74:PHE:H | 2.21 | 0.44 |
| 20:AT:57:ARG:HB2 | 20:AT:57:ARG:NH1 | 2.32 | 0.44 |
| 25:AZ:24:LYS:NZ | 25:AZ:24:LYS:CB | 2.80 | 0.44 |
| 25:AZ:342:PHE:N | 25:AZ:342:PHE:CD1 | 2.86 | 0.44 |
| 25:AZ:344:PHE:CD1 | 25:AZ:344:PHE:N | 2.86 | 0.44 |
| 28:B2:59:ARG:HA | 28:B2:62:THR:HB | 2.00 | 0.44 |
| 29:B3:29:ARG:O | 29:B3:30:ARG:C | 2.55 | 0.44 |
| 32:B6:22:ALA:HB2 | 32:B6:39:TYR:CE2 | 2.52 | 0.44 |
| 36:BA:1111:A:H2' | 36:BA:1111:A:N3 | 2.33 | 0.44 |
| 36:BA:1382:G:H8 | 36:BA:1382:G:O5' | 2.00 | 0.44 |
| 36:BA:140:G:H1' | 36:BA:141:A:H2 | 1.82 | 0.44 |
| 36:BA:1534:U:H2' | 36:BA:1535:A:O4' | 2.17 | 0.44 |
| 36:BA:1583:A:O2' | 36:BA:1586:A:N1 | 2.43 | 0.44 |
| 36:BA:1592:C:H2' | 36:BA:1593:G:H8 | 1.82 | 0.44 |
| 27:B1:50:ARG:NH2 | 36:BA:2200:C:OP2 | 2.50 | 0.44 |
| 36:BA:2740:A:C6 | 36:BA:2741:A:C6 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:45:C:H2' | 36:BA:47:C:C6 | 2.53 | 0.44 |
| 36:BA:755:C:H2' | 36:BA:756:C:C6 | 2.53 | 0.44 |
| 36:BA:911:A:N1 | 36:BA:2277:G:O2' | 2.46 | 0.44 |
| 37:BB:77:U:O2' | 37:BB:78:A:H5' | 2.18 | 0.44 |
| 38:BC:131:LEU:HD22 | 38:BC:136:LEU:CD1 | 2.42 | 0.44 |
| 39:BD:30:GLU:CD | 39:BD:63:ARG:HE | 2.21 | 0.44 |
| 36:BA:773:U:H4' | 39:BD:47:GLY:CA | 2.48 | 0.44 |
| 40:BE:34:VAL:O | 40:BE:34:VAL:HG13 | 2.17 | 0.44 |
| 36:BA:2638:G:P | 40:BE:82:ARG:HH21 | 2.41 | 0.44 |
| 42:BG:161:THR:HG21 | 42:BG:172:LEU:HD13 | 2.00 | 0.44 |
| 46:BN:61:ARG:HG3 | 46:BN:61:ARG:NH1 | 2.33 | 0.44 |
| 49:BQ:39:PRO:HG3 | 49:BQ:99:PRO:HD3 | 2.00 | 0.44 |
| 51:BS:101:LEU:C | 51:BS:101:LEU:HD12 | 2.38 | 0.44 |
| 51:BS:54:LEU:O | 51:BS:57:LYS:N | 2.51 | 0.44 |
| 52:BT:83:ILE:O | 52:BT:84:GLN:C | 2.56 | 0.44 |
| 57:BY:19:LYS:HB2 | 57:BY:20:TYR:CD1 | 2.53 | 0.44 |
| 57:BY:50:ARG:CD | 57:BY:53:PRO:HA | 2.46 | 0.44 |
| 57:BY:59:GLY:O | 57:BY:60:PHE:CD1 | 2.71 | 0.44 |
| 58:BZ:141:VAL:O | 58:BZ:143:GLY:N | 2.43 | 0.44 |
| 1:AA:1047:G:O2' | 1:AA:1048:G:H5' | 2.18 | 0.44 |
| 1:AA:1057:G:H2' | 1:AA:1058:G:O4' | 2.18 | 0.44 |
| 1:AA:538:G:OP2 | 12:AL:115:LYS:HG3 | 2.17 | 0.44 |
| 1:AA:598:U:H4' | 8:AH:94:TYR:CD1 | 2.53 | 0.44 |
| 1:AA:659:U:O2' | 1:AA:660:G:H5' | 2.18 | 0.44 |
| 2:AB:163:PHE:HD2 | 2:AB:185:ILE:HB | 1.83 | 0.44 |
| 5:AE:33:VAL:HG11 | 5:AE:109:ILE:HA | 1.99 | 0.44 |
| 5:AE:37:ARG:O | 5:AE:38:GLN:HG2 | 2.18 | 0.44 |
| 6:AF:50:TYR:HB2 | 6:AF:51:PRO:HD2 | 2.00 | 0.44 |
| 9:AI:40:LEU:C | 9:AI:42:ARG:N | 2.71 | 0.44 |
| 9:AI:99:LEU:CB | 9:AI:101:PHE:CD1 | 3.01 | 0.44 |
| 13:AM:33:ALA:O | 13:AM:37:THR:HG23 | 2.17 | 0.44 |
| 1:AA:1318:A:O3' | 19:AS:10:PHE:CD2 | 2.71 | 0.44 |
| 22:AV:44:G:H2' | 22:AV:45:U:H5' | 2.00 | 0.44 |
| 25:AZ:259:ALA:HB1 | 25:AZ:260:PRO:CD | 2.48 | 0.44 |
| 25:AZ:322:VAL:HA | 25:AZ:396:GLY:HA2 | 1.99 | 0.44 |
| 25:AZ:70:TYR:CD1 | 25:AZ:70:TYR:O | 2.71 | 0.44 |
| 28:B2:24:LEU:O | 28:B2:24:LEU:HD23 | 2.17 | 0.44 |
| 30:B4:5:ILE:N | 30:B4:5:ILE:HD13 | 2.28 | 0.44 |
| 36:BA:1120:G:O2' | 36:BA:1121:C:H5' | 2.18 | 0.44 |
| 36:BA:1204:A:H1' | 36:BA:1206:G:N7 | 2.33 | 0.44 |
| 36:BA:1242:A:N1 | 48:BP:8:PRO:CG | 2.78 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:BA:1380:G:H2' | 36:BA:1381:G:H8 | 1.83 | 0.44 |
| 36:BA:1701:A:H5' | 36:BA:1702:G:OP2 | 2.18 | 0.44 |
| 36:BA:1754:C:H4' | 52:BT:101:PHE:CD2 | 2.53 | 0.44 |
| 36:BA:2095:C:H2' | 36:BA:2096:U:C6 | 2.52 | 0.44 |
| 36:BA:2168:G:H2' | 36:BA:2169:A:H3' | 1.99 | 0.44 |
| 36:BA:2681:C:C2' | 36:BA:2681:C:O2 | 2.65 | 0.44 |
| 36:BA:2721:A:H2' | 36:BA:2722:G:O4' | 2.18 | 0.44 |
| 36:BA:375:C:H2' | 36:BA:376:C:C6 | 2.52 | 0.44 |
| 36:BA:614(A):U:C4' | 36:BA:614(B):G:C5' | 2.95 | 0.44 |
| 36:BA:782:A:N1 | 39:BD:226:MET:HE2 | 2.33 | 0.44 |
| 36:BA:569:U:H1' | 36:BA:947:G:O4' | 2.18 | 0.44 |
| 36:BA:983:A:H2' | 36:BA:984:A:C8 | 2.53 | 0.44 |
| 36:BA:984:A:C5' | 36:BA:985:C:H5 | 2.28 | 0.44 |
| 38:BC:212:VAL:HG12 | 38:BC:224:ILE:HD11 | 2.00 | 0.44 |
| 39:BD:266:SER:C | 39:BD:267:SER:O | 2.56 | 0.44 |
| 39:BD:46:GLN:CD | 39:BD:46:GLN:N | 2.72 | 0.44 |
| 43:BH:53:GLU:HB3 | 43:BH:54:ARG:H | 1.66 | 0.44 |
| 47:BO:47:ILE:HG23 | 47:BO:48:PRO:CD | 2.43 | 0.44 |
| 47:BO:81:ASP:C | 47:BO:81:ASP:OD1 | 2.56 | 0.44 |
| 49:BQ:6:ARG:C | 49:BQ:7:MET:HG3 | 2.39 | 0.44 |
| 52:BT:64:ARG:HD2 | 52:BT:73:GLU:CD | 2.38 | 0.44 |
| 54:BV:29:PRO:HG2 | 54:BV:30:GLY:H | 1.81 | 0.44 |
| 57:BY:76:CYS:O | 57:BY:77:PRO:C | 2.55 | 0.44 |
| 58:BZ:128:VAL:CG2 | 58:BZ:129:SER:H | 2.24 | 0.44 |
| 1:AA:355:C:C2 | 1:AA:356:A:C8 | 3.06 | 0.43 |
| 1:AA:441:A:H3' | 1:AA:442:C:C6 | 2.52 | 0.43 |
| 1:AA:594:G:H2' | 1:AA:595:G:C5' | 2.48 | 0.43 |
| 1:AA:633:G:C5' | 1:AA:634:C:OP2 | 2.66 | 0.43 |
| 2:AB:162:ILE:HG22 | 2:AB:183:PRO:O | 2.18 | 0.43 |
| 10:AJ:54:PHE:CE2 | 10:AJ:55:LYS:CD | 2.98 | 0.43 |
| 11:AK:61:ALA:CB | 11:AK:90:GLY:HA3 | 2.46 | 0.43 |
| 14:AN:15:LYS:HB3 | 14:AN:16:PHE:CE2 | 2.53 | 0.43 |
| 15:AO:22:THR:O | 15:AO:27:VAL:HG11 | 2.18 | 0.43 |
| 15:AO:29:VAL:HG21 | 15:AO:67:LEU:HD23 | 1.99 | 0.43 |
| 30:B4:27:THR:O | 30:B4:28:LYS:HB3 | 2.17 | 0.43 |
| 32:B6:52:VAL:HG22 | 32:B6:53:LYS:N | 2.30 | 0.43 |
| 36:BA:99:U:C3' | 36:BA:100:G:H5' | 2.48 | 0.43 |
| 36:BA:1221(A):C:O2' | 36:BA:1222:C:H5' | 2.18 | 0.43 |
| 36:BA:1253:A:H3' | 36:BA:1254:A:H5' | 2.00 | 0.43 |
| 36:BA:578:A:H5' | 36:BA:1254:A:OP1 | 2.18 | 0.43 |
| 36:BA:1528:A:C2 | 36:BA:1542:A:H2 | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:1649:G:O2' | 36:BA:1650:G:H5' | 2.18 | 0.43 |
| 36:BA:2115:G:C2' | 36:BA:2116:G:H5'' | 2.48 | 0.43 |
| 36:BA:2206:G:H21 | 36:BA:2207:G:C5' | 2.31 | 0.43 |
| 36:BA:2262:U:H2' | 36:BA:2263:C:C6 | 2.52 | 0.43 |
| 36:BA:589:C:H6 | 36:BA:589:C:O5' | 2.01 | 0.43 |
| 36:BA:59:U:O2' | 36:BA:73:A:H2' | 2.17 | 0.43 |
| 36:BA:627:A:C5 | 36:BA:637:A:N7 | 2.85 | 0.43 |
| 40:BE:38:THR:HG23 | 40:BE:39:PRO:HD2 | 1.99 | 0.43 |
| 36:BA:2745:C:H4' | 43:BH:142:GLY:O | 2.17 | 0.43 |
| 48:BP:39:LYS:CD | 48:BP:40:SER:H | 2.29 | 0.43 |
| 48:BP:85:LEU:N | 48:BP:85:LEU:HD23 | 2.33 | 0.43 |
| 48:BP:7:ARG:CB | 48:BP:8:PRO:CD | 2.95 | 0.43 |
| 48:BP:97:PRO:O | 48:BP:98:GLU:CB | 2.57 | 0.43 |
| 49:BQ:56:ARG:NH1 | 49:BQ:56:ARG:HG3 | 2.33 | 0.43 |
| 53:BU:57:PHE:O | 53:BU:58:ARG:C | 2.56 | 0.43 |
| 54:BV:4:ILE:HA | 54:BV:12:TYR:O | 2.18 | 0.43 |
| 57:BY:96:ILE:CD1 | 57:BY:99:CYS:SG | 3.07 | 0.43 |
| 1:AA:106:C:O2' | 1:AA:107:G:H5' | 2.18 | 0.43 |
| 1:AA:1073:U:O2' | 1:AA:1074:G:H5' | 2.17 | 0.43 |
| 1:AA:1260:C:OP1 | 1:AA:1284:C:H4' | 2.17 | 0.43 |
| 1:AA:1264:C:H1' | 1:AA:1272:G:N2 | 2.33 | 0.43 |
| 1:AA:455:C:O5' | 1:AA:455:C:H6 | 2.01 | 0.43 |
| 1:AA:67:C:O2' | 1:AA:171:A:H1' | 2.18 | 0.43 |
| 2:AB:115:LEU:O | 2:AB:118:LEU:HB2 | 2.19 | 0.43 |
| 8:AH:111:ILE:HG22 | 8:AH:112:LEU:N | 2.34 | 0.43 |
| 8:AH:97:VAL:HG13 | 8:AH:98:LYS:N | 2.32 | 0.43 |
| 13:AM:79:LYS:O | 13:AM:82:MET:SD | 2.76 | 0.43 |
| 3:AC:13:GLY:HA3 | 14:AN:57:ARG:NH2 | 2.33 | 0.43 |
| 16:AP:82:GLN:O | 16:AP:83:GLU:CB | 2.65 | 0.43 |
| 19:AS:20:LEU:HA | 19:AS:23:ASN:HB3 | 1.99 | 0.43 |
| 19:AS:79:THR:O | 19:AS:80:TYR:CB | 2.66 | 0.43 |
| 25:AZ:227:ASP:HB3 | 25:AZ:229:PHE:CE1 | 2.54 | 0.43 |
| 25:AZ:246:LYS:O | 25:AZ:247:VAL:HG13 | 2.18 | 0.43 |
| 25:AZ:252:GLU:O | 25:AZ:253:VAL:HG13 | 2.18 | 0.43 |
| 25:AZ:334:PHE:CD1 | 25:AZ:334:PHE:N | 2.86 | 0.43 |
| 25:AZ:334:PHE:HE2 | 25:AZ:353:VAL:HG11 | 1.82 | 0.43 |
| 26:B0:69:PHE:CE2 | 26:B0:79:VAL:HG22 | 2.53 | 0.43 |
| 28:B2:47:ASN:O | 28:B2:50:ILE:CD1 | 2.66 | 0.43 |
| 32:B6:11:LEU:HD21 | 32:B6:51:GLU:CD | 2.38 | 0.43 |
| 34:B8:32:LEU:HB3 | 34:B8:36:LYS:CE | 2.48 | 0.43 |
| 36:BA:1024:G:H3' | 36:BA:1025:G:C5' | 2.25 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:191:A:H2' | 36:BA:192:C:H6 | 1.83 | 0.43 |
| 36:BA:1958:C:O2' | 36:BA:1959:G:H5' | 2.18 | 0.43 |
| 36:BA:2168:G:O2' | 36:BA:2169:A:C8 | 2.68 | 0.43 |
| 36:BA:2199:A:H2' | 36:BA:2199:A:N3 | 2.34 | 0.43 |
| 34:B8:34:TRP:CA | 36:BA:2420:C:OP1 | 2.67 | 0.43 |
| 36:BA:2704:C:H2' | 36:BA:2705:A:C8 | 2.53 | 0.43 |
| 36:BA:581:C:H2' | 36:BA:582:G:C8 | 2.41 | 0.43 |
| 36:BA:59:U:H3 | 36:BA:68:G:H1 | 1.66 | 0.43 |
| 36:BA:79:G:H2' | 36:BA:80:G:H8 | 1.83 | 0.43 |
| 36:BA:870:A:C2 | 36:BA:871:U:H1' | 2.53 | 0.43 |
| 36:BA:893:C:O2' | 36:BA:894:C:H5' | 2.18 | 0.43 |
| 36:BA:940:G:H2' | 36:BA:941:A:O4' | 2.18 | 0.43 |
| 37:BB:43:C:H3' | 37:BB:44:G:C5' | 2.48 | 0.43 |
| 41:BF:117:ARG:HH21 | 41:BF:187:VAL:HA | 1.82 | 0.43 |
| 41:BF:142:TRP:O | 41:BF:145:GLU:HB2 | 2.17 | 0.43 |
| 42:BG:37:VAL:HG22 | 42:BG:159:VAL:HG23 | 1.99 | 0.43 |
| 46:BN:57:ALA:O | 46:BN:58:ASP:C | 2.56 | 0.43 |
| 51:BS:19:LYS:HB3 | 51:BS:20:ARG:NH2 | 2.33 | 0.43 |
| 51:BS:98:VAL:CG1 | 51:BS:100:ALA:HB2 | 2.48 | 0.43 |
| 52:BT:32:TYR:CG | 52:BT:81:PRO:HB3 | 2.53 | 0.43 |
| 53:BU:95:LEU:O | 53:BU:97:ASP:N | 2.52 | 0.43 |
| 55:BW:56:ALA:C | 55:BW:58:ALA:H | 2.20 | 0.43 |
| 58:BZ:128:VAL:CG2 | 58:BZ:129:SER:N | 2.78 | 0.43 |
| 1:AA:1007:C:H42 | 1:AA:1022:G:H1 | 1.66 | 0.43 |
| 1:AA:1112:C:N3 | 3:AC:178:LEU:N | 2.55 | 0.43 |
| 1:AA:156:G:C6 | 1:AA:166:G:O6 | 2.72 | 0.43 |
| 1:AA:599:C:O2' | 1:AA:600:C:H5' | 2.19 | 0.43 |
| 2:AB:181:PHE:O | 2:AB:183:PRO:HD3 | 2.19 | 0.43 |
| 4:AD:13:ARG:O | 4:AD:14:ARG:C | 2.57 | 0.43 |
| 4:AD:199:ASN:O | 4:AD:199:ASN:OD1 | 2.36 | 0.43 |
| 1:AA:411:A:OP2 | 4:AD:25:ARG:NH2 | 2.50 | 0.43 |
| 10:AJ:34:VAL:CG1 | 10:AJ:73:ASP:O | 2.66 | 0.43 |
| 12:AL:7:ILE:HG22 | 12:AL:8:ASN:N | 2.32 | 0.43 |
| 13:AM:108:ARG:HH11 | 13:AM:108:ARG:HG3 | 1.82 | 0.43 |
| 13:AM:23:TYR:CE1 | 13:AM:70:LEU:HD22 | 2.53 | 0.43 |
| 19:AS:70:LYS:O | 19:AS:73:GLU:HB2 | 2.18 | 0.43 |
| 25:AZ:217:VAL:O | 25:AZ:217:VAL:HG23 | 2.18 | 0.43 |
| 33:B7:16:HIS:ND1 | 36:BA:465:G:H4' | 2.33 | 0.43 |
| 34:B8:52:LYS:O | 34:B8:56:GLU:OE1 | 2.36 | 0.43 |
| 36:BA:1352:U:O2' | 36:BA:1353:A:H5' | 2.19 | 0.43 |
| 36:BA:1426:G:O5' | 36:BA:1426:G:H8 | 2.02 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BA:1780:A:H5' | 36:BA:1780:A:H8 | 1.82 | 0.43 |
| 36:BA:2510:C:O2' | 36:BA:2511:U:H5' | 2.18 | 0.43 |
| 36:BA:2808:U:H2' | 36:BA:2809:A:H5' | 2.00 | 0.43 |
| 36:BA:2866:U:C5 | 36:BA:2868:A:H1' | 2.52 | 0.43 |
| 36:BA:49:A:H4' | 36:BA:50:U:O5' | 2.18 | 0.43 |
| 36:BA:586:A:H5' | 41:BF:89:VAL:HG11 | 1.99 | 0.43 |
| 36:BA:60:G:C8 | 36:BA:63:U:C5 | 3.06 | 0.43 |
| 36:BA:910:A:C6 | 36:BA:911:A:C6 | 3.07 | 0.43 |
| 37:BB:62:C:C2 | 37:BB:63:G:C8 | 3.05 | 0.43 |
| 39:BD:112:GLN:H | 39:BD:115:GLN:NE2 | 2.15 | 0.43 |
| 40:BE:8:LYS:HD2 | 40:BE:188:VAL:CG1 | 2.48 | 0.43 |
| 42:BG:136:ARG:HG2 | 42:BG:136:ARG:NH1 | 2.33 | 0.43 |
| 42:BG:47:LYS:NZ | 42:BG:81:LYS:CB | 2.81 | 0.43 |
| 36:BA:1082:U:H5' | 45:BK:116:UNK:O | 2.18 | 0.43 |
| 47:BO:18:LYS:HB2 | 47:BO:45:GLU:HB3 | 2.00 | 0.43 |
| 36:BA:2727:G:O2' | 47:BO:70:LYS:HE2 | 2.19 | 0.43 |
| 48:BP:84:ASN:O | 48:BP:87:ASP:N | 2.47 | 0.43 |
| 49:BQ:52:VAL:O | 49:BQ:53:ALA:C | 2.55 | 0.43 |
| 37:BB:7:G:O5' | 51:BS:29:PHE:HE1 | 2.01 | 0.43 |
| 51:BS:54:LEU:HD13 | 51:BS:54:LEU:O | 2.19 | 0.43 |
| 54:BV:75:PHE:C | 54:BV:75:PHE:CD1 | 2.91 | 0.43 |
| 55:BW:5:ALA:HB3 | 55:BW:105:VAL:H | 1.83 | 0.43 |
| 36:BA:519:U:H5'' | 55:BW:25:ARG:HH12 | 1.82 | 0.43 |
| 57:BY:50:ARG:O | 57:BY:52:SER:N | 2.51 | 0.43 |
| 58:BZ:29:TYR:HE2 | 58:BZ:87:ASP:OD2 | 2.02 | 0.43 |
| 58:BZ:38:TYR:CG | 58:BZ:38:TYR:O | 2.71 | 0.43 |
| 1:AA:1161:C:H2' | 1:AA:1162:C:H6 | 1.84 | 0.43 |
| 1:AA:1270:C:C6 | 1:AA:1270:C:C3' | 3.01 | 0.43 |
| 1:AA:1423:G:H2' | 1:AA:1424:C:C6 | 2.53 | 0.43 |
| 1:AA:601:C:H2' | 1:AA:602:A:C8 | 2.54 | 0.43 |
| 2:AB:97:TRP:CH2 | 2:AB:176:GLU:CD | 2.92 | 0.43 |
| 3:AC:70:VAL:O | 3:AC:106:VAL:HG23 | 2.17 | 0.43 |
| 1:AA:542:G:P | 4:AD:10:ARG:HH22 | 2.40 | 0.43 |
| 4:AD:159:ARG:HG3 | 4:AD:159:ARG:HH11 | 1.84 | 0.43 |
| 6:AF:86:ARG:O | 6:AF:87:ARG:HG2 | 2.18 | 0.43 |
| 11:AK:126:ARG:C | 11:AK:128:ALA:N | 2.72 | 0.43 |
| 12:AL:102:ARG:HA | 12:AL:102:ARG:HD2 | 1.58 | 0.43 |
| 12:AL:41:ARG:NH2 | 12:AL:57:LYS:HZ3 | 2.14 | 0.43 |
| 17:AQ:86:GLU:O | 17:AQ:90:ILE:HG12 | 2.19 | 0.43 |
| 25:AZ:194:GLU:HG3 | 25:AZ:195:TRP:H | 1.84 | 0.43 |
| 25:AZ:171:ILE:HD13 | 25:AZ:202:LEU:CD1 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:AZ:33:PHE:O | 25:AZ:36:ALA:HB3 | 2.19 | 0.43 |
| 26:B0:52:GLY:HA3 | 26:B0:60:PHE:CZ | 2.53 | 0.43 |
| 29:B3:8:LEU:HD13 | 29:B3:29:ARG:O | 2.17 | 0.43 |
| 33:B7:40:TRP:CD2 | 36:BA:459:U:C5' | 3.01 | 0.43 |
| 36:BA:1223:G:H5' | 36:BA:1223:G:C8 | 2.49 | 0.43 |
| 36:BA:1334:G:O2' | 36:BA:1335:U:H5' | 2.19 | 0.43 |
| 36:BA:1510:G:H2' | 36:BA:1511:C:C6 | 2.54 | 0.43 |
| 36:BA:1747:G:H2' | 36:BA:1747(A):G:H8 | 1.83 | 0.43 |
| 36:BA:2206:G:N3 | 36:BA:2207:G:H5' | 2.33 | 0.43 |
| 22:AV:75:C:OP1 | 36:BA:2602:A:C5' | 2.65 | 0.43 |
| 36:BA:2747:G:O6 | 36:BA:2755:C:H5'' | 2.18 | 0.43 |
| 36:BA:2816:C:H2' | 36:BA:2817:G:H8 | 1.82 | 0.43 |
| 36:BA:289:A:H2' | 36:BA:290:G:H8 | 1.81 | 0.43 |
| 36:BA:407:G:H2' | 36:BA:408:G:C8 | 2.52 | 0.43 |
| 36:BA:753:C:O2' | 36:BA:754:C:H5' | 2.17 | 0.43 |
| 36:BA:986:C:O5' | 36:BA:986:C:H6 | 2.00 | 0.43 |
| 38:BC:196:LEU:C | 38:BC:198:ALA:N | 2.72 | 0.43 |
| 36:BA:782:A:N3 | 39:BD:226:MET:HG2 | 2.32 | 0.43 |
| 40:BE:34:VAL:O | 40:BE:34:VAL:HG22 | 2.18 | 0.43 |
| 41:BF:72:ARG:HB3 | 41:BF:72:ARG:NH1 | 2.33 | 0.43 |
| 22:AV:56:C:N3 | 42:BG:83:ARG:HD3 | 2.34 | 0.43 |
| 46:BN:14:VAL:HG12 | 46:BN:15:LEU:N | 2.34 | 0.43 |
| 46:BN:30:ILE:HG22 | 46:BN:34:LEU:HD23 | 1.99 | 0.43 |
| 46:BN:31:ALA:HA | 46:BN:34:LEU:HB2 | 2.00 | 0.43 |
| 46:BN:35:ARG:HH21 | 46:BN:42:TRP:HH2 | 1.66 | 0.43 |
| 51:BS:25:ARG:O | 51:BS:39:ILE:HA | 2.19 | 0.43 |
| 54:BV:13:ARG:HG2 | 54:BV:13:ARG:O | 2.17 | 0.43 |
| 54:BV:35:LEU:C | 54:BV:37:VAL:H | 2.22 | 0.43 |
| 54:BV:31:ALA:O | 54:BV:60:GLU:HG3 | 2.18 | 0.43 |
| 56:BX:30:VAL:HG21 | 56:BX:39:ILE:HD11 | 2.00 | 0.43 |
| 56:BX:70:LEU:HD23 | 56:BX:71:GLY:N | 2.34 | 0.43 |
| 56:BX:28:PHE:CZ | 56:BX:81:VAL:HG21 | 2.53 | 0.43 |
| 58:BZ:108:PRO:HA | 58:BZ:141:VAL:HG12 | 1.93 | 0.43 |
| 1:AA:1181:G:O2' | 1:AA:1182:G:H5' | 2.18 | 0.43 |
| 5:AE:89:ILE:HG12 | 5:AE:90:VAL:N | 2.34 | 0.43 |
| 6:AF:63:TYR:O | 6:AF:64:GLN:CB | 2.66 | 0.43 |
| 8:AH:75:ARG:HB2 | 8:AH:75:ARG:HE | 1.56 | 0.43 |
| 1:AA:1060:C:H4' | 10:AJ:52:GLY:N | 2.33 | 0.43 |
| 12:AL:25:PRO:C | 12:AL:27:LEU:H | 2.21 | 0.43 |
| 19:AS:4:SER:C | 19:AS:5:LEU:O | 2.57 | 0.43 |
| 24:AY:73:G:C6 | 24:AY:74:C:C2 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:73:G:H2' | 24:AY:74:C:C5' | 2.49 | 0.43 |
| 24:AY:77:TRP:CE2 | 25:AZ:67:HIS:CD2 | 3.07 | 0.43 |
| 25:AZ:229:PHE:CD1 | 25:AZ:229:PHE:N | 2.86 | 0.43 |
| 25:AZ:232:THR:C | 25:AZ:234:ARG:H | 2.22 | 0.43 |
| 25:AZ:330:ARG:CG | 25:AZ:395:VAL:HB | 2.45 | 0.43 |
| 36:BA:1188:U:H2' | 36:BA:1189:A:H5' | 1.99 | 0.43 |
| 36:BA:1224:C:C5 | 36:BA:1225:G:C5 | 3.06 | 0.43 |
| 36:BA:1479:G:H5' | 36:BA:1558:A:C2 | 2.53 | 0.43 |
| 36:BA:1498:C:C2' | 36:BA:1499:C:H5'' | 2.49 | 0.43 |
| 36:BA:1523:U:H2' | 36:BA:1524:G:H8 | 1.83 | 0.43 |
| 36:BA:1643:G:C4 | 36:BA:1644:C:C6 | 3.06 | 0.43 |
| 36:BA:2620:C:H2' | 36:BA:2621:A:O4' | 2.17 | 0.43 |
| 36:BA:2796:U:C3' | 36:BA:2799:C:H5' | 2.49 | 0.43 |
| 36:BA:363:G:C4 | 36:BA:363(A):A:N7 | 2.87 | 0.43 |
| 36:BA:528:A:C2 | 36:BA:2043:C:C5' | 3.00 | 0.43 |
| 36:BA:810:U:C4 | 48:BP:32:THR:HA | 2.53 | 0.43 |
| 38:BC:131:LEU:HB3 | 38:BC:136:LEU:HB2 | 2.00 | 0.43 |
| 39:BD:175:LEU:HD12 | 39:BD:185:VAL:HG21 | 2.00 | 0.43 |
| 39:BD:182:LEU:HA | 39:BD:182:LEU:HD23 | 1.73 | 0.43 |
| 39:BD:63:ARG:HH11 | 39:BD:63:ARG:HG3 | 1.84 | 0.43 |
| 40:BE:4:ILE:HD11 | 40:BE:28:ALA:HB1 | 2.01 | 0.43 |
| 40:BE:35:GLN:HG2 | 40:BE:36:ARG:O | 2.18 | 0.43 |
| 40:BE:34:VAL:CG1 | 40:BE:48:GLN:HE21 | 2.32 | 0.43 |
| 40:BE:93:VAL:C | 40:BE:95:ILE:N | 2.72 | 0.43 |
| 41:BF:102:PRO:C | 41:BF:104:LYS:N | 2.71 | 0.43 |
| 41:BF:132:VAL:CG2 | 41:BF:162:LEU:HD23 | 2.40 | 0.43 |
| 42:BG:73:ALA:CB | 42:BG:87:PRO:HG3 | 2.49 | 0.43 |
| 43:BH:19:VAL:HG12 | 43:BH:20:ALA:N | 2.33 | 0.43 |
| 46:BN:55:VAL:HG22 | 46:BN:56:ASN:H | 1.83 | 0.43 |
| 46:BN:57:ALA:O | 46:BN:58:ASP:O | 2.36 | 0.43 |
| 46:BN:68:GLU:HA | 46:BN:86:PRO:HB2 | 2.01 | 0.43 |
| 51:BS:30:ARG:HH22 | 51:BS:62:LYS:HD3 | 1.80 | 0.43 |
| 54:BV:4:ILE:HB | 54:BV:39:LEU:O | 2.18 | 0.43 |
| 57:BY:46:LYS:CG | 57:BY:47:LYS:N | 2.72 | 0.43 |
| 57:BY:17:SER:HB3 | 57:BY:71:LYS:HB3 | 1.99 | 0.43 |
| 1:AA:1003:G:N2 | 1:AA:1038:C:N3 | 2.66 | 0.43 |
| 1:AA:1152:A:H5' | 10:AJ:70:ARG:HH21 | 1.83 | 0.43 |
| 1:AA:1174:G:O2' | 1:AA:1175:G:H5' | 2.18 | 0.43 |
| 1:AA:1321:C:OP2 | 1:AA:1322:C:H2' | 2.18 | 0.43 |
| 1:AA:1406:U:C2' | 1:AA:1407:C:H5' | 2.49 | 0.43 |
| 1:AA:346:G:O2' | 1:AA:347:G:P | 2.76 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:431:A:H2' | 1:AA:432:A:O4' | 2.19 | 0.43 |
| 1:AA:630:G:H2' | 1:AA:631:G:O4' | 2.19 | 0.43 |
| 1:AA:633:G:H3' | 1:AA:634:C:H6 | 1.83 | 0.43 |
| 1:AA:791:G:H2' | 1:AA:792:A:H5' | 2.00 | 0.43 |
| 2:AB:201:ILE:O | 2:AB:202:PRO:C | 2.56 | 0.43 |
| 3:AC:83:ARG:O | 3:AC:87:LEU:HG | 2.18 | 0.43 |
| 5:AE:74:GLY:HA3 | 5:AE:116:THR:OG1 | 2.18 | 0.43 |
| 1:AA:706:A:H1' | 11:AK:29:ILE:HD11 | 2.00 | 0.43 |
| 13:AM:77:ASN:O | 13:AM:81:LEU:HG | 2.19 | 0.43 |
| 17:AQ:69:LYS:O | 17:AQ:70:ARG:HD2 | 2.19 | 0.43 |
| 19:AS:72:GLY:C | 19:AS:74:PHE:N | 2.71 | 0.43 |
| 22:AW:72:C:H2' | 22:AW:73:A:O4' | 2.19 | 0.43 |
| 23:AX:26:A:C3' | 23:AX:27:A:H5'' | 2.29 | 0.43 |
| 25:AZ:194:GLU:CG | 25:AZ:195:TRP:N | 2.78 | 0.43 |
| 30:B4:42:PHE:CD2 | 30:B4:42:PHE:O | 2.71 | 0.43 |
| 33:B7:8:ASN:HD21 | 33:B7:10:ARG:N | 2.16 | 0.43 |
| 34:B8:15:LYS:HD3 | 48:BP:65:ARG:HH22 | 1.84 | 0.43 |
| 36:BA:86:C:O2' | 36:BA:104:U:H1' | 2.19 | 0.43 |
| 36:BA:1060:U:C4 | 36:BA:1062:G:OP2 | 2.71 | 0.43 |
| 36:BA:1056:G:C2 | 36:BA:1102:C:C5 | 3.05 | 0.43 |
| 36:BA:1681:G:O2' | 36:BA:1762:A:C2' | 2.65 | 0.43 |
| 36:BA:2115:G:H2' | 36:BA:2116:G:H5'' | 1.99 | 0.43 |
| 36:BA:2410:G:C2 | 36:BA:2411:A:H1' | 2.53 | 0.43 |
| 36:BA:2514:U:H2' | 36:BA:2515:C:C6 | 2.53 | 0.43 |
| 36:BA:2580:U:C5 | 36:BA:2581:G:C6 | 3.06 | 0.43 |
| 36:BA:2720:U:C2 | 36:BA:2721:A:C8 | 3.07 | 0.43 |
| 36:BA:2852:G:O2' | 36:BA:2853:C:H5' | 2.18 | 0.43 |
| 31:B5:13:LYS:HZ1 | 36:BA:516:C:H5'' | 1.83 | 0.43 |
| 36:BA:528:A:H3' | 36:BA:528:A:H8 | 1.84 | 0.43 |
| 36:BA:532:A:N3 | 36:BA:532:A:H2' | 2.33 | 0.43 |
| 36:BA:658:C:C2 | 36:BA:659:C:C5 | 3.07 | 0.43 |
| 36:BA:804:A:H2' | 36:BA:806:C:C4 | 2.53 | 0.43 |
| 36:BA:889:C:O2' | 36:BA:890:A:P | 2.77 | 0.43 |
| 36:BA:910:A:H62 | 49:BQ:12:GLN:HA | 1.83 | 0.43 |
| 38:BC:6:ARG:HG2 | 38:BC:6:ARG:O | 2.18 | 0.43 |
| 39:BD:227:ASN:HB3 | 39:BD:228:PRO:CD | 2.49 | 0.43 |
| 39:BD:39:LYS:HB2 | 39:BD:62:TYR:HB2 | 1.99 | 0.43 |
| 40:BE:12:THR:HG23 | 40:BE:13:ARG:N | 2.33 | 0.43 |
| 46:BN:58:ASP:HB3 | 46:BN:95:PRO:HB2 | 2.00 | 0.43 |
| 49:BQ:16:ARG:HH21 | 49:BQ:18:LYS:NZ | 2.16 | 0.43 |
| 50:BR:84:ALA:HB3 | 50:BR:85:PRO:CD | 2.41 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:BR:87:TYR:C | 50:BR:89:ASP:H | 2.22 | 0.43 |
| 52:BT:102:ILE:HD12 | 52:BT:110:ILE:CD1 | 2.46 | 0.43 |
| 52:BT:34:VAL:HG22 | 52:BT:39:ARG:HG3 | 2.01 | 0.43 |
| 53:BU:22:LYS:HD3 | 53:BU:22:LYS:HA | 1.89 | 0.43 |
| 53:BU:59:ARG:C | 53:BU:61:TRP:N | 2.72 | 0.43 |
| 56:BX:21:PHE:HD2 | 56:BX:26:TYR:CE2 | 2.36 | 0.43 |
| 57:BY:62:GLU:CD | 57:BY:62:GLU:N | 2.72 | 0.43 |
| 57:BY:85:VAL:CG1 | 57:BY:86:ARG:N | 2.80 | 0.43 |
| 58:BZ:10:ARG:O | 58:BZ:36:LYS:HG3 | 2.19 | 0.43 |
| 58:BZ:48:PHE:CE2 | 58:BZ:52:SER:O | 2.71 | 0.43 |
| 1:AA:1202:G:H2' | 1:AA:1203:C:C5' | 2.46 | 0.43 |
| 1:AA:189(A):C:O2' | 1:AA:189(B):C:H5' | 2.18 | 0.43 |
| 1:AA:621:A:O2' | 1:AA:622:A:H5' | 2.19 | 0.43 |
| 1:AA:783:C:O2' | 1:AA:784:C:H5' | 2.19 | 0.43 |
| 1:AA:865:A:O2' | 1:AA:866:C:H5' | 2.18 | 0.43 |
| 2:AB:124:SER:OG | 2:AB:125:PRO:HD2 | 2.18 | 0.43 |
| 2:AB:190:THR:O | 2:AB:191:ASP:HB2 | 2.18 | 0.43 |
| 3:AC:84:ILE:O | 3:AC:84:ILE:CG1 | 2.67 | 0.43 |
| 4:AD:52:SER:O | 4:AD:55:ALA:N | 2.51 | 0.43 |
| 6:AF:3:ARG:NH1 | 6:AF:38:GLU:OE1 | 2.51 | 0.43 |
| 6:AF:71:ARG:HG3 | 6:AF:71:ARG:HH11 | 1.84 | 0.43 |
| 9:AI:4:TYR:HA | 9:AI:88:TYR:CD1 | 2.54 | 0.43 |
| 11:AK:29:ILE:HG12 | 11:AK:29:ILE:O | 2.19 | 0.43 |
| 12:AL:102:ARG:HG3 | 12:AL:102:ARG:NH1 | 2.33 | 0.43 |
| 17:AQ:90:ILE:O | 17:AQ:93:GLN:HB3 | 2.18 | 0.43 |
| 17:AQ:89:LEU:O | 17:AQ:93:GLN:N | 2.52 | 0.43 |
| 19:AS:9:VAL:CG1 | 19:AS:39:THR:HB | 2.49 | 0.43 |
| 25:AZ:199:ILE:O | 25:AZ:202:LEU:HB3 | 2.18 | 0.43 |
| 25:AZ:306:LYS:HG2 | 25:AZ:307:PRO:HD2 | 1.99 | 0.43 |
| 28:B2:64:LEU:HD23 | 28:B2:64:LEU:C | 2.37 | 0.43 |
| 32:B6:27:LYS:HG3 | 32:B6:30:THR:CB | 2.48 | 0.43 |
| 36:BA:1058:G:N1 | 36:BA:1059:G:N7 | 2.66 | 0.43 |
| 36:BA:1337:G:C4 | 36:BA:1338:G:C8 | 3.06 | 0.43 |
| 36:BA:1349:A:H5' | 36:BA:1349:A:N3 | 2.33 | 0.43 |
| 36:BA:2101:G:H2' | 36:BA:2102:U:C4' | 2.49 | 0.43 |
| 36:BA:2170:A:H4' | 38:BC:133:PRO:HB2 | 1.98 | 0.43 |
| 36:BA:2125:G:N2 | 36:BA:2173:A:H61 | 2.15 | 0.43 |
| 36:BA:2341:G:H2' | 36:BA:2342:C:C6 | 2.54 | 0.43 |
| 36:BA:2370:G:C6 | 36:BA:2371:G:C6 | 3.06 | 0.43 |
| 36:BA:1786:A:N1 | 36:BA:2606:C:O4' | 2.52 | 0.43 |
| 36:BA:1999:C:H5'' | 36:BA:2723:C:O2' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BA:2741:A:C2' | 36:BA:2742:C:H5' | 2.48 | 0.43 |
| 36:BA:326:G:H2' | 36:BA:327:G:O4' | 2.19 | 0.43 |
| 36:BA:329:G:H1 | 57:BY:19:LYS:HE3 | 1.84 | 0.43 |
| 36:BA:323:G:C2 | 36:BA:333:G:H1' | 2.54 | 0.43 |
| 36:BA:627:A:C6 | 36:BA:637:A:C8 | 3.07 | 0.43 |
| 36:BA:710:G:H2' | 36:BA:711:G:H8 | 1.83 | 0.43 |
| 36:BA:781:A:H2 | 36:BA:1776:G:N3 | 2.15 | 0.43 |
| 37:BB:53:A:N7 | 37:BB:54:G:N7 | 2.67 | 0.43 |
| 39:BD:32:SER:O | 39:BD:36:PRO:CD | 2.66 | 0.43 |
| 39:BD:85:ASP:OD1 | 39:BD:87:ASN:ND2 | 2.49 | 0.43 |
| 42:BG:9:ARG:C | 42:BG:11:TYR:H | 2.22 | 0.43 |
| 43:BH:85:LYS:HZ3 | 43:BH:132:ARG:C | 2.17 | 0.43 |
| 48:BP:115:LEU:CD2 | 48:BP:115:LEU:N | 2.82 | 0.43 |
| 48:BP:23:PRO:C | 48:BP:33:ARG:CZ | 2.87 | 0.43 |
| 49:BQ:26:TYR:CD1 | 49:BQ:28:ALA:HB2 | 2.53 | 0.43 |
| 49:BQ:39:PRO:O | 49:BQ:40:ALA:CB | 2.65 | 0.43 |
| 49:BQ:5:ARG:O | 49:BQ:6:ARG:HG2 | 2.19 | 0.43 |
| 49:BQ:78:PRO:HD2 | 49:BQ:81:VAL:HG11 | 2.00 | 0.43 |
| 52:BT:83:ILE:CD1 | 52:BT:84:GLN:HG2 | 2.49 | 0.43 |
| 52:BT:92:GLY:O | 52:BT:94:ALA:N | 2.52 | 0.43 |
| 53:BU:80:ILE:HG22 | 53:BU:80:ILE:O | 2.19 | 0.43 |
| 54:BV:16:PRO:HA | 54:BV:96:ILE:O | 2.18 | 0.43 |
| 58:BZ:127:LYS:HG3 | 58:BZ:127:LYS:O | 2.18 | 0.43 |
| 1:AA:1106:G:O2' | 1:AA:1107:C:H5' | 2.19 | 0.43 |
| 1:AA:174:C:O2' | 1:AA:175:C:H5' | 2.17 | 0.43 |
| 1:AA:512:U:H2' | 1:AA:513:C:C6 | 2.54 | 0.43 |
| 1:AA:909:A:H2' | 1:AA:910:C:O4' | 2.19 | 0.43 |
| 2:AB:214:ILE:O | 2:AB:218:ALA:CB | 2.67 | 0.43 |
| 3:AC:145:GLY:O | 3:AC:146:ALA:O | 2.37 | 0.43 |
| 4:AD:132:ARG:O | 4:AD:132:ARG:HD2 | 2.18 | 0.43 |
| 4:AD:15:GLU:OE1 | 4:AD:59:ARG:NE | 2.52 | 0.43 |
| 6:AF:14:LEU:HD13 | 6:AF:18:GLN:CB | 2.49 | 0.43 |
| 7:AG:111:ARG:NH1 | 7:AG:111:ARG:HG2 | 2.33 | 0.43 |
| 7:AG:120:ILE:HG22 | 7:AG:124:LEU:HD12 | 2.00 | 0.43 |
| 9:AI:46:ALA:HB2 | 9:AI:74:ILE:HG23 | 2.01 | 0.43 |
| 12:AL:104:VAL:O | 12:AL:105:TYR:C | 2.57 | 0.43 |
| 19:AS:13:ASP:C | 19:AS:15:LEU:N | 2.72 | 0.43 |
| 20:AT:69:GLY:O | 20:AT:73:HIS:CD2 | 2.71 | 0.43 |
| 20:AT:93:GLU:CD | 20:AT:94:ALA:N | 2.72 | 0.43 |
| 22:AW:43:C:H2' | 22:AW:44:G:C1' | 2.49 | 0.43 |
| 25:AZ:107:SER:OG | 25:AZ:137:LYS:NZ | 2.41 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:AY:76:A:N1 | 25:AZ:269:GLY:C | 2.72 | 0.43 |
| 25:AZ:46:ASP:OD2 | 25:AZ:47:TYR:N | 2.47 | 0.43 |
| 27:B1:3:LYS:HB3 | 27:B1:4:VAL:H | 1.60 | 0.43 |
| 28:B2:31:GLU:CB | 28:B2:53:LEU:HD11 | 2.49 | 0.43 |
| 29:B3:8:LEU:HD12 | 29:B3:28:LEU:HB2 | 2.00 | 0.43 |
| 34:B8:11:LYS:HG2 | 34:B8:11:LYS:O | 2.19 | 0.43 |
| 36:BA:1052:C:O2' | 36:BA:1053:C:P | 2.76 | 0.43 |
| 36:BA:1116:C:H2' | 36:BA:1117:G:C8 | 2.46 | 0.43 |
| 36:BA:1471:A:H2' | 36:BA:1472:A:C8 | 2.54 | 0.43 |
| 36:BA:1495:A:C4 | 36:BA:1496:A:H2 | 2.36 | 0.43 |
| 36:BA:1591:G:H8 | 36:BA:1591:G:H5' | 1.84 | 0.43 |
| 36:BA:1934:C:O2' | 36:BA:1935:G:H5' | 2.19 | 0.43 |
| 36:BA:2674:G:H2' | 36:BA:2675:A:H8 | 1.84 | 0.43 |
| 36:BA:2681:C:H5 | 36:BA:2725:A:H62 | 1.62 | 0.43 |
| 36:BA:301:G:C6 | 36:BA:317:G:C5 | 3.07 | 0.43 |
| 36:BA:67:U:H2' | 36:BA:68:G:H8 | 1.84 | 0.43 |
| 36:BA:7:G:O2' | 36:BA:8:A:H5' | 2.19 | 0.43 |
| 36:BA:962:G:O2' | 36:BA:963:U:H5' | 2.19 | 0.43 |
| 38:BC:30:LYS:HZ3 | 38:BC:178:ALA:HB1 | 1.80 | 0.43 |
| 40:BE:104:VAL:HG12 | 40:BE:105:THR:N | 2.33 | 0.43 |
| 40:BE:119:ARG:NH1 | 40:BE:158:GLY:HA3 | 2.34 | 0.43 |
| 41:BF:110:LEU:C | 41:BF:110:LEU:HD13 | 2.39 | 0.43 |
| 41:BF:3:GLU:O | 41:BF:19:GLU:CB | 2.66 | 0.43 |
| 42:BG:101:ILE:O | 42:BG:104:GLU:HB3 | 2.18 | 0.43 |
| 43:BH:65:HIS:CE1 | 43:BH:69:ARG:NH1 | 2.87 | 0.43 |
| 43:BH:83:TYR:CD1 | 43:BH:84:SER:N | 2.87 | 0.43 |
| 45:BK:48:UNK:O | 45:BK:49:UNK:CB | 2.66 | 0.43 |
| 46:BN:108:PRO:HG2 | 46:BN:113:GLY:CA | 2.48 | 0.43 |
| 47:BO:7:TYR:CE1 | 47:BO:20:MET:HB2 | 2.54 | 0.43 |
| 34:B8:13:ARG:HD3 | 48:BP:61:ARG:O | 2.19 | 0.43 |
| 48:BP:65:ARG:O | 48:BP:68:GLN:OE1 | 2.36 | 0.43 |
| 50:BR:44:LEU:HD13 | 50:BR:44:LEU:O | 2.17 | 0.43 |
| 36:BA:2864:G:OP1 | 52:BT:119:LYS:HD2 | 2.19 | 0.43 |
| 52:BT:90:GLN:O | 52:BT:91:ARG:C | 2.57 | 0.43 |
| 54:BV:55:ALA:HB1 | 54:BV:101:GLY:HA2 | 2.00 | 0.43 |
| 55:BW:50:VAL:HG13 | 55:BW:50:VAL:O | 2.18 | 0.43 |
| 58:BZ:35:ARG:CZ | 58:BZ:35:ARG:HA | 2.48 | 0.43 |
| 1:AA:1134:G:C2 | 1:AA:1142:G:C6 | 3.06 | 0.43 |
| 1:AA:1303:C:N4 | 1:AA:1304:G:C6 | 2.86 | 0.43 |
| 1:AA:1354:C:O2' | 1:AA:1355:G:H5' | 2.18 | 0.43 |
| 1:AA:1399:C:C2 | 1:AA:1502:A:N6 | 2.87 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:153:C:N4 | 1:AA:168:G:H1 | 2.17 | 0.43 |
| 1:AA:402:G:O2' | 1:AA:403:C:H5' | 2.18 | 0.43 |
| 1:AA:498:U:O2' | 1:AA:499:A:P | 2.77 | 0.43 |
| 2:AB:220:ASP:OD1 | 2:AB:223:ILE:HD12 | 2.19 | 0.43 |
| 2:AB:7:VAL:HG13 | 2:AB:11:LEU:CD1 | 2.48 | 0.43 |
| 4:AD:104:VAL:HA | 4:AD:107:ARG:HB2 | 2.01 | 0.43 |
| 5:AE:28:PHE:CD1 | 5:AE:28:PHE:N | 2.87 | 0.43 |
| 5:AE:95:ALA:O | 5:AE:96:PRO:C | 2.56 | 0.43 |
| 6:AF:35:ALA:HB1 | 6:AF:65:VAL:CG1 | 2.49 | 0.43 |
| 9:AI:11:LYS:O | 9:AI:11:LYS:CG | 2.66 | 0.43 |
| 9:AI:128:ARG:HG2 | 9:AI:128:ARG:OXT | 2.19 | 0.43 |
| 10:AJ:9:ARG:HG2 | 10:AJ:69:ASN:OD1 | 2.19 | 0.43 |
| 1:AA:254:G:OP1 | 17:AQ:67:LYS:O | 2.37 | 0.43 |
| 20:AT:57:ARG:HH11 | 20:AT:103:GLY:N | 2.16 | 0.43 |
| 22:AV:14:A:N6 | 22:AV:21:A:C2 | 2.87 | 0.43 |
| 22:AV:72:C:C3' | 22:AV:73:A:C5' | 2.96 | 0.43 |
| 22:AW:19:G:C6 | 36:BA:2169:A:O2' | 2.62 | 0.43 |
| 25:AZ:248:LYS:O | 25:AZ:267:VAL:HG21 | 2.19 | 0.43 |
| 26:B0:12:ASN:HA | 26:B0:14:ARG:HH12 | 1.84 | 0.43 |
| 27:B1:14:VAL:HG12 | 27:B1:14:VAL:O | 2.17 | 0.43 |
| 35:B9:9:ARG:HD2 | 35:B9:16:VAL:CG2 | 2.49 | 0.43 |
| 36:BA:1267:U:C5 | 36:BA:2012:G:N2 | 2.87 | 0.43 |
| 36:BA:1530:C:O5' | 36:BA:1530:C:H6 | 2.02 | 0.43 |
| 36:BA:1598:C:C5' | 56:BX:36:LYS:CD | 2.97 | 0.43 |
| 36:BA:919:G:N2 | 36:BA:2269:A:OP2 | 2.51 | 0.43 |
| 36:BA:2275:C:O2 | 49:BQ:85:LYS:CD | 2.67 | 0.43 |
| 36:BA:252:G:O2' | 36:BA:253:C:H5' | 2.19 | 0.43 |
| 36:BA:272(I):U:O2' | 36:BA:272(J):C:H5' | 2.18 | 0.43 |
| 36:BA:2889:C:H2' | 36:BA:2891:G:O4' | 2.19 | 0.43 |
| 36:BA:324:A:N6 | 36:BA:338:G:O2' | 2.52 | 0.43 |
| 36:BA:341:G:H2' | 36:BA:342:G:H8 | 1.83 | 0.43 |
| 36:BA:536:A:OP1 | 53:BU:53:ARG:NH1 | 2.51 | 0.43 |
| 36:BA:600:G:H2' | 36:BA:601:C:C6 | 2.54 | 0.43 |
| 36:BA:647:G:N2 | 36:BA:2350:C:H4' | 2.33 | 0.43 |
| 36:BA:78:A:H2' | 36:BA:79:G:C8 | 2.53 | 0.43 |
| 37:BB:17:C:O2' | 37:BB:18:G:H5' | 2.18 | 0.43 |
| 39:BD:118:VAL:CG2 | 39:BD:119:ALA:H | 2.30 | 0.43 |
| 39:BD:117:VAL:CG2 | 39:BD:128:GLY:C | 2.87 | 0.43 |
| 39:BD:197:GLY:C | 39:BD:199:ALA:N | 2.71 | 0.43 |
| 39:BD:44:ASN:HD22 | 39:BD:45:ASN:N | 2.17 | 0.43 |
| 39:BD:52:ARG:HH11 | 39:BD:52:ARG:HD3 | 1.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BF:157:VAL:HG21 | 41:BF:194:MET:HG2 | 2.00 | 0.43 |
| 41:BF:195:ASP:O | 41:BF:199:TRP:HB2 | 2.18 | 0.43 |
| 41:BF:64:ILE:HD12 | 41:BF:78:ILE:HG23 | 2.01 | 0.43 |
| 36:BA:1248:G:P | 41:BF:92:PRO:HG3 | 2.59 | 0.43 |
| 42:BG:105:LYS:HD2 | 42:BG:142:PRO:HG3 | 2.00 | 0.43 |
| 42:BG:159:VAL:HG13 | 42:BG:159:VAL:O | 2.18 | 0.43 |
| 42:BG:7:LEU:O | 42:BG:11:TYR:N | 2.52 | 0.43 |
| 45:BK:24:UNK:O | 45:BK:28:UNK:CB | 2.67 | 0.43 |
| 47:BO:105:GLU:O | 47:BO:109:LYS:CG | 2.67 | 0.43 |
| 48:BP:50:ARG:CG | 48:BP:51:PHE:N | 2.79 | 0.43 |
| 34:B8:13:ARG:NH1 | 48:BP:59:LEU:HG | 2.33 | 0.43 |
| 50:BR:104:ARG:HD3 | 50:BR:107:ASP:CG | 2.39 | 0.43 |
| 51:BS:13:ARG:O | 51:BS:15:ARG:N | 2.52 | 0.43 |
| 55:BW:17:VAL:O | 55:BW:19:LEU:N | 2.52 | 0.43 |
| 56:BX:47:PHE:C | 56:BX:49:VAL:H | 2.17 | 0.43 |
| 57:BY:32:PRO:O | 57:BY:35:TYR:N | 2.52 | 0.43 |
| 58:BZ:108:PRO:C | 58:BZ:110:GLY:N | 2.69 | 0.43 |
| 58:BZ:135:GLU:HB3 | 58:BZ:136:PHE:H | 1.66 | 0.43 |
| 58:BZ:19:ARG:C | 58:BZ:21:ALA:H | 2.22 | 0.43 |
| 1:AA:1314:C:H2' | 1:AA:1315:U:H6 | 1.84 | 0.43 |
| 1:AA:66:G:C4' | 1:AA:173:U:C5 | 2.98 | 0.43 |
| 1:AA:179:A:O2' | 1:AA:180:U:H5' | 2.18 | 0.43 |
| 1:AA:186:C:C2 | 1:AA:187:C:C5 | 3.07 | 0.43 |
| 1:AA:439:A:H2' | 1:AA:441:A:O4' | 2.18 | 0.43 |
| 1:AA:84:U:H2' | 1:AA:88:A:H5' | 2.00 | 0.43 |
| 2:AB:36:ARG:HH11 | 2:AB:36:ARG:HG3 | 1.84 | 0.43 |
| 2:AB:74:LYS:O | 2:AB:76:GLN:N | 2.52 | 0.43 |
| 15:AO:24:SER:O | 15:AO:25:THR:C | 2.58 | 0.43 |
| 16:AP:8:ARG:CB | 16:AP:28:ARG:HH22 | 2.32 | 0.43 |
| 17:AQ:5:VAL:HA | 17:AQ:59:ILE:O | 2.19 | 0.43 |
| 22:AW:56:C:H2' | 22:AW:57:G:C8 | 2.54 | 0.43 |
| 24:AY:54:5MU:H2' | 24:AY:55:PSU:O4' | 2.19 | 0.43 |
| 25:AZ:139:ASP:O | 25:AZ:140:MET:HE2 | 2.19 | 0.43 |
| 25:AZ:290:LEU:HD12 | 25:AZ:298:VAL:HG21 | 2.01 | 0.43 |
| 28:B2:29:LYS:O | 28:B2:32:LEU:N | 2.51 | 0.43 |
| 33:B7:38:GLY:O | 36:BA:458:G:C5' | 2.58 | 0.43 |
| 36:BA:1124:C:H2' | 36:BA:1125:G:O4' | 2.18 | 0.43 |
| 36:BA:1218:C:H2' | 36:BA:1218:C:O2 | 2.17 | 0.43 |
| 36:BA:1331:A:O2' | 36:BA:1332:G:H5'' | 2.19 | 0.43 |
| 36:BA:139:G:C6 | 36:BA:140:G:H2' | 2.53 | 0.43 |
| 36:BA:1429:G:H2' | 36:BA:1430:C:H6 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:1614:A:H2' | 36:BA:1615:C:C5' | 2.39 | 0.43 |
| 36:BA:1790:C:H2' | 36:BA:1791:A:C5 | 2.54 | 0.43 |
| 36:BA:191:A:O2' | 36:BA:192:C:C5' | 2.66 | 0.43 |
| 36:BA:2175:C:O4' | 38:BC:215:THR:HG21 | 2.19 | 0.43 |
| 36:BA:2552:U:H2' | 36:BA:2554:U:H5'' | 2.01 | 0.43 |
| 36:BA:2645:G:OP2 | 36:BA:2645:G:H8 | 2.02 | 0.43 |
| 36:BA:272(I):U:C2' | 36:BA:272(J):C:H5' | 2.49 | 0.43 |
| 36:BA:2809:A:H2' | 36:BA:2810:A:C8 | 2.53 | 0.43 |
| 36:BA:736:C:O2' | 36:BA:737:C:H5' | 2.19 | 0.43 |
| 37:BB:107:G:O2' | 37:BB:108:U:H5' | 2.18 | 0.43 |
| 39:BD:75:ILE:HG21 | 39:BD:99:ASP:HB2 | 2.00 | 0.43 |
| 40:BE:119:ARG:HG3 | 40:BE:160:TYR:CD2 | 2.53 | 0.43 |
| 41:BF:130:ALA:HB3 | 41:BF:142:TRP:HD1 | 1.84 | 0.43 |
| 42:BG:111:LEU:HD21 | 42:BG:179:PRO:CD | 2.49 | 0.43 |
| 42:BG:88:ILE:HG22 | 42:BG:89:GLY:N | 2.34 | 0.43 |
| 49:BQ:32:TYR:CD1 | 49:BQ:32:TYR:N | 2.86 | 0.43 |
| 36:BA:2840:C:H4' | 50:BR:53:HIS:CD2 | 2.54 | 0.43 |
| 55:BW:91:GLY:O | 55:BW:92:ARG:O | 2.36 | 0.43 |
| 58:BZ:11:GLU:CD | 58:BZ:11:GLU:N | 2.71 | 0.43 |
| 58:BZ:153:SER:H | 58:BZ:167:PRO:HB2 | 1.84 | 0.43 |
| 58:BZ:38:TYR:O | 58:BZ:38:TYR:CD1 | 2.72 | 0.43 |
| 1:AA:1006:C:H2' | 1:AA:1007:C:C6 | 2.54 | 0.42 |
| 1:AA:1004:A:C5' | 1:AA:1025:U:O4 | 2.66 | 0.42 |
| 1:AA:1497:G:C2' | 1:AA:1498:U:H5' | 2.49 | 0.42 |
| 1:AA:537:G:H2' | 1:AA:538:G:H8 | 1.84 | 0.42 |
| 1:AA:666:G:H5' | 1:AA:726:C:H1' | 2.01 | 0.42 |
| 3:AC:3:ASN:OD1 | 3:AC:3:ASN:N | 2.52 | 0.42 |
| 4:AD:121:VAL:O | 4:AD:134:ASP:HA | 2.18 | 0.42 |
| 5:AE:60:TYR:CZ | 5:AE:64:ARG:NH2 | 2.86 | 0.42 |
| 5:AE:75:THR:HB | 5:AE:117:ASP:O | 2.19 | 0.42 |
| 5:AE:82:VAL:HG21 | 5:AE:138:ALA:CA | 2.49 | 0.42 |
| 8:AH:77:GLU:OE2 | 8:AH:81:HIS:NE2 | 2.46 | 0.42 |
| 1:AA:1371:G:OP2 | 9:AI:11:LYS:HD2 | 2.19 | 0.42 |
| 1:AA:256:U:H5' | 17:AQ:17:LYS:NZ | 2.34 | 0.42 |
| 26:B0:14:ARG:CG | 26:B0:14:ARG:NH1 | 2.81 | 0.42 |
| 27:B1:29:GLY:O | 27:B1:30:VAL:CG2 | 2.65 | 0.42 |
| 34:B8:30:ARG:NH1 | 36:BA:2419:U:O4 | 2.51 | 0.42 |
| 36:BA:1013:C:C2' | 36:BA:1014:U:H5' | 2.50 | 0.42 |
| 36:BA:1253:A:C3' | 36:BA:1254:A:H5' | 2.48 | 0.42 |
| 36:BA:1490:A:C2 | 39:BD:75:ILE:HD12 | 2.54 | 0.42 |
| 36:BA:1636:C:H2' | 36:BA:1637:A:H8 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:2199:A:C5' | 36:BA:2200:C:OP2 | 2.66 | 0.42 |
| 36:BA:2284:C:H2' | 36:BA:2285:C:C6 | 2.48 | 0.42 |
| 36:BA:2478:A:C2' | 36:BA:2479:G:H5' | 2.49 | 0.42 |
| 36:BA:2726:U:H6 | 47:BO:67:LYS:NZ | 2.17 | 0.42 |
| 36:BA:2768:C:O2' | 36:BA:2769:C:H5' | 2.19 | 0.42 |
| 36:BA:2854:G:O2' | 36:BA:2855:C:H5' | 2.18 | 0.42 |
| 36:BA:29:U:H2' | 36:BA:30:G:H8 | 1.84 | 0.42 |
| 36:BA:622:G:C2' | 36:BA:623:G:H5' | 2.48 | 0.42 |
| 36:BA:752:A:HO2' | 36:BA:753:C:P | 2.39 | 0.42 |
| 36:BA:847:U:OP2 | 36:BA:928:G:O6 | 2.36 | 0.42 |
| 36:BA:970:C:H2' | 36:BA:971:C:H6 | 1.83 | 0.42 |
| 38:BC:132:GLY:N | 38:BC:133:PRO:HD3 | 2.33 | 0.42 |
| 36:BA:2124:G:N2 | 38:BC:217:THR:O | 2.52 | 0.42 |
| 38:BC:3:HIS:O | 38:BC:8:ARG:HG3 | 2.18 | 0.42 |
| 43:BH:18:GLU:CB | 43:BH:25:LYS:HB2 | 2.48 | 0.42 |
| 46:BN:45:ASN:N | 46:BN:45:ASN:HD22 | 2.15 | 0.42 |
| 51:BS:85:VAL:HG22 | 51:BS:106:ARG:HB2 | 1.99 | 0.42 |
| 52:BT:62:THR:HG22 | 52:BT:75:ILE:HG13 | 2.01 | 0.42 |
| 36:BA:1227:G:H5' | 53:BU:13:LYS:HZ2 | 1.83 | 0.42 |
| 53:BU:95:LEU:HD12 | 54:BV:11:GLN:NE2 | 2.32 | 0.42 |
| 58:BZ:119:GLU:HG2 | 58:BZ:122:ARG:HH11 | 1.82 | 0.42 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:C6 | 2.54 | 0.42 |
| 1:AA:1152:A:OP1 | 10:AJ:68:HIS:CD2 | 2.70 | 0.42 |
| 1:AA:949:A:C2 | 1:AA:1233:G:N3 | 2.88 | 0.42 |
| 1:AA:17:U:H2' | 1:AA:18:C:H6 | 1.80 | 0.42 |
| 1:AA:389:A:N3 | 1:AA:389:A:H2' | 2.33 | 0.42 |
| 1:AA:46:G:O2' | 1:AA:365:U:H1' | 2.19 | 0.42 |
| 1:AA:625:G:H2' | 1:AA:626:U:C6 | 2.53 | 0.42 |
| 1:AA:692:U:OP1 | 11:AK:124:LYS:HE2 | 2.19 | 0.42 |
| 1:AA:735:C:H2' | 1:AA:736:C:C6 | 2.53 | 0.42 |
| 1:AA:866:C:H2' | 1:AA:867:G:O4' | 2.19 | 0.42 |
| 2:AB:17:PHE:H | 2:AB:17:PHE:HD2 | 1.66 | 0.42 |
| 4:AD:175:SER:OG | 4:AD:184:LYS:HB2 | 2.18 | 0.42 |
| 5:AE:71:LEU:HD13 | 5:AE:114:GLY:O | 2.20 | 0.42 |
| 10:AJ:6:ILE:CD1 | 10:AJ:23:ILE:HG21 | 2.48 | 0.42 |
| 10:AJ:57:LYS:O | 10:AJ:57:LYS:HD2 | 2.19 | 0.42 |
| 11:AK:89:ALA:C | 11:AK:91:ARG:H | 2.22 | 0.42 |
| 17:AQ:62:SER:HB2 | 17:AQ:72:ARG:HG3 | 2.01 | 0.42 |
| 18:AR:45:SER:OG | 18:AR:46:GLU:N | 2.49 | 0.42 |
| 19:AS:29:ARG:O | 19:AS:31:ILE:N | 2.53 | 0.42 |
| 20:AT:57:ARG:CZ | 20:AT:102:GLY:HA3 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AW:39:U:O4' | 22:AW:39:U:O2 | 2.36 | 0.42 |
| 24:AY:4:G:C3' | 24:AY:5:G:H5'' | 2.48 | 0.42 |
| 24:AY:77:TRP:NE1 | 25:AZ:67:HIS:CD2 | 2.87 | 0.42 |
| 25:AZ:219:LYS:HB3 | 25:AZ:220:PRO:HD2 | 2.00 | 0.42 |
| 25:AZ:257:GLY:O | 25:AZ:258:LEU:HB2 | 2.19 | 0.42 |
| 25:AZ:27:LEU:O | 25:AZ:31:LEU:HG | 2.19 | 0.42 |
| 25:AZ:332:THR:HB | 25:AZ:333:GLY:H | 1.54 | 0.42 |
| 29:B3:31:LEU:O | 29:B3:32:GLN:CB | 2.66 | 0.42 |
| 32:B6:15:GLU:OE1 | 32:B6:18:ARG:CG | 2.66 | 0.42 |
| 32:B6:25:LYS:HE2 | 34:B8:34:TRP:HE1 | 1.83 | 0.42 |
| 36:BA:1152:C:H2' | 36:BA:1153:C:H6 | 1.84 | 0.42 |
| 36:BA:1169:G:H2' | 36:BA:1170:G:O4' | 2.17 | 0.42 |
| 36:BA:1291:C:C2' | 36:BA:1292:U:C5' | 2.95 | 0.42 |
| 36:BA:1756:G:H4' | 36:BA:1758:G:O4' | 2.19 | 0.42 |
| 36:BA:2166:G:H2' | 36:BA:2167:U:C6 | 2.54 | 0.42 |
| 36:BA:2167:U:N3 | 36:BA:2171:A:N6 | 2.64 | 0.42 |
| 36:BA:402:A:C2' | 36:BA:403:U:H5' | 2.48 | 0.42 |
| 36:BA:909:A:H2' | 36:BA:912:C:C5 | 2.53 | 0.42 |
| 37:BB:16:G:O2' | 37:BB:17:C:H6 | 1.99 | 0.42 |
| 36:BA:2125:G:O4' | 38:BC:217:THR:HG23 | 2.19 | 0.42 |
| 39:BD:108:PRO:HB3 | 39:BD:143:HIS:CE1 | 2.54 | 0.42 |
| 39:BD:118:VAL:CG2 | 39:BD:119:ALA:N | 2.81 | 0.42 |
| 39:BD:261:LYS:HZ2 | 39:BD:263:ARG:CZ | 2.30 | 0.42 |
| 36:BA:692:C:C5' | 39:BD:42:GLY:H | 2.32 | 0.42 |
| 40:BE:181:LEU:HD21 | 52:BT:7:ILE:HG23 | 2.02 | 0.42 |
| 36:BA:2787:C:H1' | 40:BE:61:ARG:HD3 | 2.00 | 0.42 |
| 41:BF:125:LEU:CD2 | 41:BF:125:LEU:N | 2.80 | 0.42 |
| 42:BG:15:VAL:HG12 | 42:BG:19:LEU:HD11 | 2.01 | 0.42 |
| 42:BG:60:LEU:O | 42:BG:60:LEU:HD13 | 2.20 | 0.42 |
| 42:BG:8:LYS:O | 42:BG:11:TYR:HB3 | 2.19 | 0.42 |
| 42:BG:40:ASN:HB2 | 42:BG:91:ARG:HB2 | 2.00 | 0.42 |
| 51:BS:87:PHE:CD2 | 51:BS:88:ASP:N | 2.83 | 0.42 |
| 52:BT:121:ILE:HG22 | 52:BT:122:ASP:N | 2.34 | 0.42 |
| 52:BT:83:ILE:CG1 | 52:BT:84:GLN:HG2 | 2.48 | 0.42 |
| 52:BT:88:ILE:HG22 | 52:BT:89:VAL:HG23 | 1.99 | 0.42 |
| 54:BV:89:GLN:OE1 | 54:BV:89:GLN:HA | 2.19 | 0.42 |
| 36:BA:747:U:O3' | 55:BW:89:ALA:HB3 | 2.19 | 0.42 |
| 1:AA:1152:A:H2' | 1:AA:1153:C:H6 | 1.83 | 0.42 |
| 1:AA:1216:G:OP2 | 14:AN:2:ALA:HB2 | 2.20 | 0.42 |
| 1:AA:314:C:O2' | 1:AA:315:A:H5' | 2.19 | 0.42 |
| 1:AA:413:G:H1' | 1:AA:428:G:N2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:731:G:H5' | 1:AA:766:A:H4' | 2.01 | 0.42 |
| 1:AA:858:G:N1 | 1:AA:869:G:C8 | 2.87 | 0.42 |
| 2:AB:200:ILE:HG22 | 2:AB:202:PRO:HD3 | 2.00 | 0.42 |
| 2:AB:59:GLU:CA | 2:AB:221:LEU:HD11 | 2.48 | 0.42 |
| 3:AC:112:SER:OG | 3:AC:115:LEU:HG | 2.20 | 0.42 |
| 5:AE:24:ARG:HG2 | 5:AE:24:ARG:HH11 | 1.85 | 0.42 |
| 5:AE:63:ARG:O | 5:AE:64:ARG:CB | 2.67 | 0.42 |
| 9:AI:82:ALA:C | 9:AI:84:ALA:N | 2.73 | 0.42 |
| 10:AJ:27:ALA:HA | 10:AJ:30:SER:OG | 2.19 | 0.42 |
| 10:AJ:32:ALA:HB2 | 10:AJ:76:ASN:HB2 | 2.00 | 0.42 |
| 11:AK:25:TYR:CE1 | 11:AK:87:THR:HB | 2.52 | 0.42 |
| 12:AL:82:VAL:O | 12:AL:106:ASP:HB2 | 2.18 | 0.42 |
| 15:AO:21:ASP:OD2 | 15:AO:21:ASP:C | 2.57 | 0.42 |
| 19:AS:61:TYR:O | 19:AS:62:ILE:CB | 2.66 | 0.42 |
| 19:AS:45:VAL:HA | 19:AS:62:ILE:HG13 | 2.00 | 0.42 |
| 25:AZ:93:ILE:CG1 | 25:AZ:122:LEU:HD13 | 2.50 | 0.42 |
| 25:AZ:171:ILE:HG12 | 25:AZ:202:LEU:HA | 2.01 | 0.42 |
| 30:B4:18:CYS:SG | 30:B4:19:GLY:N | 2.93 | 0.42 |
| 32:B6:11:LEU:HA | 32:B6:11:LEU:HD22 | 1.83 | 0.42 |
| 36:BA:1106:G:C2' | 36:BA:1107:G:H5' | 2.49 | 0.42 |
| 36:BA:1351:C:H2' | 36:BA:1352:U:C6 | 2.54 | 0.42 |
| 36:BA:1615:C:H2' | 36:BA:1617:C:C5 | 2.54 | 0.42 |
| 36:BA:2059:A:O3' | 41:BF:69:HIS:HA | 2.19 | 0.42 |
| 36:BA:210:C:H2' | 36:BA:211:A:C8 | 2.54 | 0.42 |
| 36:BA:236:C:H2' | 36:BA:237:C:C6 | 2.54 | 0.42 |
| 36:BA:2456:C:O2' | 36:BA:2457:U:H5' | 2.19 | 0.42 |
| 36:BA:2704:C:H2' | 36:BA:2705:A:O4' | 2.20 | 0.42 |
| 36:BA:2796:U:C2' | 36:BA:2799:C:H5' | 2.49 | 0.42 |
| 36:BA:286:C:H42 | 36:BA:355:G:H1 | 1.68 | 0.42 |
| 36:BA:955:C:N4 | 36:BA:956:G:C5 | 2.87 | 0.42 |
| 37:BB:104:U:O2' | 58:BZ:72:ARG:HD2 | 2.19 | 0.42 |
| 39:BD:209:ALA:C | 39:BD:210:GLY:O | 2.53 | 0.42 |
| 40:BE:14:ILE:HG13 | 40:BE:21:VAL:HG23 | 2.00 | 0.42 |
| 41:BF:20:LEU:C | 41:BF:23:ASP:OD2 | 2.57 | 0.42 |
| 42:BG:168:GLU:O | 42:BG:169:ALA:C | 2.58 | 0.42 |
| 42:BG:76:SER:HB3 | 42:BG:83:ARG:CB | 2.45 | 0.42 |
| 43:BH:135:GLY:HA3 | 43:BH:141:VAL:HG22 | 2.01 | 0.42 |
| 50:BR:111:LEU:HD12 | 50:BR:111:LEU:N | 2.35 | 0.42 |
| 50:BR:12:ARG:HD3 | 50:BR:16:HIS:HD2 | 1.83 | 0.42 |
| 51:BS:54:LEU:O | 51:BS:56:LEU:N | 2.52 | 0.42 |
| 52:BT:121:ILE:O | 52:BT:124:ASP:HB2 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 56:BX:52:VAL:CG2 | 56:BX:84:ALA:HA | 2.49 | 0.42 |
| 58:BZ:102:LEU:HD21 | 58:BZ:124:ILE:CG1 | 2.50 | 0.42 |
| 58:BZ:7:ALA:HB3 | 58:BZ:61:LEU:CD2 | 2.49 | 0.42 |
| 1:AA:1032:G:H2' | 1:AA:1033:G:H8 | 1.82 | 0.42 |
| 1:AA:1060:C:C5 | 3:AC:2:GLY:CA | 3.02 | 0.42 |
| 1:AA:1313:U:C2 | 1:AA:1314:C:C5 | 3.07 | 0.42 |
| 3:AC:70:VAL:HG12 | 3:AC:72:LYS:N | 2.33 | 0.42 |
| 3:AC:73:PRO:O | 3:AC:76:VAL:HG22 | 2.20 | 0.42 |
| 7:AG:77:SER:HB2 | 7:AG:84:ASN:ND2 | 2.32 | 0.42 |
| 9:AI:9:ARG:HG3 | 9:AI:14:VAL:HG13 | 2.02 | 0.42 |
| 11:AK:115:PRO:C | 11:AK:117:ASN:H | 2.23 | 0.42 |
| 15:AO:70:LEU:HD12 | 15:AO:70:LEU:HA | 1.82 | 0.42 |
| 19:AS:10:PHE:CE2 | 19:AS:37:ARG:O | 2.72 | 0.42 |
| 20:AT:10:LEU:O | 20:AT:13:LEU:CD2 | 2.68 | 0.42 |
| 20:AT:86:ARG:O | 20:AT:90:GLN:HG2 | 2.18 | 0.42 |
| 25:AZ:195:TRP:O | 25:AZ:198:LYS:HB2 | 2.20 | 0.42 |
| 25:AZ:34:VAL:HG21 | 25:AZ:199:ILE:CG2 | 2.44 | 0.42 |
| 25:AZ:35:THR:HG22 | 25:AZ:203:LEU:HD13 | 2.00 | 0.42 |
| 26:B0:7:LEU:HD13 | 49:BQ:85:LYS:HG3 | 2.01 | 0.42 |
| 27:B1:37:ILE:HD12 | 27:B1:37:ILE:C | 2.39 | 0.42 |
| 29:B3:26:LEU:CD2 | 29:B3:43:ILE:HG23 | 2.49 | 0.42 |
| 32:B6:20:ASN:OD1 | 32:B6:21:TYR:N | 2.52 | 0.42 |
| 32:B6:53:LYS:CG | 32:B6:54:ILE:N | 2.83 | 0.42 |
| 34:B8:30:ARG:CZ | 36:BA:2419:U:O4 | 2.66 | 0.42 |
| 36:BA:1005:C:H2' | 36:BA:1006:C:C6 | 2.55 | 0.42 |
| 36:BA:85:G:N2 | 36:BA:103:A:C2 | 2.85 | 0.42 |
| 36:BA:1431:U:H2' | 36:BA:1432:C:O4' | 2.19 | 0.42 |
| 36:BA:1445(A):C:H2' | 36:BA:1446:C:H6 | 1.85 | 0.42 |
| 36:BA:1720:U:H2' | 36:BA:1721:G:H5'' | 2.01 | 0.42 |
| 36:BA:2014:A:H2' | 36:BA:2015:A:C8 | 2.54 | 0.42 |
| 36:BA:2111:C:H1' | 36:BA:2118:U:H4' | 2.00 | 0.42 |
| 34:B8:33:ASN:HD22 | 36:BA:2419:U:H5'' | 1.81 | 0.42 |
| 36:BA:2476:A:O2' | 36:BA:2477:C:H5'' | 2.18 | 0.42 |
| 36:BA:271(H):G:HO2' | 36:BA:271(I):G:P | 2.43 | 0.42 |
| 36:BA:288:C:H2' | 36:BA:288:C:O2 | 2.19 | 0.42 |
| 36:BA:2894:G:N3 | 36:BA:2894:G:H2' | 2.35 | 0.42 |
| 36:BA:645:C:C2' | 36:BA:645:C:O2 | 2.66 | 0.42 |
| 38:BC:116:THR:H | 38:BC:119:VAL:CG2 | 2.31 | 0.42 |
| 38:BC:161:ILE:HD13 | 38:BC:173:ALA:CB | 2.40 | 0.42 |
| 39:BD:142:VAL:HG21 | 39:BD:191:ALA:CB | 2.49 | 0.42 |
| 39:BD:182:LEU:HB2 | 39:BD:272:ALA:HB3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BE:154:LYS:O | 40:BE:156:MET:HG3 | 2.20 | 0.42 |
| 40:BE:49:LEU:HD22 | 40:BE:49:LEU:N | 2.34 | 0.42 |
| 41:BF:107:LYS:O | 41:BF:109:GLY:N | 2.52 | 0.42 |
| 41:BF:28:ILE:HD13 | 41:BF:28:ILE:H | 1.83 | 0.42 |
| 36:BA:443:A:N7 | 41:BF:45:ARG:HG2 | 2.34 | 0.42 |
| 41:BF:65:TRP:CH2 | 41:BF:75:HIS:HD2 | 2.38 | 0.42 |
| 41:BF:43:LYS:HA | 41:BF:98:SER:HA | 2.00 | 0.42 |
| 41:BF:8:GLN:HG3 | 41:BF:9:ILE:N | 2.35 | 0.42 |
| 42:BG:109:VAL:HG21 | 42:BG:142:PRO:HB3 | 2.02 | 0.42 |
| 42:BG:61:ALA:HB2 | 42:BG:68:PRO:HD3 | 2.01 | 0.42 |
| 42:BG:81:LYS:HB3 | 42:BG:82:LEU:H | 1.59 | 0.42 |
| 43:BH:17:VAL:CG1 | 43:BH:18:GLU:N | 2.81 | 0.42 |
| 43:BH:50:VAL:CG1 | 43:BH:51:ARG:N | 2.80 | 0.42 |
| 45:BK:5:UNK:O | 45:BK:6:UNK:C | 2.67 | 0.42 |
| 36:BA:631:A:H5'' | 48:BP:65:ARG:HH11 | 1.80 | 0.42 |
| 50:BR:38:VAL:HB | 50:BR:39:PRO:CD | 2.36 | 0.42 |
| 51:BS:101:LEU:C | 51:BS:102:ALA:O | 2.58 | 0.42 |
| 51:BS:93:LYS:HA | 51:BS:93:LYS:HD2 | 1.74 | 0.42 |
| 53:BU:27:LEU:C | 53:BU:29:SER:H | 2.21 | 0.42 |
| 1:AA:1228:C:H4' | 13:AM:116:THR:HA | 2.00 | 0.42 |
| 1:AA:143:A:H2 | 1:AA:220:G:H1 | 1.67 | 0.42 |
| 1:AA:291:C:O2' | 1:AA:292:G:H5' | 2.19 | 0.42 |
| 1:AA:356:A:C2 | 1:AA:368:U:O2 | 2.72 | 0.42 |
| 1:AA:728:A:H2' | 1:AA:729:A:C8 | 2.54 | 0.42 |
| 2:AB:19:HIS:O | 2:AB:39:ILE:CG2 | 2.65 | 0.42 |
| 3:AC:188:LEU:CD1 | 3:AC:195:VAL:CG1 | 2.98 | 0.42 |
| 3:AC:36:ASP:OD2 | 3:AC:59:ARG:NH2 | 2.52 | 0.42 |
| 4:AD:150:GLU:C | 4:AD:152:SER:H | 2.23 | 0.42 |
| 5:AE:13:ILE:HA | 5:AE:29:GLY:O | 2.19 | 0.42 |
| 6:AF:48:LEU:HD13 | 6:AF:52:ILE:CD1 | 2.49 | 0.42 |
| 7:AG:18:TYR:CG | 7:AG:59:LEU:HD13 | 2.55 | 0.42 |
| 8:AH:27:PRO:HG3 | 8:AH:58:TYR:CE2 | 2.54 | 0.42 |
| 10:AJ:44:VAL:HG12 | 10:AJ:45:ARG:N | 2.34 | 0.42 |
| 13:AM:23:TYR:C | 13:AM:23:TYR:HD1 | 2.22 | 0.42 |
| 16:AP:8:ARG:HB2 | 16:AP:28:ARG:NH2 | 2.35 | 0.42 |
| 17:AQ:52:LYS:O | 17:AQ:55:ASP:OD1 | 2.37 | 0.42 |
| 1:AA:1320:C:H41 | 19:AS:37:ARG:HB3 | 1.84 | 0.42 |
| 20:AT:26:ASN:CB | 20:AT:71:THR:OG1 | 2.65 | 0.42 |
| 20:AT:72:LEU:HD11 | 20:AT:80:ARG:HE | 1.83 | 0.42 |
| 22:AW:34:G:O2' | 22:AW:35:A:H5' | 2.18 | 0.42 |
| 25:AZ:12:VAL:HG13 | 25:AZ:100:ASP:OD2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:174:SER:OG | 25:AZ:177:LEU:HB2 | 2.19 | 0.42 |
| 26:B0:32:ARG:O | 26:B0:35:ASN:HB2 | 2.19 | 0.42 |
| 36:BA:1274:A:C2 | 36:BA:1302:A:C2 | 3.08 | 0.42 |
| 36:BA:1576:U:H2' | 36:BA:1577:C:H6 | 1.84 | 0.42 |
| 36:BA:1644:C:C2' | 36:BA:1644:C:O2 | 2.67 | 0.42 |
| 36:BA:1914:C:O2 | 36:BA:1914:C:O4' | 2.36 | 0.42 |
| 36:BA:1963:U:C2' | 36:BA:1963:U:O2 | 2.65 | 0.42 |
| 36:BA:2102:U:H2' | 36:BA:2103:C:C1' | 2.49 | 0.42 |
| 36:BA:235:U:H2' | 36:BA:236:C:H6 | 1.84 | 0.42 |
| 36:BA:2572:A:C8 | 40:BE:144:ARG:HB3 | 2.54 | 0.42 |
| 36:BA:2641:G:C8 | 36:BA:2641:G:C5' | 2.96 | 0.42 |
| 36:BA:2679:A:H5' | 40:BE:165:VAL:HG21 | 2.01 | 0.42 |
| 36:BA:527:C:N4 | 36:BA:2779:U:OP1 | 2.53 | 0.42 |
| 36:BA:284:U:O2' | 36:BA:285:C:H5' | 2.20 | 0.42 |
| 36:BA:2881:C:O2' | 36:BA:2882:A:H5' | 2.19 | 0.42 |
| 36:BA:631:A:OP1 | 48:BP:64:LYS:HE2 | 2.19 | 0.42 |
| 36:BA:857:C:C4 | 36:BA:858:U:C4 | 3.07 | 0.42 |
| 38:BC:49:ILE:HG21 | 38:BC:208:PHE:CE1 | 2.54 | 0.42 |
| 39:BD:117:VAL:HG21 | 39:BD:128:GLY:CA | 2.50 | 0.42 |
| 40:BE:132:HIS:CG | 40:BE:135:HIS:CE1 | 3.07 | 0.42 |
| 40:BE:176:ILE:HG22 | 40:BE:178:GLU:CB | 2.50 | 0.42 |
| 40:BE:47:VAL:CG2 | 40:BE:85:ASN:HA | 2.49 | 0.42 |
| 41:BF:176:LEU:HB3 | 41:BF:177:ALA:H | 1.59 | 0.42 |
| 42:BG:99:MET:O | 42:BG:103:LEU:HB2 | 2.20 | 0.42 |
| 43:BH:33:LEU:HD12 | 43:BH:75:ALA:CA | 2.47 | 0.42 |
| 44:BJ:114:UNK:O | 44:BJ:115:UNK:CB | 2.67 | 0.42 |
| 46:BN:1:MET:SD | 46:BN:2:LYS:N | 2.93 | 0.42 |
| 46:BN:6:PRO:CB | 46:BN:41:ASP:OD1 | 2.66 | 0.42 |
| 48:BP:112:LEU:O | 48:BP:127:ALA:HB1 | 2.20 | 0.42 |
| 48:BP:25:SER:O | 48:BP:27:HIS:N | 2.51 | 0.42 |
| 49:BQ:101:ARG:HH11 | 49:BQ:101:ARG:CG | 2.32 | 0.42 |
| 49:BQ:58:PHE:CD1 | 49:BQ:58:PHE:O | 2.73 | 0.42 |
| 51:BS:48:LEU:CD1 | 51:BS:48:LEU:H | 2.32 | 0.42 |
| 52:BT:28:VAL:HG12 | 52:BT:29:ARG:HD3 | 2.00 | 0.42 |
| 53:BU:31:SER:C | 53:BU:33:ARG:H | 2.22 | 0.42 |
| 54:BV:3:ALA:O | 54:BV:13:ARG:HA | 2.20 | 0.42 |
| 55:BW:75:TYR:N | 55:BW:75:TYR:CD1 | 2.88 | 0.42 |
| 57:BY:81:LYS:HZ3 | 57:BY:99:CYS:HB2 | 1.83 | 0.42 |
| 58:BZ:30:ASN:HA | 58:BZ:89:PHE:CE2 | 2.53 | 0.42 |
| 1:AA:1030:C:N4 | 1:AA:1032:G:N2 | 2.67 | 0.42 |
| 1:AA:1055:A:H2' | 3:AC:156:ARG:HD2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1139:G:C5' | 1:AA:1140:C:OP1 | 2.63 | 0.42 |
| 1:AA:1269:A:C2 | 1:AA:1313:U:H1' | 2.55 | 0.42 |
| 1:AA:443:C:H2' | 1:AA:444:C:C6 | 2.55 | 0.42 |
| 1:AA:823:G:H2' | 1:AA:824:C:C6 | 2.55 | 0.42 |
| 2:AB:82:ARG:HH11 | 2:AB:82:ARG:HG2 | 1.83 | 0.42 |
| 7:AG:91:VAL:O | 7:AG:92:SER:C | 2.58 | 0.42 |
| 11:AK:52:GLY:N | 11:AK:55:LYS:CE | 2.76 | 0.42 |
| 16:AP:45:THR:HG22 | 16:AP:47:ASP:CB | 2.48 | 0.42 |
| 18:AR:36:ASN:C | 18:AR:38:GLU:N | 2.73 | 0.42 |
| 21:AU:10:ARG:O | 21:AU:11:GLY:C | 2.58 | 0.42 |
| 25:AZ:344:PHE:HD2 | 25:AZ:384:LEU:HD23 | 1.84 | 0.42 |
| 25:AZ:329:GLY:O | 25:AZ:393:ARG:NE | 2.53 | 0.42 |
| 27:B1:48:LYS:HE3 | 27:B1:59:THR:CB | 2.50 | 0.42 |
| 27:B1:8:SER:HB3 | 27:B1:66:HIS:CD2 | 2.54 | 0.42 |
| 29:B3:54:VAL:CG1 | 29:B3:55:ARG:N | 2.81 | 0.42 |
| 31:B5:20:ARG:O | 31:B5:23:HIS:HB2 | 2.19 | 0.42 |
| 32:B6:26:ASN:HD22 | 32:B6:32:ASN:CG | 2.17 | 0.42 |
| 32:B6:10:LEU:CD1 | 34:B8:34:TRP:CD1 | 3.02 | 0.42 |
| 36:BA:1304:C:O2' | 36:BA:1305:C:H5' | 2.19 | 0.42 |
| 36:BA:1495:A:N3 | 36:BA:1496:A:H2 | 2.13 | 0.42 |
| 36:BA:1853:A:H2' | 36:BA:1854:A:C8 | 2.55 | 0.42 |
| 36:BA:1837:C:O2 | 36:BA:1927:A:H2 | 2.02 | 0.42 |
| 36:BA:2163:C:OP1 | 36:BA:2172:U:H5 | 2.02 | 0.42 |
| 36:BA:2206:G:H3' | 36:BA:2207:G:C5' | 2.49 | 0.42 |
| 36:BA:2476:A:C2 | 36:BA:2477:C:C6 | 3.02 | 0.42 |
| 36:BA:438:G:H2' | 36:BA:440:G:H8 | 1.85 | 0.42 |
| 36:BA:259:G:N2 | 36:BA:621:A:C8 | 2.75 | 0.42 |
| 36:BA:723:G:H2' | 36:BA:724:U:O4' | 2.20 | 0.42 |
| 38:BC:64:LEU:HD22 | 38:BC:188:ASN:HB3 | 2.02 | 0.42 |
| 38:BC:86:ALA:O | 38:BC:91:ALA:HB3 | 2.19 | 0.42 |
| 38:BC:99:ILE:HD12 | 38:BC:102:LYS:HZ2 | 1.84 | 0.42 |
| 36:BA:1818:U:H2' | 39:BD:157:ARG:HG3 | 2.02 | 0.42 |
| 36:BA:1816:G:N7 | 39:BD:62:TYR:CE1 | 2.88 | 0.42 |
| 39:BD:72:LYS:NZ | 39:BD:75:ILE:HG13 | 2.33 | 0.42 |
| 40:BE:103:ASP:OD2 | 40:BE:168:MET:HE2 | 2.20 | 0.42 |
| 42:BG:133:LEU:HD12 | 42:BG:157:ILE:HB | 2.00 | 0.42 |
| 48:BP:112:LEU:HD13 | 48:BP:112:LEU:O | 2.19 | 0.42 |
| 48:BP:45:LEU:CD2 | 48:BP:46:LYS:H | 2.32 | 0.42 |
| 52:BT:50:ILE:HD12 | 52:BT:50:ILE:N | 2.35 | 0.42 |
| 55:BW:1:MET:HE1 | 55:BW:62:HIS:HB3 | 2.01 | 0.42 |
| 56:BX:10:ALA:O | 56:BX:28:PHE:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:BY:20:TYR:HB3 | 57:BY:23:ARG:HG3 | 2.02 | 0.42 |
| 58:BZ:115:GLY:HA2 | 58:BZ:175:VAL:O | 2.18 | 0.42 |
| 58:BZ:8:TYR:CD1 | 58:BZ:8:TYR:N | 2.86 | 0.42 |
| 1:AA:1002:G:O5' | 1:AA:1002:G:H8 | 2.02 | 0.42 |
| 1:AA:1003:G:O2' | 1:AA:1004:A:H4' | 2.18 | 0.42 |
| 1:AA:1231:G:C6 | 1:AA:1232:U:C4 | 3.08 | 0.42 |
| 1:AA:1402:C:O2 | 1:AA:1500:A:N1 | 2.52 | 0.42 |
| 1:AA:663:A:O2' | 1:AA:664:G:H5' | 2.19 | 0.42 |
| 1:AA:93:G:H3' | 1:AA:96:U:C5 | 2.54 | 0.42 |
| 1:AA:966:G:O2' | 1:AA:967:C:H5' | 2.20 | 0.42 |
| 1:AA:971:G:H5'' | 1:AA:972:C:H5'' | 2.01 | 0.42 |
| 2:AB:69:LEU:HB2 | 2:AB:159:PRO:HG2 | 2.01 | 0.42 |
| 3:AC:82:GLU:HB2 | 3:AC:83:ARG:H | 1.70 | 0.42 |
| 4:AD:118:ARG:O | 4:AD:119:GLN:C | 2.58 | 0.42 |
| 5:AE:147:ASP:CA | 5:AE:150:ARG:NH1 | 2.82 | 0.42 |
| 6:AF:8:ILE:CD1 | 6:AF:26:ILE:HD13 | 2.48 | 0.42 |
| 9:AI:4:TYR:HD2 | 9:AI:85:LEU:HA | 1.85 | 0.42 |
| 10:AJ:20:ALA:O | 10:AJ:22:LYS:N | 2.51 | 0.42 |
| 13:AM:65:LYS:O | 13:AM:65:LYS:HG3 | 2.20 | 0.42 |
| 14:AN:15:LYS:HD3 | 14:AN:16:PHE:CE2 | 2.55 | 0.42 |
| 17:AQ:53:LEU:HD23 | 17:AQ:53:LEU:C | 2.40 | 0.42 |
| 22:AV:12:U:H5'' | 36:BA:1908:C:O2' | 2.20 | 0.42 |
| 25:AZ:106:VAL:HG12 | 25:AZ:107:SER:N | 2.34 | 0.42 |
| 25:AZ:248:LYS:HB2 | 25:AZ:248:LYS:HZ2 | 1.85 | 0.42 |
| 25:AZ:302:GLN:HB3 | 25:AZ:302:GLN:HE21 | 1.69 | 0.42 |
| 25:AZ:342:PHE:O | 25:AZ:348:ASP:HA | 2.19 | 0.42 |
| 25:AZ:351:GLY:HA3 | 25:AZ:374:LEU:HD23 | 2.01 | 0.42 |
| 26:B0:27:GLU:OE1 | 36:BA:856:C:H1' | 2.19 | 0.42 |
| 27:B1:23:LYS:CD | 27:B1:28:GLY:HA3 | 2.49 | 0.42 |
| 28:B2:61:LEU:O | 28:B2:62:THR:C | 2.57 | 0.42 |
| 36:BA:1042:G:N2 | 36:BA:1043:C:H1' | 2.35 | 0.42 |
| 36:BA:323:G:O2' | 36:BA:1205:U:N3 | 2.51 | 0.42 |
| 36:BA:1386:C:O2' | 36:BA:1387:C:H5' | 2.20 | 0.42 |
| 36:BA:1495:A:C2 | 36:BA:1496:A:C2 | 3.08 | 0.42 |
| 36:BA:1553:A:H2' | 36:BA:1554:A:H5'' | 2.02 | 0.42 |
| 36:BA:1787:A:O4' | 36:BA:2589:A:H4' | 2.20 | 0.42 |
| 36:BA:2092:U:C5 | 36:BA:2226:C:OP2 | 2.73 | 0.42 |
| 36:BA:2443:C:O2' | 36:BA:2444:G:H5' | 2.20 | 0.42 |
| 36:BA:2453:A:O2' | 36:BA:2454:G:H5' | 2.20 | 0.42 |
| 36:BA:2484:G:O2' | 36:BA:2485:G:H5' | 2.20 | 0.42 |
| 36:BA:2568:C:H6 | 36:BA:2568:C:O5' | 2.03 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:BA:2657:A:N3 | 36:BA:2657:A:H5' | 2.35 | 0.42 |
| 36:BA:2712:U:HO2' | 36:BA:2712(A):A:H3' | 1.84 | 0.42 |
| 36:BA:2822:G:OP1 | 40:BE:159:HIS:NE2 | 2.52 | 0.42 |
| 36:BA:486:C:H2' | 36:BA:487:C:C6 | 2.50 | 0.42 |
| 33:B7:12:ARG:HG3 | 36:BA:686:G:O6 | 2.19 | 0.42 |
| 36:BA:890:A:H2' | 36:BA:892:G:O4' | 2.20 | 0.42 |
| 36:BA:972:G:OP2 | 36:BA:974:G:H5'' | 2.20 | 0.42 |
| 37:BB:68:C:O2' | 37:BB:69:G:H5' | 2.19 | 0.42 |
| 38:BC:70:LYS:CE | 38:BC:177:LYS:HZ3 | 2.32 | 0.42 |
| 39:BD:79:VAL:N | 39:BD:115:GLN:O | 2.52 | 0.42 |
| 40:BE:201:THR:OG1 | 40:BE:202:LYS:N | 2.52 | 0.42 |
| 42:BG:40:ASN:OD1 | 42:BG:156:ASP:HB2 | 2.19 | 0.42 |
| 42:BG:167:GLU:O | 42:BG:170:ARG:HB3 | 2.19 | 0.42 |
| 43:BH:76:VAL:HG12 | 43:BH:77:LYS:N | 2.34 | 0.42 |
| 44:BJ:48:UNK:O | 44:BJ:49:UNK:CB | 2.66 | 0.42 |
| 46:BN:137:LYS:HB3 | 46:BN:138:LEU:H | 1.56 | 0.42 |
| 46:BN:65:LYS:HD3 | 46:BN:69:GLN:HE21 | 1.84 | 0.42 |
| 48:BP:112:LEU:HD22 | 48:BP:112:LEU:C | 2.40 | 0.42 |
| 48:BP:121:LYS:HA | 48:BP:122:PRO:HD3 | 1.91 | 0.42 |
| 36:BA:662:G:P | 48:BP:18:ARG:HD2 | 2.60 | 0.42 |
| 48:BP:39:LYS:CD | 48:BP:40:SER:N | 2.83 | 0.42 |
| 49:BQ:108:GLY:HA3 | 58:BZ:116:VAL:HG11 | 2.01 | 0.42 |
| 52:BT:35:LYS:HZ1 | 52:BT:41:ARG:HD2 | 1.84 | 0.42 |
| 52:BT:62:THR:HA | 52:BT:74:ARG:O | 2.20 | 0.42 |
| 58:BZ:18:LEU:CD2 | 58:BZ:18:LEU:H | 2.33 | 0.42 |
| 1:AA:1222:G:C2' | 1:AA:1223:C:H5' | 2.49 | 0.42 |
| 1:AA:1269:A:H2 | 1:AA:1325:C:O2 | 2.01 | 0.42 |
| 1:AA:1443:G:C6 | 1:AA:1460:A:C2 | 3.07 | 0.42 |
| 1:AA:192:U:O2' | 20:AT:57:ARG:HG3 | 2.20 | 0.42 |
| 1:AA:501:C:H1' | 1:AA:549:C:H1' | 2.02 | 0.42 |
| 1:AA:743:U:O2' | 1:AA:744:C:H5' | 2.20 | 0.42 |
| 1:AA:81:U:C2 | 1:AA:83:U:H5 | 2.38 | 0.42 |
| 1:AA:986:A:H2' | 1:AA:987:G:O4' | 2.19 | 0.42 |
| 2:AB:20:GLU:HG3 | 2:AB:190:THR:O | 2.18 | 0.42 |
| 2:AB:67:THR:HG22 | 2:AB:90:MET:HE3 | 2.02 | 0.42 |
| 3:AC:53:ALA:O | 3:AC:69:HIS:HB2 | 2.20 | 0.42 |
| 4:AD:50:ARG:HA | 4:AD:51:PRO:HD3 | 1.87 | 0.42 |
| 5:AE:41:VAL:CG1 | 5:AE:113:ALA:HB2 | 2.49 | 0.42 |
| 5:AE:69:VAL:HA | 5:AE:70:PRO:HD2 | 1.92 | 0.42 |
| 7:AG:113:GLU:HB2 | 7:AG:119:ARG:CG | 2.47 | 0.42 |
| 10:AJ:24:VAL:CG2 | 10:AJ:37:PRO:HG3 | 2.42 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:55:LYS:HE3 | 10:AJ:55:LYS:CA | 2.49 | 0.42 |
| 15:AO:36:ILE:HG23 | 15:AO:56:LEU:HD11 | 2.02 | 0.42 |
| 16:AP:45:THR:C | 16:AP:47:ASP:N | 2.68 | 0.42 |
| 1:AA:264:U:H4' | 17:AQ:63:ARG:HD3 | 2.01 | 0.42 |
| 6:AF:89:MET:SD | 18:AR:76:LEU:HD21 | 2.60 | 0.42 |
| 20:AT:74:LYS:HD3 | 20:AT:74:LYS:N | 2.35 | 0.42 |
| 21:AU:24:ARG:HG2 | 21:AU:24:ARG:O | 2.20 | 0.42 |
| 25:AZ:383:GLY:H | 25:AZ:400:VAL:HB | 1.85 | 0.42 |
| 26:B0:55:ARG:HE | 26:B0:55:ARG:HB3 | 1.49 | 0.42 |
| 27:B1:86:SER:HB2 | 27:B1:89:GLU:HB2 | 2.01 | 0.42 |
| 29:B3:45:GLY:O | 29:B3:48:GLU:N | 2.52 | 0.42 |
| 34:B8:6:THR:HG22 | 34:B8:63:PRO:HD3 | 2.01 | 0.42 |
| 36:BA:996:A:N6 | 36:BA:1159:U:H3 | 2.17 | 0.42 |
| 36:BA:1266:G:O6 | 55:BW:13:SER:OG | 2.23 | 0.42 |
| 36:BA:1336:A:H2' | 36:BA:1337:G:C8 | 2.53 | 0.42 |
| 36:BA:144:C:H2' | 36:BA:145:G:C8 | 2.54 | 0.42 |
| 36:BA:1718:G:C8 | 36:BA:1718:G:H5' | 2.51 | 0.42 |
| 36:BA:2192:G:H2' | 36:BA:2193:G:H5' | 2.02 | 0.42 |
| 36:BA:21:A:C2 | 36:BA:22:C:C2 | 3.08 | 0.42 |
| 36:BA:2346:A:H5' | 36:BA:2383:G:O4' | 2.20 | 0.42 |
| 36:BA:2375:G:N3 | 36:BA:2379:G:N1 | 2.67 | 0.42 |
| 36:BA:2642:G:O2' | 36:BA:2643:G:H5' | 2.20 | 0.42 |
| 36:BA:2739:U:O2 | 36:BA:2766:G:N2 | 2.52 | 0.42 |
| 36:BA:355:G:H2' | 36:BA:356:G:C8 | 2.54 | 0.42 |
| 38:BC:100:ILE:O | 38:BC:100:ILE:HG22 | 2.19 | 0.42 |
| 38:BC:11:LEU:HD23 | 38:BC:220:PRO:CB | 2.49 | 0.42 |
| 38:BC:123:VAL:CG1 | 38:BC:124:GLY:N | 2.82 | 0.42 |
| 38:BC:148:ASN:HD22 | 38:BC:151:GLU:CD | 2.23 | 0.42 |
| 39:BD:35:LYS:HG2 | 39:BD:62:TYR:O | 2.20 | 0.42 |
| 39:BD:35:LYS:HB2 | 39:BD:63:ARG:CG | 2.50 | 0.42 |
| 40:BE:167:VAL:O | 40:BE:170:LEU:HD11 | 2.20 | 0.42 |
| 43:BH:101:ARG:HG2 | 43:BH:117:PRO:HG3 | 2.02 | 0.42 |
| 46:BN:18:ALA:HB2 | 46:BN:26:LEU:HD13 | 2.02 | 0.42 |
| 47:BO:22:ILE:HA | 47:BO:22:ILE:HD13 | 1.81 | 0.42 |
| 49:BQ:97:VAL:HG11 | 49:BQ:103:MET:HE2 | 2.02 | 0.42 |
| 50:BR:29:LEU:HD23 | 50:BR:70:LEU:HD11 | 2.01 | 0.42 |
| 51:BS:106:ARG:HD2 | 51:BS:106:ARG:C | 2.40 | 0.42 |
| 46:BN:2:LYS:HZ2 | 54:BV:12:TYR:HB3 | 1.84 | 0.42 |
| 55:BW:47:VAL:HA | 55:BW:50:VAL:HG12 | 2.02 | 0.42 |
| 56:BX:13:LEU:O | 56:BX:14:SER:HB3 | 2.19 | 0.42 |
| 56:BX:50:LYS:HG3 | 56:BX:51:VAL:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:BY:43:ASN:HB3 | 57:BY:64:GLU:CA | 2.30 | 0.42 |
| 1:AA:119:A:C4' | 1:AA:120:A:O5' | 2.66 | 0.42 |
| 1:AA:124:G:C6 | 1:AA:125:U:C4 | 3.08 | 0.42 |
| 1:AA:1530:G:H2' | 1:AA:1531:A:C8 | 2.55 | 0.42 |
| 1:AA:176:C:C4 | 1:AA:177:C:N4 | 2.88 | 0.42 |
| 1:AA:32:A:H2' | 1:AA:33:A:C8 | 2.55 | 0.42 |
| 1:AA:374:A:C6 | 1:AA:375:U:C4 | 3.07 | 0.42 |
| 2:AB:185:ILE:HG23 | 2:AB:199:TYR:HB2 | 2.01 | 0.42 |
| 4:AD:4:TYR:C | 4:AD:4:TYR:CD1 | 2.92 | 0.42 |
| 4:AD:65:ARG:NH1 | 4:AD:70:ILE:O | 2.52 | 0.42 |
| 4:AD:91:SER:O | 4:AD:93:PHE:N | 2.53 | 0.42 |
| 6:AF:25:ILE:O | 6:AF:25:ILE:CD1 | 2.66 | 0.42 |
| 6:AF:48:LEU:HD13 | 6:AF:52:ILE:HG13 | 2.01 | 0.42 |
| 7:AG:92:SER:HB3 | 7:AG:95:ARG:HB3 | 2.01 | 0.42 |
| 8:AH:114:THR:OG1 | 8:AH:117:GLY:O | 2.35 | 0.42 |
| 7:AG:37:ASN:HD21 | 9:AI:41:VAL:H | 1.67 | 0.42 |
| 9:AI:4:TYR:HA | 9:AI:88:TYR:CE1 | 2.55 | 0.42 |
| 13:AM:39:ILE:HD11 | 13:AM:56:LEU:HB2 | 2.02 | 0.42 |
| 13:AM:82:MET:CB | 13:AM:93:ARG:NH1 | 2.82 | 0.42 |
| 15:AO:23:GLY:O | 15:AO:24:SER:CB | 2.68 | 0.42 |
| 1:AA:189(F):U:O2 | 17:AQ:63:ARG:NH2 | 2.53 | 0.42 |
| 19:AS:62:ILE:HA | 19:AS:66:MET:CE | 2.50 | 0.42 |
| 20:AT:89:ARG:CB | 20:AT:104:LEU:HD11 | 2.39 | 0.42 |
| 20:AT:48:LYS:HD2 | 20:AT:51:GLU:OE2 | 2.20 | 0.42 |
| 20:AT:82:SER:O | 20:AT:86:ARG:HD3 | 2.20 | 0.42 |
| 21:AU:3:LYS:HB3 | 21:AU:14:TRP:CD1 | 2.55 | 0.42 |
| 25:AZ:22:HIS:CD2 | 25:AZ:107:SER:HB3 | 2.55 | 0.42 |
| 25:AZ:67:HIS:ND1 | 25:AZ:80:VAL:HG22 | 2.35 | 0.42 |
| 26:B0:12:ASN:N | 26:B0:12:ASN:OD1 | 2.53 | 0.42 |
| 26:B0:47:PRO:HB3 | 26:B0:51:VAL:O | 2.20 | 0.42 |
| 27:B1:89:GLU:O | 27:B1:92:LYS:HD2 | 2.19 | 0.42 |
| 28:B2:37:PHE:C | 28:B2:39:ALA:H | 2.22 | 0.42 |
| 29:B3:26:LEU:HB2 | 29:B3:28:LEU:CD2 | 2.46 | 0.42 |
| 34:B8:32:LEU:HD13 | 36:BA:2391:G:OP1 | 2.20 | 0.42 |
| 34:B8:46:ARG:NH1 | 34:B8:46:ARG:HG2 | 2.34 | 0.42 |
| 36:BA:1022:G:C5 | 36:BA:1140:C:C4 | 3.08 | 0.42 |
| 36:BA:1264:G:O5' | 36:BA:1264:G:H8 | 2.02 | 0.42 |
| 36:BA:1278:A:O2' | 36:BA:1279:G:H5' | 2.20 | 0.42 |
| 36:BA:570:G:C5 | 36:BA:2030:A:C2 | 3.08 | 0.42 |
| 36:BA:2137:C:N4 | 36:BA:2154:G:H22 | 2.15 | 0.42 |
| 36:BA:2455:G:C2 | 36:BA:2498:C:N4 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BA:2562:U:H2' | 36:BA:2563:U:H5' | 2.00 | 0.42 |
| 36:BA:2741:A:H2' | 36:BA:2742:C:O4' | 2.18 | 0.42 |
| 36:BA:2858:C:H5 | 36:BA:2859:G:C5 | 2.38 | 0.42 |
| 36:BA:363:G:H2' | 36:BA:363(A):A:C8 | 2.55 | 0.42 |
| 36:BA:756:C:O2' | 36:BA:757:U:H5' | 2.20 | 0.42 |
| 37:BB:39:A:C2 | 37:BB:44:G:N3 | 2.88 | 0.42 |
| 37:BB:81:G:H5' | 37:BB:81:G:N3 | 2.35 | 0.42 |
| 38:BC:20:TYR:O | 38:BC:225:ASN:N | 2.53 | 0.42 |
| 38:BC:94:VAL:O | 38:BC:95:GLY:C | 2.57 | 0.42 |
| 36:BA:764:A:OP1 | 39:BD:208:LYS:HE3 | 2.20 | 0.42 |
| 36:BA:1800:C:P | 39:BD:266:SER:HG | 2.43 | 0.42 |
| 39:BD:3:VAL:H | 39:BD:20:ASP:HB2 | 1.85 | 0.42 |
| 42:BG:136:ARG:HG2 | 42:BG:136:ARG:HH11 | 1.85 | 0.42 |
| 42:BG:18:GLU:O | 42:BG:22:ARG:N | 2.44 | 0.42 |
| 42:BG:47:LYS:HZ1 | 42:BG:81:LYS:CB | 2.32 | 0.42 |
| 48:BP:136:GLU:O | 48:BP:139:LYS:N | 2.51 | 0.42 |
| 48:BP:21:ARG:O | 48:BP:22:GLY:C | 2.58 | 0.42 |
| 50:BR:21:TYR:HB3 | 50:BR:47:PHE:CD2 | 2.55 | 0.42 |
| 51:BS:28:VAL:CG1 | 51:BS:29:PHE:N | 2.81 | 0.42 |
| 52:BT:125:ARG:HG2 | 52:BT:125:ARG:NH1 | 2.35 | 0.42 |
| 52:BT:66:VAL:HA | 52:BT:71:GLY:HA2 | 2.02 | 0.42 |
| 54:BV:95:LEU:C | 54:BV:95:LEU:CD2 | 2.88 | 0.42 |
| 55:BW:1:MET:HE2 | 55:BW:2:GLU:N | 2.35 | 0.42 |
| 57:BY:46:LYS:H | 57:BY:62:GLU:CG | 2.33 | 0.42 |
| 58:BZ:77:ASP:OD2 | 58:BZ:79:ARG:O | 2.38 | 0.42 |
| 1:AA:1253:G:H1' | 1:AA:1355:G:O2' | 2.19 | 0.42 |
| 1:AA:1277:C:O2' | 1:AA:1279:A:H1' | 2.20 | 0.42 |
| 1:AA:1269:A:H2 | 1:AA:1313:U:C2 | 2.38 | 0.42 |
| 1:AA:192:U:O2' | 1:AA:193:C:H5' | 2.19 | 0.42 |
| 3:AC:23:TYR:C | 3:AC:23:TYR:CD2 | 2.92 | 0.42 |
| 4:AD:9:CYS:HA | 4:AD:12:CYS:HB2 | 2.01 | 0.42 |
| 6:AF:22:GLU:C | 6:AF:24:GLU:N | 2.73 | 0.42 |
| 8:AH:103:VAL:CB | 8:AH:109:ILE:H | 2.33 | 0.42 |
| 8:AH:50:ARG:HA | 8:AH:59:LEU:HD23 | 2.01 | 0.42 |
| 9:AI:18:PHE:HB2 | 9:AI:62:TYR:HB3 | 2.02 | 0.42 |
| 11:AK:63:LEU:N | 11:AK:63:LEU:HD23 | 2.35 | 0.42 |
| 12:AL:55:VAL:HG22 | 12:AL:56:ALA:H | 1.83 | 0.42 |
| 1:AA:523:A:N1 | 12:AL:92:ASP:HB2 | 2.35 | 0.42 |
| 13:AM:12:ASN:N | 13:AM:12:ASN:ND2 | 2.61 | 0.42 |
| 13:AM:29:ARG:O | 13:AM:30:ALA:C | 2.58 | 0.42 |
| 13:AM:66:LEU:O | 13:AM:70:LEU:CB | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 14:AN:23:ARG:O | 14:AN:24:CYS:C | 2.56 | 0.42 |
| 17:AQ:36:ILE:H | 17:AQ:36:ILE:HG12 | 1.68 | 0.42 |
| 22:AV:21:A:H2' | 22:AV:22:G:C5' | 2.42 | 0.42 |
| 35:B9:4:ARG:HG2 | 35:B9:34:GLN:HE21 | 1.85 | 0.42 |
| 36:BA:1680:U:O2 | 36:BA:1763:G:H3' | 2.20 | 0.42 |
| 36:BA:1757:U:H2' | 36:BA:1758:G:OP1 | 2.20 | 0.42 |
| 36:BA:1887:C:C2' | 36:BA:1888:G:H5'' | 2.49 | 0.42 |
| 36:BA:194:G:H2' | 36:BA:195:A:O4' | 2.19 | 0.42 |
| 36:BA:2132:U:O4 | 38:BC:5:LYS:HE3 | 2.19 | 0.42 |
| 36:BA:2246:G:O2' | 36:BA:2247:A:H5' | 2.20 | 0.42 |
| 36:BA:2490:G:H4' | 36:BA:2491:U:OP1 | 2.20 | 0.42 |
| 36:BA:2712:U:O2 | 36:BA:2712:U:H5'' | 2.19 | 0.42 |
| 36:BA:2718:G:C6 | 36:BA:2719:G:C5 | 3.07 | 0.42 |
| 36:BA:2801(A):A:H4' | 36:BA:2802:G:H2' | 2.02 | 0.42 |
| 36:BA:2840:C:O2' | 36:BA:2841:C:H5' | 2.19 | 0.42 |
| 36:BA:309:G:H1' | 36:BA:329:G:O2' | 2.19 | 0.42 |
| 36:BA:392:C:O2' | 36:BA:393:C:H5' | 2.20 | 0.42 |
| 36:BA:454:A:H4' | 36:BA:455:C:OP2 | 2.20 | 0.42 |
| 36:BA:483:A:H1' | 57:BY:60:PHE:HZ | 1.85 | 0.42 |
| 36:BA:577:G:C6 | 36:BA:578:A:C6 | 3.08 | 0.42 |
| 36:BA:654(Q):C:H2' | 36:BA:654(R):C:C6 | 2.55 | 0.42 |
| 36:BA:860:U:O4' | 36:BA:860:U:O2 | 2.38 | 0.42 |
| 37:BB:34:U:H5'' | 37:BB:35:U:OP1 | 2.19 | 0.42 |
| 37:BB:78:A:C2 | 37:BB:100:A:C4 | 3.07 | 0.42 |
| 37:BB:77:U:C2' | 37:BB:78:A:H5' | 2.50 | 0.42 |
| 37:BB:98:G:H2' | 37:BB:99:G:C5' | 2.50 | 0.42 |
| 38:BC:112:ALA:O | 38:BC:113:VAL:HG23 | 2.20 | 0.42 |
| 38:BC:208:PHE:O | 38:BC:209:LEU:HD23 | 2.20 | 0.42 |
| 46:BN:103:VAL:O | 46:BN:106:MET:HB2 | 2.20 | 0.42 |
| 47:BO:104:ARG:NE | 52:BT:33:LYS:HD2 | 2.35 | 0.42 |
| 52:BT:124:ASP:HB3 | 52:BT:125:ARG:NH1 | 2.33 | 0.42 |
| 53:BU:79:PHE:CE1 | 53:BU:83:LEU:CD2 | 3.02 | 0.42 |
| 53:BU:92:ARG:HD2 | 54:BV:11:GLN:CD | 2.39 | 0.42 |
| 55:BW:20:VAL:HG23 | 55:BW:47:VAL:HG21 | 2.01 | 0.42 |
| 55:BW:51:LEU:O | 55:BW:54:ALA:HB3 | 2.19 | 0.42 |
| 1:AA:1103:C:H2' | 1:AA:1104:G:O4' | 2.20 | 0.41 |
| 1:AA:1485:U:O2' | 1:AA:1486:G:H5' | 2.20 | 0.41 |
| 1:AA:358:U:O4' | 25:AZ:233:GLY:HA2 | 2.20 | 0.41 |
| 1:AA:393:A:H2' | 1:AA:394:G:H5' | 2.00 | 0.41 |
| 1:AA:498:U:O2' | 1:AA:499:A:O5' | 2.38 | 0.41 |
| 1:AA:748:C:H1' | 1:AA:749:C:H5 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:858:G:C4' | 1:AA:858:G:C8 | 3.03 | 0.41 |
| 2:AB:209:ARG:HD3 | 2:AB:239:VAL:CG1 | 2.50 | 0.41 |
| 3:AC:76:VAL:CG2 | 3:AC:103:VAL:HG11 | 2.50 | 0.41 |
| 7:AG:7:ALA:O | 7:AG:8:GLU:HB2 | 2.20 | 0.41 |
| 11:AK:13:GLN:HB3 | 11:AK:75:TYR:O | 2.20 | 0.41 |
| 20:AT:50:GLU:C | 20:AT:52:ALA:N | 2.73 | 0.41 |
| 20:AT:82:SER:O | 20:AT:86:ARG:HB3 | 2.19 | 0.41 |
| 22:AV:27:G:O2' | 22:AV:28:G:H5' | 2.20 | 0.41 |
| 25:AZ:289:LEU:HA | 25:AZ:289:LEU:HD12 | 1.85 | 0.41 |
| 25:AZ:324:LYS:HD2 | 25:AZ:326:GLU:HG2 | 2.02 | 0.41 |
| 25:AZ:89:ILE:HD13 | 25:AZ:389:ARG:HH12 | 1.84 | 0.41 |
| 26:B0:23:VAL:C | 26:B0:24:LYS:HD3 | 2.39 | 0.41 |
| 31:B5:7:PRO:HG2 | 36:BA:2016:U:O2 | 2.20 | 0.41 |
| 33:B7:30:VAL:CG1 | 36:BA:466:A:H5'' | 2.50 | 0.41 |
| 33:B7:6:GLN:HA | 33:B7:7:PRO:HD2 | 1.82 | 0.41 |
| 36:BA:1137:G:O2' | 36:BA:2039:C:H5'' | 2.20 | 0.41 |
| 36:BA:1332:G:N2 | 36:BA:1610:A:C8 | 2.88 | 0.41 |
| 36:BA:1967:C:H2' | 36:BA:1968:G:C5' | 2.50 | 0.41 |
| 36:BA:1987:G:C8 | 36:BA:1987:G:H5'' | 2.55 | 0.41 |
| 36:BA:1996:C:H5 | 47:BO:32:TYR:OH | 2.03 | 0.41 |
| 36:BA:2029:G:C4 | 36:BA:2031:A:OP2 | 2.73 | 0.41 |
| 36:BA:2103:C:H2' | 36:BA:2104:G:C5' | 2.50 | 0.41 |
| 36:BA:2312:U:H4' | 42:BG:71:THR:CG2 | 2.50 | 0.41 |
| 36:BA:415:A:C2 | 36:BA:2409:G:N1 | 2.88 | 0.41 |
| 36:BA:2455:G:H2' | 36:BA:2456:C:C6 | 2.55 | 0.41 |
| 36:BA:2696:U:H2' | 36:BA:2697:G:C8 | 2.55 | 0.41 |
| 36:BA:306:U:H2' | 36:BA:307:G:O4' | 2.21 | 0.41 |
| 36:BA:85:G:H5'' | 36:BA:85:G:H8 | 1.84 | 0.41 |
| 36:BA:968:G:H2' | 36:BA:969:U:H6 | 1.84 | 0.41 |
| 38:BC:162:GLU:O | 38:BC:173:ALA:HB2 | 2.20 | 0.41 |
| 38:BC:184:LYS:H | 38:BC:184:LYS:HE2 | 1.81 | 0.41 |
| 40:BE:6:GLY:HA2 | 40:BE:51:PHE:CE2 | 2.53 | 0.41 |
| 41:BF:154:VAL:HG12 | 41:BF:155:LEU:N | 2.34 | 0.41 |
| 41:BF:179:GLU:HB3 | 41:BF:205:ARG:NH2 | 2.34 | 0.41 |
| 41:BF:2:LYS:HG3 | 41:BF:25:PRO:HB2 | 2.02 | 0.41 |
| 47:BO:29:ASN:O | 47:BO:30:ALA:C | 2.55 | 0.41 |
| 48:BP:85:LEU:CD2 | 48:BP:116:GLY:HA3 | 2.50 | 0.41 |
| 50:BR:28:LEU:HD12 | 50:BR:114:VAL:CG2 | 2.47 | 0.41 |
| 51:BS:96:GLY:C | 51:BS:98:VAL:N | 2.72 | 0.41 |
| 52:BT:108:ARG:HA | 52:BT:111:ARG:NH1 | 2.35 | 0.41 |
| 52:BT:32:TYR:CG | 52:BT:81:PRO:CB | 3.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 56:BX:52:VAL:HG23 | 56:BX:84:ALA:HA | 2.02 | 0.41 |
| 57:BY:13:VAL:HG11 | 57:BY:28:LYS:HD3 | 2.01 | 0.41 |
| 57:BY:27:VAL:C | 57:BY:28:LYS:HG3 | 2.40 | 0.41 |
| 58:BZ:28:MET:SD | 58:BZ:33:LEU:HG | 2.60 | 0.41 |
| 37:BB:75:G:N3 | 58:BZ:85:HIS:HE1 | 2.18 | 0.41 |
| 1:AA:1111:A:O2' | 1:AA:1112:C:H5' | 2.20 | 0.41 |
| 1:AA:389:A:C6 | 1:AA:390:C:H1' | 2.54 | 0.41 |
| 1:AA:553:A:H2' | 1:AA:554:C:C6 | 2.55 | 0.41 |
| 1:AA:955:U:H5' | 13:AM:120:LYS:NZ | 2.35 | 0.41 |
| 2:AB:103:THR:HA | 2:AB:180:LEU:HD11 | 2.02 | 0.41 |
| 2:AB:91:PRO:HG2 | 2:AB:155:LEU:HD23 | 2.01 | 0.41 |
| 2:AB:83:MET:C | 2:AB:85:ALA:H | 2.23 | 0.41 |
| 8:AH:81:HIS:N | 8:AH:138:TRP:O | 2.52 | 0.41 |
| 9:AI:11:LYS:C | 9:AI:13:ALA:H | 2.24 | 0.41 |
| 9:AI:97:LYS:O | 9:AI:98:PRO:C | 2.59 | 0.41 |
| 13:AM:70:LEU:HD23 | 13:AM:70:LEU:C | 2.39 | 0.41 |
| 17:AQ:59:ILE:HG22 | 17:AQ:60:ILE:N | 2.35 | 0.41 |
| 17:AQ:6:LEU:HB3 | 17:AQ:23:VAL:HG11 | 2.02 | 0.41 |
| 20:AT:80:ARG:NH1 | 20:AT:80:ARG:HG2 | 2.36 | 0.41 |
| 22:AW:56:C:C2 | 22:AW:57:G:N7 | 2.88 | 0.41 |
| 25:AZ:352:VAL:HG12 | 25:AZ:353:VAL:H | 1.84 | 0.41 |
| 27:B1:4:VAL:CG2 | 27:B1:11:ARG:HG2 | 2.49 | 0.41 |
| 32:B6:22:ALA:HB2 | 32:B6:39:TYR:CZ | 2.55 | 0.41 |
| 32:B6:42:TRP:CD2 | 36:BA:2348:U:O2' | 2.74 | 0.41 |
| 36:BA:1028:A:N6 | 36:BA:1125:G:H2' | 2.35 | 0.41 |
| 36:BA:1493:C:C2' | 36:BA:1493:C:O2 | 2.68 | 0.41 |
| 36:BA:1518:U:H2' | 36:BA:1519:G:O4' | 2.19 | 0.41 |
| 36:BA:1539:G:C2' | 36:BA:1540:U:H5' | 2.50 | 0.41 |
| 36:BA:1987:G:H8 | 36:BA:1987:G:H5" | 1.85 | 0.41 |
| 36:BA:2010:G:H5" | 55:BW:42:ARG:HB2 | 2.02 | 0.41 |
| 36:BA:201:C:C2' | 36:BA:202:U:H5' | 2.50 | 0.41 |
| 36:BA:2284:C:C2 | 36:BA:2285:C:C5 | 3.08 | 0.41 |
| 36:BA:2533:A:H2' | 36:BA:2534:A:O4' | 2.20 | 0.41 |
| 36:BA:2580:U:H4' | 40:BE:130:GLY:CA | 2.50 | 0.41 |
| 27:B1:18:ILE:HD12 | 36:BA:380:U:H5' | 2.02 | 0.41 |
| 36:BA:520:G:H2' | 36:BA:521:G:C8 | 2.55 | 0.41 |
| 36:BA:676:A:N1 | 36:BA:802:A:N1 | 2.69 | 0.41 |
| 36:BA:807:U:H1' | 36:BA:2445:G:OP1 | 2.20 | 0.41 |
| 29:B3:13:ILE:HD11 | 36:BA:989:G:C8 | 2.55 | 0.41 |
| 38:BC:7:TYR:CZ | 38:BC:11:LEU:HD21 | 2.54 | 0.41 |
| 40:BE:55:ASN:O | 40:BE:56:PRO:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BF:148:LEU:HB3 | 41:BF:172:TRP:CZ3 | 2.53 | 0.41 |
| 42:BG:56:ALA:CA | 42:BG:153:ARG:HH21 | 2.27 | 0.41 |
| 43:BH:106:THR:HG22 | 43:BH:112:PRO:CA | 2.45 | 0.41 |
| 46:BN:18:ALA:HB3 | 46:BN:26:LEU:CD2 | 2.49 | 0.41 |
| 46:BN:26:LEU:HG | 46:BN:30:ILE:CD1 | 2.49 | 0.41 |
| 47:BO:104:ARG:NH1 | 52:BT:35:LYS:HD3 | 2.35 | 0.41 |
| 48:BP:114:ILE:CG2 | 48:BP:130:PHE:HD1 | 2.30 | 0.41 |
| 48:BP:83:VAL:HG12 | 48:BP:112:LEU:CD2 | 2.42 | 0.41 |
| 50:BR:104:ARG:HD3 | 50:BR:107:ASP:OD2 | 2.21 | 0.41 |
| 52:BT:28:VAL:O | 52:BT:29:ARG:HB2 | 2.19 | 0.41 |
| 36:BA:484:C:P | 57:BY:49:VAL:HG13 | 2.59 | 0.41 |
| 36:BA:483:A:O3' | 57:BY:49:VAL:HG22 | 2.20 | 0.41 |
| 58:BZ:7:ALA:O | 58:BZ:61:LEU:HA | 2.19 | 0.41 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:O4' | 2.20 | 0.41 |
| 1:AA:1163:C:H2' | 1:AA:1164:G:H8 | 1.84 | 0.41 |
| 1:AA:1288:A:H1' | 1:AA:1352:C:O2' | 2.20 | 0.41 |
| 1:AA:174:C:H2' | 1:AA:175:C:C6 | 2.55 | 0.41 |
| 1:AA:321:A:O2' | 1:AA:322:C:H5' | 2.19 | 0.41 |
| 1:AA:375:U:C4 | 1:AA:376:G:N7 | 2.88 | 0.41 |
| 1:AA:407:G:H2' | 1:AA:408:A:H8 | 1.86 | 0.41 |
| 1:AA:452:A:H1' | 1:AA:453:A:H5'' | 2.03 | 0.41 |
| 1:AA:633:G:H3' | 1:AA:634:C:C6 | 2.54 | 0.41 |
| 1:AA:803:G:H2' | 1:AA:804:U:O4' | 2.20 | 0.41 |
| 1:AA:825:G:O2' | 1:AA:826:C:H5' | 2.20 | 0.41 |
| 1:AA:877:C:H5'' | 8:AH:88:LYS:HD3 | 2.03 | 0.41 |
| 1:AA:973:G:H3' | 1:AA:974:A:H5'' | 2.02 | 0.41 |
| 2:AB:82:ARG:O | 2:AB:86:GLU:HG3 | 2.20 | 0.41 |
| 3:AC:154:SER:HB2 | 3:AC:165:THR:HB | 2.02 | 0.41 |
| 4:AD:67:ILE:O | 4:AD:67:ILE:HG22 | 2.21 | 0.41 |
| 4:AD:74:GLN:O | 4:AD:78:LEU:HB2 | 2.20 | 0.41 |
| 5:AE:41:VAL:HG11 | 5:AE:113:ALA:HB2 | 2.03 | 0.41 |
| 5:AE:5:ASP:OD1 | 5:AE:5:ASP:O | 2.36 | 0.41 |
| 7:AG:18:TYR:C | 7:AG:20:ASP:N | 2.73 | 0.41 |
| 7:AG:63:LYS:O | 7:AG:63:LYS:HD2 | 2.21 | 0.41 |
| 8:AH:104:ARG:O | 8:AH:105:ARG:C | 2.59 | 0.41 |
| 19:AS:62:ILE:HA | 19:AS:66:MET:HE1 | 2.01 | 0.41 |
| 25:AZ:138:VAL:C | 25:AZ:140:MET:N | 2.68 | 0.41 |
| 25:AZ:13:ASN:ND2 | 25:AZ:241:ARG:CG | 2.82 | 0.41 |
| 26:B0:12:ASN:C | 26:B0:14:ARG:H | 2.24 | 0.41 |
| 26:B0:24:LYS:O | 26:B0:25:ARG:CG | 2.68 | 0.41 |
| 26:B0:50:ASN:ND2 | 26:B0:63:VAL:HG21 | 2.32 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:B1:30:VAL:O | 36:BA:2395:C:O2' | 2.37 | 0.41 |
| 32:B6:15:GLU:OE2 | 32:B6:41:PRO:HB2 | 2.15 | 0.41 |
| 36:BA:1168:G:O2' | 36:BA:1169:G:H5' | 2.20 | 0.41 |
| 36:BA:1259:G:H2' | 36:BA:1260:G:C8 | 2.55 | 0.41 |
| 36:BA:1411:C:H2' | 36:BA:1412:A:H8 | 1.85 | 0.41 |
| 36:BA:1670:C:OP2 | 36:BA:1671:U:O4 | 2.38 | 0.41 |
| 36:BA:2038:G:H2' | 36:BA:2039:C:C6 | 2.55 | 0.41 |
| 36:BA:2146:C:H4' | 36:BA:2147:G:C5 | 2.54 | 0.41 |
| 36:BA:2294:C:H2' | 36:BA:2294:C:O2 | 2.20 | 0.41 |
| 36:BA:2405:G:HO2' | 36:BA:2406:U:P | 2.43 | 0.41 |
| 36:BA:1296:G:OP1 | 36:BA:2709:G:H4' | 2.21 | 0.41 |
| 36:BA:2809:A:H62 | 36:BA:2891:G:H2' | 1.85 | 0.41 |
| 36:BA:493:G:H2' | 36:BA:494:G:O4' | 2.19 | 0.41 |
| 36:BA:528:A:C8 | 36:BA:528:A:H3' | 2.54 | 0.41 |
| 36:BA:848:G:O6 | 36:BA:928:G:H2' | 2.20 | 0.41 |
| 37:BB:15:A:H1' | 37:BB:110:G:C4 | 2.55 | 0.41 |
| 38:BC:38:ASP:OD2 | 38:BC:177:LYS:HB3 | 2.20 | 0.41 |
| 39:BD:165:ILE:HG23 | 39:BD:173:VAL:CG2 | 2.50 | 0.41 |
| 40:BE:199:ARG:HG2 | 40:BE:200:GLU:N | 2.27 | 0.41 |
| 40:BE:76:ARG:O | 40:BE:77:ILE:C | 2.58 | 0.41 |
| 42:BG:7:LEU:HD22 | 42:BG:176:LEU:HD23 | 2.02 | 0.41 |
| 43:BH:44:VAL:CG1 | 43:BH:45:VAL:N | 2.82 | 0.41 |
| 43:BH:83:TYR:O | 43:BH:84:SER:C | 2.58 | 0.41 |
| 46:BN:7:LYS:O | 46:BN:8:GLN:O | 2.38 | 0.41 |
| 47:BO:6:THR:HG22 | 47:BO:7:TYR:N | 2.35 | 0.41 |
| 48:BP:96:THR:HG22 | 48:BP:126:VAL:HB | 2.02 | 0.41 |
| 48:BP:95:VAL:HG23 | 48:BP:125:VAL:HA | 2.02 | 0.41 |
| 48:BP:97:PRO:C | 48:BP:99:LEU:H | 2.23 | 0.41 |
| 49:BQ:20:ALA:O | 49:BQ:21:THR:OG1 | 2.33 | 0.41 |
| 50:BR:67:LEU:CD1 | 50:BR:71:GLN:O | 2.67 | 0.41 |
| 51:BS:22:GLY:O | 51:BS:23:ARG:O | 2.38 | 0.41 |
| 51:BS:28:VAL:CG1 | 51:BS:29:PHE:H | 2.31 | 0.41 |
| 51:BS:68:GLN:C | 51:BS:70:GLY:N | 2.74 | 0.41 |
| 53:BU:110:VAL:O | 53:BU:113:ALA:HB3 | 2.20 | 0.41 |
| 53:BU:115:ALA:C | 53:BU:117:GLN:H | 2.22 | 0.41 |
| 54:BV:7:THR:HG23 | 54:BV:7:THR:O | 2.21 | 0.41 |
| 57:BY:12:THR:CG2 | 57:BY:13:VAL:N | 2.83 | 0.41 |
| 49:BQ:63:LYS:HZ3 | 58:BZ:175:VAL:HG11 | 1.86 | 0.41 |
| 58:BZ:18:LEU:H | 58:BZ:18:LEU:HD22 | 1.86 | 0.41 |
| 1:AA:1054:C:OP2 | 1:AA:1197:G:OP2 | 2.37 | 0.41 |
| 1:AA:1129:C:OP1 | 1:AA:1130:A:H5" | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:341:C:O2' | 1:AA:342:C:H5' | 2.21 | 0.41 |
| 1:AA:663:A:H5' | 1:AA:836:G:OP1 | 2.20 | 0.41 |
| 1:AA:707:C:H4' | 11:AK:20:TYR:CD1 | 2.55 | 0.41 |
| 1:AA:771:G:H2' | 1:AA:772:U:C6 | 2.56 | 0.41 |
| 6:AF:19:LEU:C | 6:AF:19:LEU:HD23 | 2.40 | 0.41 |
| 7:AG:26:PHE:HB2 | 7:AG:62:PHE:HZ | 1.86 | 0.41 |
| 7:AG:71:PRO:O | 7:AG:91:VAL:CG1 | 2.67 | 0.41 |
| 8:AH:49:GLU:HG2 | 8:AH:62:TYR:HE2 | 1.85 | 0.41 |
| 9:AI:118:LYS:HB3 | 9:AI:118:LYS:HE2 | 1.67 | 0.41 |
| 10:AJ:48:THR:HG23 | 10:AJ:62:HIS:ND1 | 2.35 | 0.41 |
| 11:AK:46:GLY:O | 11:AK:48:ILE:O | 2.38 | 0.41 |
| 12:AL:71:PRO:HG3 | 12:AL:99:HIS:HD2 | 1.85 | 0.41 |
| 13:AM:13:LYS:O | 13:AM:14:ARG:C | 2.59 | 0.41 |
| 24:AY:10:G:C2 | 24:AY:26:A:H1' | 2.55 | 0.41 |
| 25:AZ:133:VAL:CG1 | 25:AZ:134:PHE:N | 2.83 | 0.41 |
| 25:AZ:14:VAL:HA | 25:AZ:101:GLY:O | 2.20 | 0.41 |
| 25:AZ:221:PHE:CA | 25:AZ:244:ARG:HG3 | 2.49 | 0.41 |
| 26:B0:11:ARG:C | 26:B0:14:ARG:HH22 | 2.22 | 0.41 |
| 27:B1:19:GLN:OE1 | 27:B1:19:GLN:HA | 2.20 | 0.41 |
| 28:B2:25:VAL:O | 28:B2:27:GLU:N | 2.54 | 0.41 |
| 28:B2:63:VAL:C | 28:B2:65:ASN:N | 2.72 | 0.41 |
| 33:B7:40:TRP:CD2 | 36:BA:459:U:H5'' | 2.56 | 0.41 |
| 36:BA:1113:U:H2' | 36:BA:1114:G:C8 | 2.55 | 0.41 |
| 36:BA:1112:G:O2' | 36:BA:1113:U:H5' | 2.21 | 0.41 |
| 36:BA:1131:G:H21 | 46:BN:73:THR:CG2 | 2.29 | 0.41 |
| 36:BA:1144:G:O2' | 36:BA:1145:C:H5' | 2.21 | 0.41 |
| 36:BA:1331:A:O2' | 36:BA:1332:G:H8 | 2.02 | 0.41 |
| 36:BA:149:A:H2' | 36:BA:150:C:O4' | 2.19 | 0.41 |
| 36:BA:1666:G:O2' | 36:BA:1667:G:H5' | 2.19 | 0.41 |
| 36:BA:570:G:C6 | 36:BA:2030:A:C2 | 3.08 | 0.41 |
| 36:BA:1129:A:H4' | 36:BA:2515:C:O2' | 2.21 | 0.41 |
| 36:BA:744:G:H2' | 36:BA:745:G:C5' | 2.50 | 0.41 |
| 36:BA:848:G:C2 | 36:BA:933:A:H1' | 2.55 | 0.41 |
| 38:BC:106:GLY:O | 38:BC:107:TRP:HB2 | 2.19 | 0.41 |
| 38:BC:192:PHE:C | 38:BC:194:ARG:N | 2.73 | 0.41 |
| 38:BC:200:LYS:HE3 | 38:BC:208:PHE:HB2 | 2.01 | 0.41 |
| 38:BC:34:THR:O | 38:BC:35:ALA:HB2 | 2.20 | 0.41 |
| 38:BC:64:LEU:HA | 38:BC:65:PRO:HD3 | 1.92 | 0.41 |
| 39:BD:75:ILE:N | 39:BD:75:ILE:CD1 | 2.80 | 0.41 |
| 40:BE:115:GLY:HA2 | 40:BE:157:ALA:CB | 2.49 | 0.41 |
| 41:BF:123:LEU:HD12 | 41:BF:124:LEU:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BF:164:ARG:HD3 | 41:BF:175:THR:OG1 | 2.20 | 0.41 |
| 41:BF:34:TRP:CZ3 | 48:BP:12:ALA:HA | 2.55 | 0.41 |
| 43:BH:38:SER:C | 43:BH:40:GLU:H | 2.23 | 0.41 |
| 48:BP:121:LYS:HB2 | 48:BP:123:LEU:HD22 | 2.00 | 0.41 |
| 48:BP:23:PRO:HB2 | 48:BP:33:ARG:CG | 2.37 | 0.41 |
| 54:BV:16:PRO:O | 54:BV:96:ILE:O | 2.38 | 0.41 |
| 54:BV:57:VAL:HG22 | 54:BV:58:VAL:N | 2.35 | 0.41 |
| 57:BY:4:LYS:HG3 | 57:BY:5:MET:N | 2.34 | 0.41 |
| 58:BZ:102:LEU:HD21 | 58:BZ:124:ILE:HG12 | 2.01 | 0.41 |
| 1:AA:1318:A:C1' | 19:AS:37:ARG:HH21 | 2.34 | 0.41 |
| 1:AA:142:G:N3 | 1:AA:196:A:H2 | 2.19 | 0.41 |
| 1:AA:445:G:H2' | 1:AA:446:G:H8 | 1.86 | 0.41 |
| 1:AA:488:C:O2' | 1:AA:489:C:H5' | 2.20 | 0.41 |
| 6:AF:74:ASP:HB3 | 6:AF:77:ARG:NH2 | 2.34 | 0.41 |
| 7:AG:111:ARG:HE | 7:AG:123:GLU:HB2 | 1.84 | 0.41 |
| 8:AH:104:ARG:NH2 | 8:AH:138:TRP:CZ2 | 2.88 | 0.41 |
| 8:AH:116:LYS:HD3 | 8:AH:127:LEU:HD12 | 2.01 | 0.41 |
| 8:AH:18:ARG:HD3 | 8:AH:18:ARG:HA | 1.69 | 0.41 |
| 9:AI:8:GLY:HA2 | 9:AI:79:LEU:HD12 | 2.01 | 0.41 |
| 9:AI:97:LYS:HB3 | 9:AI:98:PRO:HD3 | 2.03 | 0.41 |
| 14:AN:23:ARG:NH1 | 14:AN:30:ALA:HB2 | 2.36 | 0.41 |
| 17:AQ:81:ARG:O | 17:AQ:83:ASP:N | 2.54 | 0.41 |
| 18:AR:24:ALA:C | 18:AR:26:LEU:H | 2.23 | 0.41 |
| 19:AS:35:SER:C | 19:AS:37:ARG:H | 2.23 | 0.41 |
| 20:AT:50:GLU:CB | 20:AT:100:ILE:HD13 | 2.48 | 0.41 |
| 31:B5:54:GLY:O | 31:B5:55:ARG:C | 2.57 | 0.41 |
| 36:BA:1458:C:H4' | 36:BA:1459:G:O4' | 2.21 | 0.41 |
| 36:BA:1771:C:O2' | 36:BA:1786:A:H8 | 1.93 | 0.41 |
| 36:BA:2111:C:O2 | 36:BA:2111:C:H2' | 2.20 | 0.41 |
| 36:BA:2136:C:H2' | 36:BA:2137:C:H6 | 1.86 | 0.41 |
| 36:BA:45:C:OP2 | 36:BA:215:G:H2' | 2.20 | 0.41 |
| 36:BA:2188:C:H2' | 36:BA:2189:U:C6 | 2.56 | 0.41 |
| 36:BA:964:C:O2' | 36:BA:2273:A:N3 | 2.43 | 0.41 |
| 36:BA:2585:U:O2 | 36:BA:2585:U:O4' | 2.38 | 0.41 |
| 36:BA:2726:U:H4' | 47:BO:1:MET:HE3 | 2.03 | 0.41 |
| 36:BA:2761:G:H8 | 36:BA:2761:G:H5' | 1.85 | 0.41 |
| 36:BA:407:G:C2 | 36:BA:408:G:C5 | 3.08 | 0.41 |
| 36:BA:699:A:H2' | 36:BA:700:G:O4' | 2.21 | 0.41 |
| 36:BA:828:U:H2' | 36:BA:829:A:C8 | 2.55 | 0.41 |
| 36:BA:920:G:O2' | 36:BA:921:G:H5' | 2.20 | 0.41 |
| 37:BB:100:A:C4 | 37:BB:101:G:C8 | 3.07 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BB:39:A:C2 | 37:BB:44:G:C2 | 3.08 | 0.41 |
| 37:BB:94:C:H2' | 37:BB:95:C:C6 | 2.56 | 0.41 |
| 38:BC:66:HIS:CE1 | 38:BC:184:LYS:HD3 | 2.55 | 0.41 |
| 38:BC:212:VAL:HG11 | 38:BC:224:ILE:HD11 | 2.02 | 0.41 |
| 39:BD:134:ARG:HG2 | 39:BD:187:GLY:O | 2.21 | 0.41 |
| 40:BE:143:ASN:ND2 | 40:BE:143:ASN:N | 2.69 | 0.41 |
| 41:BF:110:LEU:HD12 | 41:BF:206:ILE:CD1 | 2.51 | 0.41 |
| 41:BF:159:GLY:CA | 41:BF:164:ARG:HH21 | 2.28 | 0.41 |
| 42:BG:107:LEU:HD21 | 42:BG:178:PHE:CD1 | 2.56 | 0.41 |
| 43:BH:66:GLY:O | 43:BH:67:LEU:C | 2.58 | 0.41 |
| 43:BH:92:ILE:C | 43:BH:94:TYR:H | 2.23 | 0.41 |
| 48:BP:110:TYR:CZ | 48:BP:111:ARG:NE | 2.89 | 0.41 |
| 50:BR:69:ASP:O | 50:BR:70:LEU:C | 2.57 | 0.41 |
| 51:BS:30:ARG:HH22 | 51:BS:62:LYS:HG2 | 1.83 | 0.41 |
| 53:BU:97:ASP:O | 53:BU:100:VAL:N | 2.51 | 0.41 |
| 37:BB:92:C:H5'' | 58:BZ:79:ARG:HH12 | 1.85 | 0.41 |
| 1:AA:1008:C:N4 | 1:AA:1021:G:H1 | 2.12 | 0.41 |
| 1:AA:1310:G:H2' | 1:AA:1311:G:C8 | 2.55 | 0.41 |
| 1:AA:1431:C:H2' | 1:AA:1432:G:H5' | 2.02 | 0.41 |
| 1:AA:77:G:H2' | 1:AA:77:G:N3 | 2.36 | 0.41 |
| 1:AA:807:A:H2' | 1:AA:808:C:C6 | 2.55 | 0.41 |
| 2:AB:105:PHE:CE1 | 2:AB:155:LEU:HD12 | 2.55 | 0.41 |
| 2:AB:162:ILE:HG23 | 2:AB:184:VAL:HA | 2.03 | 0.41 |
| 2:AB:100:GLY:N | 2:AB:176:GLU:OE2 | 2.47 | 0.41 |
| 2:AB:60:ASP:HB3 | 2:AB:64:ARG:NH2 | 2.32 | 0.41 |
| 2:AB:8:LYS:HE2 | 2:AB:217:ARG:HH22 | 1.86 | 0.41 |
| 7:AG:21:VAL:HG23 | 7:AG:22:LEU:N | 2.35 | 0.41 |
| 9:AI:53:VAL:C | 9:AI:55:ALA:N | 2.73 | 0.41 |
| 9:AI:95:LYS:HD3 | 9:AI:96:LEU:HB2 | 2.02 | 0.41 |
| 1:AA:528:C:H41 | 12:AL:49:ASN:ND2 | 2.18 | 0.41 |
| 12:AL:69:TYR:HB2 | 12:AL:90:VAL:HG21 | 2.02 | 0.41 |
| 16:AP:42:ARG:O | 16:AP:43:LYS:C | 2.58 | 0.41 |
| 1:AA:128:G:O2' | 17:AQ:3:LYS:HE2 | 2.20 | 0.41 |
| 17:AQ:86:GLU:O | 17:AQ:87:LYS:C | 2.58 | 0.41 |
| 18:AR:40:LEU:O | 18:AR:41:LYS:C | 2.59 | 0.41 |
| 19:AS:49:ILE:H | 19:AS:49:ILE:CD1 | 2.15 | 0.41 |
| 1:AA:1456:G:H8 | 20:AT:58:LYS:HD3 | 1.85 | 0.41 |
| 25:AZ:231:ILE:CG2 | 25:AZ:234:ARG:HG3 | 2.51 | 0.41 |
| 26:B0:56:ASP:OD1 | 26:B0:56:ASP:O | 2.39 | 0.41 |
| 27:B1:14:VAL:HG13 | 27:B1:39:LYS:HG3 | 2.03 | 0.41 |
| 33:B7:35:ARG:O | 33:B7:38:GLY:N | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:123:G:H2' | 36:BA:124:G:O4' | 2.19 | 0.41 |
| 36:BA:1301:A:O2' | 36:BA:1302:A:P | 2.78 | 0.41 |
| 36:BA:1313:U:H3' | 36:BA:1314:C:H5' | 2.03 | 0.41 |
| 36:BA:1541:G:O2' | 36:BA:1542:A:H5'' | 2.21 | 0.41 |
| 36:BA:1602:U:H3' | 36:BA:1603:A:H5' | 2.01 | 0.41 |
| 36:BA:2006:C:H2' | 36:BA:2007:C:H6 | 1.84 | 0.41 |
| 36:BA:2063:C:C4 | 36:BA:2064:C:C4 | 3.09 | 0.41 |
| 36:BA:2713:A:C3' | 36:BA:2714:G:C5' | 2.96 | 0.41 |
| 36:BA:687:C:H42 | 36:BA:787:U:H4' | 1.85 | 0.41 |
| 36:BA:74:A:C5' | 36:BA:75:G:O4' | 2.64 | 0.41 |
| 38:BC:10:LEU:N | 38:BC:10:LEU:CD2 | 2.83 | 0.41 |
| 38:BC:163:PHE:CD2 | 38:BC:192:PHE:HE1 | 2.37 | 0.41 |
| 39:BD:71:ASP:CB | 39:BD:103:ARG:HH22 | 2.33 | 0.41 |
| 39:BD:35:LYS:NZ | 39:BD:36:PRO:HD3 | 2.36 | 0.41 |
| 40:BE:93:VAL:C | 40:BE:95:ILE:H | 2.23 | 0.41 |
| 41:BF:129:PHE:C | 41:BF:131:GLY:N | 2.73 | 0.41 |
| 41:BF:139:PHE:CE2 | 41:BF:167:ALA:HB2 | 2.56 | 0.41 |
| 41:BF:18:ARG:O | 41:BF:19:GLU:HB3 | 2.21 | 0.41 |
| 42:BG:110:ALA:HB1 | 42:BG:140:ILE:HD13 | 2.03 | 0.41 |
| 43:BH:43:VAL:HB | 43:BH:46:GLU:OE2 | 2.20 | 0.41 |
| 43:BH:51:ARG:O | 43:BH:52:VAL:CB | 2.69 | 0.41 |
| 44:BJ:90:UNK:O | 44:BJ:91:UNK:C | 2.68 | 0.41 |
| 50:BR:116:LEU:O | 50:BR:117:VAL:O | 2.38 | 0.41 |
| 50:BR:9:LYS:O | 50:BR:10:LEU:HD23 | 2.20 | 0.41 |
| 52:BT:10:VAL:C | 52:BT:12:SER:N | 2.74 | 0.41 |
| 52:BT:45:PHE:CE2 | 52:BT:74:ARG:HB2 | 2.55 | 0.41 |
| 52:BT:85:LYS:O | 52:BT:86:ILE:C | 2.58 | 0.41 |
| 53:BU:93:LYS:H | 53:BU:93:LYS:CD | 2.28 | 0.41 |
| 55:BW:1:MET:CE | 55:BW:62:HIS:CD2 | 3.04 | 0.41 |
| 58:BZ:163:LEU:HD23 | 58:BZ:163:LEU:O | 2.20 | 0.41 |
| 1:AA:1152:A:H5' | 10:AJ:70:ARG:HH22 | 1.82 | 0.41 |
| 1:AA:1283:G:O2' | 1:AA:1284:C:OP2 | 2.39 | 0.41 |
| 1:AA:1368:G:O2' | 1:AA:1369:C:H5' | 2.20 | 0.41 |
| 1:AA:340:U:C2 | 1:AA:350:G:N2 | 2.88 | 0.41 |
| 1:AA:484:G:H4' | 1:AA:485:G:O5' | 2.21 | 0.41 |
| 1:AA:493:G:H8 | 1:AA:493:G:O5' | 2.04 | 0.41 |
| 1:AA:975:A:C8 | 1:AA:975:A:H5' | 2.55 | 0.41 |
| 1:AA:993:G:H4' | 1:AA:994:A:OP2 | 2.20 | 0.41 |
| 7:AG:26:PHE:CB | 7:AG:101:LEU:HD22 | 2.49 | 0.41 |
| 7:AG:113:GLU:HG2 | 7:AG:119:ARG:HG2 | 2.00 | 0.41 |
| 1:AA:653:A:P | 8:AH:56:LYS:HZ1 | 2.44 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:AT:36:LEU:HA | 20:AT:36:LEU:HD22 | 1.93 | 0.41 |
| 22:AW:57:G:O2' | 22:AW:58:A:H5' | 2.20 | 0.41 |
| 24:AY:73:G:C2' | 24:AY:74:C:H5' | 2.50 | 0.41 |
| 25:AZ:272:MET:HE2 | 25:AZ:285:ASN:H | 1.86 | 0.41 |
| 25:AZ:355:LEU:HA | 25:AZ:356:PRO:HD3 | 1.96 | 0.41 |
| 26:B0:31:VAL:O | 26:B0:64:ASP:HA | 2.20 | 0.41 |
| 28:B2:21:LEU:HD11 | 28:B2:63:VAL:CG1 | 2.49 | 0.41 |
| 31:B5:52:TYR:OH | 36:BA:2884:U:H1' | 2.21 | 0.41 |
| 32:B6:27:LYS:O | 32:B6:29:ASN:N | 2.54 | 0.41 |
| 32:B6:8:LYS:HA | 32:B6:8:LYS:HD2 | 1.84 | 0.41 |
| 33:B7:29:LYS:O | 33:B7:33:ARG:HB2 | 2.21 | 0.41 |
| 34:B8:27:THR:HG22 | 48:BP:62:LEU:CD2 | 2.51 | 0.41 |
| 36:BA:1011:G:C6 | 36:BA:1151:G:C6 | 3.08 | 0.41 |
| 36:BA:121:G:C2 | 36:BA:131:G:C5 | 3.08 | 0.41 |
| 36:BA:120:U:C2 | 36:BA:149:A:N6 | 2.88 | 0.41 |
| 36:BA:1503:U:C4 | 36:BA:1504:C:N4 | 2.83 | 0.41 |
| 36:BA:1593:G:N3 | 36:BA:1593:G:H2' | 2.35 | 0.41 |
| 36:BA:1676:A:N6 | 36:BA:1677:A:C6 | 2.89 | 0.41 |
| 36:BA:2165:G:H2' | 36:BA:2166:G:C8 | 2.55 | 0.41 |
| 36:BA:2178:C:O2 | 36:BA:2178:C:O4' | 2.37 | 0.41 |
| 36:BA:2267:A:H5'' | 36:BA:2268:A:C5' | 2.50 | 0.41 |
| 36:BA:482:A:H2' | 36:BA:482:A:N3 | 2.36 | 0.41 |
| 36:BA:556:G:H2' | 36:BA:557:U:C6 | 2.56 | 0.41 |
| 38:BC:104:LEU:O | 38:BC:105:ASP:HB3 | 2.21 | 0.41 |
| 41:BF:160:ASN:HD21 | 41:BF:162:LEU:HB2 | 1.83 | 0.41 |
| 41:BF:117:ARG:NH2 | 41:BF:186:ILE:O | 2.51 | 0.41 |
| 41:BF:29:ASN:HD22 | 41:BF:32:LEU:CB | 2.33 | 0.41 |
| 43:BH:158:HIS:O | 43:BH:159:GLU:HB3 | 2.21 | 0.41 |
| 43:BH:70:THR:C | 43:BH:72:ILE:N | 2.74 | 0.41 |
| 48:BP:25:SER:C | 48:BP:27:HIS:N | 2.74 | 0.41 |
| 49:BQ:54:MET:CE | 49:BQ:64:ILE:HG23 | 2.51 | 0.41 |
| 51:BS:104:GLY:C | 51:BS:106:ARG:N | 2.72 | 0.41 |
| 51:BS:31:SER:OG | 51:BS:32:LEU:N | 2.54 | 0.41 |
| 51:BS:85:VAL:HB | 51:BS:86:ALA:H | 1.66 | 0.41 |
| 53:BU:82:GLY:O | 53:BU:84:LYS:N | 2.54 | 0.41 |
| 55:BW:21:VAL:C | 55:BW:23:LEU:N | 2.74 | 0.41 |
| 57:BY:31:LEU:HD23 | 57:BY:36:ALA:O | 2.21 | 0.41 |
| 58:BZ:119:GLU:CG | 58:BZ:122:ARG:NH1 | 2.79 | 0.41 |
| 58:BZ:8:TYR:O | 58:BZ:9:TYR:C | 2.59 | 0.41 |
| 1:AA:1174:G:H2' | 1:AA:1175:G:H8 | 1.86 | 0.41 |
| 1:AA:1307:U:O3' | 13:AM:110:ARG:HD2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:226:G:C2' | 1:AA:227:G:H5' | 2.51 | 0.41 |
| 1:AA:723:U:C2' | 1:AA:723:U:O2 | 2.65 | 0.41 |
| 1:AA:858:G:H8 | 1:AA:858:G:H5'' | 1.84 | 0.41 |
| 2:AB:16:HIS:HB3 | 2:AB:210:SER:CB | 2.51 | 0.41 |
| 3:AC:142:MET:C | 3:AC:144:SER:N | 2.73 | 0.41 |
| 4:AD:57:ARG:HB3 | 4:AD:206:PHE:HB2 | 2.02 | 0.41 |
| 8:AH:1:MET:HE1 | 8:AH:3:THR:HG23 | 2.03 | 0.41 |
| 9:AI:70:LYS:O | 9:AI:73:GLN:N | 2.53 | 0.41 |
| 13:AM:49:THR:O | 13:AM:51:ALA:N | 2.53 | 0.41 |
| 13:AM:90:LEU:CA | 13:AM:93:ARG:HB2 | 2.42 | 0.41 |
| 14:AN:39:LEU:HD11 | 14:AN:47:LEU:HD12 | 2.02 | 0.41 |
| 17:AQ:13:ASP:C | 17:AQ:15:MET:H | 2.23 | 0.41 |
| 17:AQ:24:GLU:HA | 17:AQ:39:SER:HA | 2.02 | 0.41 |
| 25:AZ:342:PHE:H | 25:AZ:342:PHE:HD1 | 1.69 | 0.41 |
| 25:AZ:319:SER:H | 25:AZ:401:THR:HB | 1.86 | 0.41 |
| 29:B3:12:PRO:O | 29:B3:15:TYR:HD1 | 2.04 | 0.41 |
| 32:B6:17:LYS:CB | 32:B6:18:ARG:NH1 | 2.84 | 0.41 |
| 32:B6:28:ARG:NH1 | 32:B6:28:ARG:HG2 | 2.35 | 0.41 |
| 35:B9:31:LYS:HE3 | 36:BA:2528:U:H5'' | 2.02 | 0.41 |
| 36:BA:1141:U:H6 | 46:BN:63:THR:CG2 | 2.33 | 0.41 |
| 36:BA:816:C:N3 | 36:BA:1192:G:N2 | 2.69 | 0.41 |
| 36:BA:1209:G:H21 | 36:BA:1210:A:H62 | 1.67 | 0.41 |
| 36:BA:1375:C:H2' | 36:BA:1376:C:H6 | 1.86 | 0.41 |
| 36:BA:1413:G:H2' | 36:BA:1414:G:H8 | 1.86 | 0.41 |
| 36:BA:1947:C:H2' | 36:BA:1948:G:H5' | 2.02 | 0.41 |
| 36:BA:2155:G:C6 | 36:BA:2156:G:C2 | 3.09 | 0.41 |
| 36:BA:2189:U:C3' | 36:BA:2190:G:H4' | 2.50 | 0.41 |
| 36:BA:2618:G:C6 | 36:BA:2619:C:C4 | 3.09 | 0.41 |
| 36:BA:272(I):U:C4 | 36:BA:363(B):G:C6 | 3.09 | 0.41 |
| 36:BA:2787:C:C2' | 36:BA:2787:C:O2 | 2.69 | 0.41 |
| 36:BA:353:G:N3 | 36:BA:353:G:H2' | 2.36 | 0.41 |
| 36:BA:472:A:C2' | 36:BA:473:G:H5' | 2.49 | 0.41 |
| 36:BA:520:G:H2' | 36:BA:521:G:H8 | 1.85 | 0.41 |
| 36:BA:588:U:C6 | 36:BA:588:U:OP2 | 2.74 | 0.41 |
| 36:BA:890:A:C2' | 36:BA:892:G:H5' | 2.51 | 0.41 |
| 36:BA:882:G:H22 | 36:BA:894:C:H42 | 1.67 | 0.41 |
| 37:BB:13:A:C2' | 37:BB:14:U:H5'' | 2.51 | 0.41 |
| 38:BC:18:LYS:HE3 | 38:BC:20:TYR:OH | 2.20 | 0.41 |
| 36:BA:2177:C:H4' | 38:BC:46:LYS:HD3 | 2.02 | 0.41 |
| 40:BE:65:GLY:HA2 | 40:BE:70:ALA:HB1 | 2.02 | 0.41 |
| 41:BF:9:ILE:HG23 | 41:BF:13:SER:C | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BH:158:HIS:CE1 | 43:BH:169:VAL:O | 2.73 | 0.41 |
| 43:BH:37:VAL:CG1 | 43:BH:38:SER:N | 2.84 | 0.41 |
| 43:BH:54:ARG:HG2 | 43:BH:54:ARG:NH1 | 2.35 | 0.41 |
| 46:BN:56:ASN:N | 46:BN:125:GLY:N | 2.67 | 0.41 |
| 46:BN:57:ALA:C | 46:BN:58:ASP:O | 2.57 | 0.41 |
| 46:BN:86:PRO:HD2 | 46:BN:89:LYS:HG3 | 2.01 | 0.41 |
| 47:BO:14:THR:CG2 | 47:BO:94:ARG:HB2 | 2.50 | 0.41 |
| 47:BO:14:THR:HG22 | 47:BO:94:ARG:HB2 | 2.02 | 0.41 |
| 49:BQ:125:LEU:HD13 | 49:BQ:125:LEU:HA | 1.88 | 0.41 |
| 50:BR:113:LEU:HD23 | 50:BR:114:VAL:N | 2.35 | 0.41 |
| 51:BS:58:LEU:CD2 | 51:BS:65:VAL:HG13 | 2.46 | 0.41 |
| 51:BS:65:VAL:O | 51:BS:69:VAL:N | 2.47 | 0.41 |
| 52:BT:40:THR:O | 52:BT:41:ARG:O | 2.38 | 0.41 |
| 52:BT:32:TYR:CB | 52:BT:81:PRO:HB3 | 2.48 | 0.41 |
| 54:BV:38:LEU:CD1 | 54:BV:57:VAL:HB | 2.47 | 0.41 |
| 57:BY:35:TYR:CD2 | 57:BY:68:HIS:HE1 | 2.32 | 0.41 |
| 58:BZ:125:LEU:HB3 | 58:BZ:164:ALA:O | 2.21 | 0.41 |
| 1:AA:1127:G:O2' | 1:AA:1128:C:H5' | 2.21 | 0.41 |
| 1:AA:1213:A:C4 | 1:AA:1215:G:C8 | 3.09 | 0.41 |
| 1:AA:1261:A:C2' | 1:AA:1262:C:H5' | 2.51 | 0.41 |
| 1:AA:565:U:H3' | 1:AA:566:G:H2' | 2.03 | 0.41 |
| 1:AA:78:G:H1 | 1:AA:91:C:H42 | 1.69 | 0.41 |
| 1:AA:977:A:N6 | 1:AA:1224:G:O5' | 2.54 | 0.41 |
| 2:AB:28:PHE:O | 2:AB:28:PHE:CD1 | 2.73 | 0.41 |
| 2:AB:61:LEU:CD1 | 2:AB:64:ARG:NH1 | 2.83 | 0.41 |
| 2:AB:68:ILE:HA | 2:AB:161:ALA:O | 2.21 | 0.41 |
| 3:AC:141:VAL:CG1 | 3:AC:149:ALA:HB2 | 2.50 | 0.41 |
| 3:AC:142:MET:HE1 | 3:AC:171:GLY:HA3 | 2.03 | 0.41 |
| 5:AE:84:PHE:N | 5:AE:87:SER:O | 2.43 | 0.41 |
| 5:AE:92:LYS:HA | 5:AE:93:PRO:HD3 | 1.92 | 0.41 |
| 7:AG:108:ALA:N | 7:AG:123:GLU:HG2 | 2.36 | 0.41 |
| 7:AG:51:GLN:HA | 7:AG:51:GLN:OE1 | 2.21 | 0.41 |
| 7:AG:93:PRO:O | 7:AG:96:GLN:HB3 | 2.21 | 0.41 |
| 9:AI:64:THR:O | 9:AI:64:THR:HG22 | 2.21 | 0.41 |
| 9:AI:82:ALA:C | 9:AI:84:ALA:H | 2.25 | 0.41 |
| 11:AK:124:LYS:NZ | 11:AK:124:LYS:CB | 2.84 | 0.41 |
| 11:AK:18:ARG:HB3 | 11:AK:33:THR:OG1 | 2.21 | 0.41 |
| 14:AN:3:ARG:HG2 | 14:AN:3:ARG:O | 2.21 | 0.41 |
| 22:AW:37:A:H3' | 22:AW:38:A:H8 | 1.85 | 0.41 |
| 25:AZ:318:ALA:CA | 25:AZ:401:THR:HG22 | 2.40 | 0.41 |
| 25:AZ:51:ASP:OD1 | 25:AZ:62:THR:HG23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AZ:88:TYR:CD1 | 25:AZ:88:TYR:N | 2.88 | 0.41 |
| 26:B0:75:LEU:HD23 | 26:B0:75:LEU:O | 2.20 | 0.41 |
| 32:B6:33:LYS:O | 32:B6:34:LEU:CB | 2.68 | 0.41 |
| 36:BA:1155:A:HO2' | 36:BA:1156:A:H2' | 1.85 | 0.41 |
| 36:BA:2377:A:O2' | 36:BA:2378:A:C5' | 2.67 | 0.41 |
| 36:BA:2880:C:C2 | 36:BA:2881:C:C5 | 3.09 | 0.41 |
| 36:BA:449:A:O2' | 53:BU:3:ARG:CD | 2.69 | 0.41 |
| 36:BA:553:G:O2' | 36:BA:554:U:H5' | 2.20 | 0.41 |
| 36:BA:654(N):G:H2' | 36:BA:654(O):G:C5' | 2.51 | 0.41 |
| 38:BC:61:THR:HG23 | 38:BC:142:ALA:O | 2.21 | 0.41 |
| 39:BD:97:TYR:HE1 | 39:BD:103:ARG:CG | 2.34 | 0.41 |
| 39:BD:73:VAL:HG12 | 39:BD:74:GLY:N | 2.36 | 0.41 |
| 40:BE:7:VAL:HG21 | 52:BT:1:MET:SD | 2.61 | 0.41 |
| 40:BE:80:GLU:C | 40:BE:81:ILE:HG12 | 2.41 | 0.41 |
| 41:BF:164:ARG:CD | 41:BF:175:THR:OG1 | 2.69 | 0.41 |
| 41:BF:98:SER:O | 41:BF:99:TYR:HB3 | 2.21 | 0.41 |
| 13:AM:7:VAL:HG23 | 42:BG:115:ARG:HA | 2.02 | 0.41 |
| 43:BH:99:VAL:HG12 | 43:BH:100:GLY:N | 2.35 | 0.41 |
| 46:BN:12:ARG:CG | 46:BN:50:ASP:OD2 | 2.65 | 0.41 |
| 47:BO:104:ARG:CB | 47:BO:104:ARG:CZ | 2.99 | 0.41 |
| 47:BO:23:ARG:HG3 | 47:BO:24:VAL:N | 2.36 | 0.41 |
| 50:BR:72:ASP:HB3 | 50:BR:75:LEU:CB | 2.50 | 0.41 |
| 47:BO:73:ASP:CG | 52:BT:32:TYR:HE1 | 2.23 | 0.41 |
| 52:BT:49:VAL:HG13 | 52:BT:49:VAL:O | 2.21 | 0.41 |
| 55:BW:84:ARG:HG2 | 55:BW:84:ARG:NH1 | 2.35 | 0.41 |
| 1:AA:1266:G:C4 | 1:AA:1268:A:C2 | 3.08 | 0.41 |
| 1:AA:1326:C:H5' | 21:AU:18:TYR:O | 2.21 | 0.41 |
| 1:AA:1432:G:OP1 | 52:BT:108:ARG:HG2 | 2.21 | 0.41 |
| 1:AA:346:G:O2' | 1:AA:347:G:O5' | 2.38 | 0.41 |
| 1:AA:407:G:H2' | 1:AA:408:A:C8 | 2.56 | 0.41 |
| 1:AA:542:G:O2' | 1:AA:543:C:H5' | 2.21 | 0.41 |
| 1:AA:973:G:H2' | 1:AA:974:A:OP1 | 2.21 | 0.41 |
| 5:AE:90:VAL:O | 5:AE:120:THR:HA | 2.21 | 0.41 |
| 5:AE:125:SER:O | 5:AE:126:ARG:HG3 | 2.21 | 0.41 |
| 7:AG:119:ARG:O | 7:AG:120:ILE:C | 2.59 | 0.41 |
| 9:AI:16:ARG:NH2 | 9:AI:64:THR:HG21 | 2.35 | 0.41 |
| 9:AI:65:VAL:O | 9:AI:66:ARG:HB2 | 2.21 | 0.41 |
| 10:AJ:20:ALA:C | 10:AJ:22:LYS:N | 2.73 | 0.41 |
| 10:AJ:28:ARG:HH12 | 10:AJ:33:GLN:CD | 2.23 | 0.41 |
| 12:AL:126:LYS:HD2 | 12:AL:126:LYS:HA | 1.86 | 0.41 |
| 15:AO:29:VAL:HG21 | 15:AO:67:LEU:CD2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:AP:8:ARG:NH2 | 16:AP:15:PRO:HG3 | 2.36 | 0.41 |
| 19:AS:36:ARG:HB3 | 19:AS:51:VAL:CG1 | 2.50 | 0.41 |
| 22:AW:18:G:O4' | 22:AW:58:A:C2 | 2.74 | 0.41 |
| 24:AY:60:U:OP2 | 24:AY:60:U:H6 | 2.04 | 0.41 |
| 25:AZ:136:ASN:O | 25:AZ:137:LYS:CB | 2.69 | 0.41 |
| 25:AZ:342:PHE:CB | 25:AZ:344:PHE:CE1 | 3.04 | 0.41 |
| 25:AZ:388:ILE:HG22 | 25:AZ:395:VAL:HG22 | 2.03 | 0.41 |
| 26:B0:56:ASP:OD1 | 26:B0:56:ASP:C | 2.58 | 0.41 |
| 31:B5:33:CYS:CB | 31:B5:36:CYS:HG | 2.32 | 0.41 |
| 34:B8:59:LYS:HE3 | 34:B8:59:LYS:HB2 | 1.83 | 0.41 |
| 36:BA:1045:A:N3 | 36:BA:1047:G:C2 | 2.89 | 0.41 |
| 36:BA:1813:G:H1' | 39:BD:50:THR:HG1 | 1.84 | 0.41 |
| 36:BA:1827:C:O2' | 36:BA:1828:G:H5' | 2.21 | 0.41 |
| 36:BA:2159:G:H2' | 36:BA:2160:G:O4' | 2.21 | 0.41 |
| 36:BA:217:G:H2' | 36:BA:218:A:O4' | 2.21 | 0.41 |
| 36:BA:2242:G:H2' | 36:BA:2243:U:O5' | 2.21 | 0.41 |
| 36:BA:2366:A:O2' | 36:BA:2367:G:H5' | 2.21 | 0.41 |
| 36:BA:2519:U:OP1 | 36:BA:2519:U:H3' | 2.21 | 0.41 |
| 36:BA:2525:G:O2' | 36:BA:2526:G:H5' | 2.21 | 0.41 |
| 38:BC:195:ALA:O | 38:BC:199:HIS:ND1 | 2.54 | 0.41 |
| 38:BC:50:ASP:OD1 | 38:BC:52:ARG:NH1 | 2.54 | 0.41 |
| 39:BD:35:LYS:CG | 39:BD:63:ARG:HG3 | 2.49 | 0.41 |
| 39:BD:88:ARG:CZ | 39:BD:88:ARG:HB3 | 2.51 | 0.41 |
| 42:BG:113:ARG:O | 42:BG:115:ARG:N | 2.54 | 0.41 |
| 42:BG:142:PRO:C | 42:BG:143:GLU:HG2 | 2.39 | 0.41 |
| 43:BH:81:GLU:HA | 43:BH:83:TYR:CE2 | 2.56 | 0.41 |
| 44:BJ:23:UNK:HA | 44:BJ:118:UNK:HA | 2.03 | 0.41 |
| 46:BN:45:ASN:O | 46:BN:46:VAL:HB | 2.21 | 0.41 |
| 48:BP:6:LEU:HG | 48:BP:9:ASN:CB | 2.51 | 0.41 |
| 52:BT:99:LEU:HB2 | 52:BT:101:PHE:CE1 | 2.56 | 0.41 |
| 52:BT:113:LYS:HA | 52:BT:113:LYS:HD3 | 1.95 | 0.41 |
| 52:BT:22:PHE:HE2 | 52:BT:85:LYS:NZ | 2.19 | 0.41 |
| 52:BT:28:VAL:CG1 | 52:BT:29:ARG:NH1 | 2.84 | 0.41 |
| 54:BV:5:VAL:O | 54:BV:11:GLN:HA | 2.21 | 0.41 |
| 54:BV:4:ILE:HG22 | 54:BV:39:LEU:HD23 | 2.03 | 0.41 |
| 55:BW:103:ILE:H | 55:BW:103:ILE:HG13 | 1.53 | 0.41 |
| 57:BY:28:LYS:C | 57:BY:38:ILE:HG22 | 2.42 | 0.41 |
| 1:AA:1004:A:C6 | 1:AA:1037:C:N4 | 2.89 | 0.41 |
| 1:AA:101:A:H2 | 1:AA:152:A:O2' | 2.03 | 0.41 |
| 1:AA:189(J):G:C2' | 1:AA:189(K):U:H5' | 2.51 | 0.41 |
| 1:AA:738:C:H2' | 1:AA:739:C:C6 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:582:U:C2 | 1:AA:760:G:C6 | 3.09 | 0.41 |
| 3:AC:164:ARG:HB2 | 3:AC:164:ARG:HE | 1.71 | 0.41 |
| 5:AE:45:PHE:CD2 | 5:AE:47:LYS:HD2 | 2.56 | 0.41 |
| 1:AA:1240:U:C4' | 7:AG:38:LEU:HD21 | 2.50 | 0.41 |
| 20:AT:45:GLN:HA | 20:AT:91:LEU:HB3 | 2.03 | 0.41 |
| 1:AA:1305:G:OP1 | 21:AU:2:GLY:N | 2.54 | 0.41 |
| 22:AW:45:U:H6 | 22:AW:45:U:H3' | 1.85 | 0.41 |
| 22:AW:71:G:O2' | 22:AW:72:C:H5' | 2.20 | 0.41 |
| 25:AZ:202:LEU:O | 25:AZ:205:ALA:HB3 | 2.21 | 0.41 |
| 25:AZ:222:LEU:HD12 | 25:AZ:303:VAL:HG11 | 2.02 | 0.41 |
| 25:AZ:371:THR:CG2 | 25:AZ:372:VAL:N | 2.78 | 0.41 |
| 25:AZ:98:GLN:HB2 | 25:AZ:99:MET:H | 1.68 | 0.41 |
| 27:B1:7:ILE:HD12 | 27:B1:70:VAL:HG22 | 2.03 | 0.41 |
| 28:B2:24:LEU:HD23 | 28:B2:24:LEU:C | 2.41 | 0.41 |
| 29:B3:6:VAL:O | 29:B3:6:VAL:HG23 | 2.21 | 0.41 |
| 31:B5:10:LYS:HG3 | 36:BA:1263:U:O4' | 2.20 | 0.41 |
| 31:B5:16:ARG:NH1 | 31:B5:17:ASP:OD1 | 2.54 | 0.41 |
| 32:B6:30:THR:O | 32:B6:31:PRO:C | 2.60 | 0.41 |
| 33:B7:12:ARG:HG3 | 33:B7:12:ARG:NH1 | 2.36 | 0.41 |
| 34:B8:50:LEU:O | 34:B8:52:LYS:N | 2.49 | 0.41 |
| 36:BA:1055:G:N2 | 36:BA:1085:A:N3 | 2.69 | 0.41 |
| 36:BA:1177:A:H5'' | 36:BA:1178:C:O5' | 2.21 | 0.41 |
| 36:BA:1258:C:O2' | 36:BA:1259:G:H5' | 2.21 | 0.41 |
| 36:BA:1403:C:C5' | 36:BA:1471:A:H1' | 2.34 | 0.41 |
| 36:BA:1543:C:H3' | 36:BA:1544:A:H5' | 1.97 | 0.41 |
| 36:BA:1557:C:H5'' | 36:BA:1558:A:OP2 | 2.21 | 0.41 |
| 36:BA:185:U:H2' | 36:BA:186:G:C8 | 2.56 | 0.41 |
| 36:BA:1858:G:H1' | 36:BA:1884:A:N6 | 2.36 | 0.41 |
| 36:BA:2033:A:O2' | 36:BA:2034:U:OP1 | 2.37 | 0.41 |
| 36:BA:2171:A:O2' | 36:BA:2172:U:C5 | 2.72 | 0.41 |
| 36:BA:2346:A:H5' | 36:BA:2383:G:C1' | 2.51 | 0.41 |
| 36:BA:2478:A:H2' | 36:BA:2479:G:C5' | 2.51 | 0.41 |
| 36:BA:311:A:H5' | 36:BA:332:A:N3 | 2.35 | 0.41 |
| 36:BA:654(N):G:O6 | 36:BA:654(O):G:N2 | 2.54 | 0.41 |
| 36:BA:730:C:H2' | 36:BA:731:C:H6 | 1.85 | 0.41 |
| 38:BC:103:ILE:HG23 | 38:BC:107:TRP:CD1 | 2.56 | 0.41 |
| 38:BC:139:ASN:OD1 | 38:BC:140:PRO:HD2 | 2.21 | 0.41 |
| 39:BD:267:SER:C | 39:BD:270:ILE:HD11 | 2.40 | 0.41 |
| 40:BE:96:PHE:O | 40:BE:175:VAL:HG11 | 2.20 | 0.41 |
| 40:BE:29:GLY:H | 40:BE:51:PHE:HZ | 1.69 | 0.41 |
| 40:BE:54:GLN:O | 40:BE:55:ASN:HB2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BE:82:ARG:O | 40:BE:84:PHE:N | 2.54 | 0.41 |
| 41:BF:62:ARG:NH1 | 41:BF:62:ARG:CG | 2.84 | 0.41 |
| 36:BA:2305:A:O2' | 42:BG:136:ARG:HG2 | 2.20 | 0.41 |
| 46:BN:22:THR:HA | 46:BN:61:ARG:CB | 2.50 | 0.41 |
| 46:BN:2:LYS:NZ | 54:BV:13:ARG:H | 2.19 | 0.41 |
| 46:BN:60:ILE:HD13 | 46:BN:99:LEU:CD2 | 2.38 | 0.41 |
| 48:BP:104:GLY:C | 48:BP:105:LEU:HD12 | 2.42 | 0.41 |
| 49:BQ:12:GLN:HG2 | 49:BQ:73:PRO:HD2 | 2.03 | 0.41 |
| 51:BS:58:LEU:CG | 51:BS:59:LYS:N | 2.69 | 0.41 |
| 51:BS:89:ARG:HB3 | 51:BS:92:TYR:HB2 | 2.03 | 0.41 |
| 55:BW:1:MET:O | 55:BW:64:MET:HE3 | 2.21 | 0.41 |
| 1:AA:1054:C:OP1 | 1:AA:1197:G:OP1 | 2.39 | 0.40 |
| 1:AA:1342:C:O2' | 9:AI:124:GLN:HG3 | 2.21 | 0.40 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.57 | 0.40 |
| 1:AA:348:G:C2' | 1:AA:349:A:H5' | 2.51 | 0.40 |
| 1:AA:490:G:O2' | 1:AA:491:G:H5' | 2.21 | 0.40 |
| 1:AA:963:G:N2 | 10:AJ:55:LYS:CD | 2.71 | 0.40 |
| 2:AB:219:VAL:O | 2:AB:223:ILE:HG13 | 2.21 | 0.40 |
| 1:AA:738:C:P | 6:AF:92:LYS:HE3 | 2.61 | 0.40 |
| 7:AG:136:LYS:HB3 | 7:AG:136:LYS:HE3 | 1.92 | 0.40 |
| 9:AI:26:VAL:HG12 | 9:AI:28:VAL:HG23 | 2.03 | 0.40 |
| 9:AI:53:VAL:O | 9:AI:55:ALA:N | 2.53 | 0.40 |
| 10:AJ:14:LYS:HB2 | 10:AJ:14:LYS:HE3 | 1.71 | 0.40 |
| 12:AL:117:ARG:NH2 | 12:AL:124:LYS:HB2 | 2.37 | 0.40 |
| 13:AM:86:CYS:O | 13:AM:89:GLY:N | 2.54 | 0.40 |
| 13:AM:90:LEU:O | 13:AM:91:ARG:CG | 2.67 | 0.40 |
| 14:AN:12:ARG:CB | 14:AN:12:ARG:HH11 | 2.33 | 0.40 |
| 14:AN:21:TYR:N | 14:AN:21:TYR:CD1 | 2.88 | 0.40 |
| 15:AO:26:GLU:OE2 | 15:AO:77:ARG:HD2 | 2.21 | 0.40 |
| 15:AO:64:ARG:HG3 | 15:AO:64:ARG:HH11 | 1.86 | 0.40 |
| 23:AX:23:G:C5 | 24:AY:36:A:C2 | 3.09 | 0.40 |
| 25:AZ:130:TYR:CD1 | 25:AZ:211:PRO:HD3 | 2.57 | 0.40 |
| 25:AZ:221:PHE:HA | 25:AZ:244:ARG:HG3 | 2.03 | 0.40 |
| 25:AZ:31:LEU:O | 25:AZ:35:THR:HG23 | 2.20 | 0.40 |
| 27:B1:10:LYS:O | 27:B1:44:PRO:HG3 | 2.20 | 0.40 |
| 28:B2:37:PHE:C | 28:B2:39:ALA:N | 2.74 | 0.40 |
| 35:B9:19:ARG:NH1 | 36:BA:2755:C:C5 | 2.89 | 0.40 |
| 36:BA:1022:G:OP2 | 46:BN:69:GLN:NE2 | 2.44 | 0.40 |
| 36:BA:1061:U:H4' | 36:BA:1070:A:C4' | 2.51 | 0.40 |
| 36:BA:1060:U:O2' | 36:BA:1061:U:OP2 | 2.30 | 0.40 |
| 36:BA:1247:A:OP1 | 41:BF:95:ARG:NH2 | 2.48 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BA:13:A:C6 | 36:BA:525:U:C2 | 3.09 | 0.40 |
| 36:BA:1511:C:C4 | 36:BA:1512:U:C5 | 3.09 | 0.40 |
| 36:BA:1697:G:C3' | 36:BA:1698:A:H5'' | 2.40 | 0.40 |
| 36:BA:1790:C:H2' | 36:BA:1791:A:C4 | 2.56 | 0.40 |
| 36:BA:2368:C:O2' | 36:BA:2369:A:H5' | 2.21 | 0.40 |
| 22:AV:76:A:H5'' | 36:BA:2602:A:N7 | 2.36 | 0.40 |
| 36:BA:514:A:O2' | 36:BA:515:A:H5' | 2.21 | 0.40 |
| 36:BA:529:A:H4' | 36:BA:530:G:O5' | 2.20 | 0.40 |
| 36:BA:565:C:H4' | 36:BA:1253:A:N1 | 2.35 | 0.40 |
| 36:BA:582:G:H2' | 36:BA:583:G:H8 | 1.86 | 0.40 |
| 37:BB:66:A:C2 | 37:BB:109:C:C2 | 3.10 | 0.40 |
| 38:BC:124:GLY:HA2 | 38:BC:128:GLY:HA3 | 2.03 | 0.40 |
| 38:BC:189:ILE:HG22 | 38:BC:190:ARG:N | 2.35 | 0.40 |
| 39:BD:43:ARG:HB2 | 39:BD:54:ARG:HB2 | 2.02 | 0.40 |
| 39:BD:73:VAL:O | 39:BD:75:ILE:N | 2.47 | 0.40 |
| 40:BE:48:GLN:CD | 40:BE:78:LEU:HD13 | 2.40 | 0.40 |
| 42:BG:138:GLN:C | 42:BG:140:ILE:H | 2.24 | 0.40 |
| 42:BG:178:PHE:CB | 42:BG:180:PHE:CE1 | 3.04 | 0.40 |
| 43:BH:17:VAL:CG1 | 43:BH:18:GLU:H | 2.28 | 0.40 |
| 43:BH:85:LYS:HD3 | 43:BH:133:VAL:H | 1.86 | 0.40 |
| 46:BN:101:HIS:C | 46:BN:103:VAL:N | 2.74 | 0.40 |
| 48:BP:140:ALA:O | 48:BP:141:ALA:HB3 | 2.21 | 0.40 |
| 48:BP:65:ARG:HB3 | 48:BP:68:GLN:NE2 | 2.36 | 0.40 |
| 36:BA:2723:C:C5' | 50:BR:2:ARG:HE | 2.34 | 0.40 |
| 50:BR:38:VAL:CB | 50:BR:39:PRO:CD | 2.97 | 0.40 |
| 51:BS:29:PHE:CE2 | 51:BS:31:SER:HB2 | 2.56 | 0.40 |
| 52:BT:19:LEU:HA | 52:BT:20:PRO:HD3 | 1.80 | 0.40 |
| 52:BT:76:PHE:HA | 52:BT:77:PRO:HD3 | 1.72 | 0.40 |
| 53:BU:113:ALA:C | 53:BU:115:ALA:N | 2.75 | 0.40 |
| 53:BU:115:ALA:C | 53:BU:117:GLN:N | 2.73 | 0.40 |
| 57:BY:27:VAL:HG12 | 57:BY:29:GLU:OE1 | 2.20 | 0.40 |
| 57:BY:31:LEU:HD22 | 57:BY:31:LEU:H | 1.87 | 0.40 |
| 58:BZ:76:LEU:O | 58:BZ:77:ASP:CB | 2.64 | 0.40 |
| 1:AA:102:G:C5 | 1:AA:103:C:C5 | 3.09 | 0.40 |
| 1:AA:1039:C:C6 | 1:AA:1040:U:C5 | 3.09 | 0.40 |
| 1:AA:1145:C:O2' | 1:AA:1146:A:C8 | 2.71 | 0.40 |
| 1:AA:1188:A:H2' | 1:AA:1189:C:H5' | 2.02 | 0.40 |
| 1:AA:1415:G:C6 | 1:AA:1486:G:C5 | 3.09 | 0.40 |
| 1:AA:165:C:O2' | 1:AA:166:G:H5' | 2.21 | 0.40 |
| 1:AA:173:U:H5' | 1:AA:197:A:C1' | 2.48 | 0.40 |
| 1:AA:189(H):G:O2' | 1:AA:189(I):G:C8 | 2.73 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:7:VAL:HA | 2:AB:11:LEU:CD1 | 2.50 | 0.40 |
| 2:AB:224:GLN:O | 2:AB:227:GLY:N | 2.54 | 0.40 |
| 2:AB:30:ARG:HG3 | 2:AB:31:TYR:N | 2.36 | 0.40 |
| 2:AB:30:ARG:CG | 2:AB:31:TYR:N | 2.84 | 0.40 |
| 2:AB:58:ILE:O | 2:AB:61:LEU:N | 2.54 | 0.40 |
| 3:AC:174:PRO:HB2 | 3:AC:177:THR:HB | 2.03 | 0.40 |
| 4:AD:59:ARG:HA | 4:AD:59:ARG:NE | 2.35 | 0.40 |
| 9:AI:11:LYS:C | 9:AI:13:ALA:N | 2.74 | 0.40 |
| 9:AI:95:LYS:HZ3 | 9:AI:96:LEU:CD1 | 2.35 | 0.40 |
| 12:AL:124:LYS:HD2 | 12:AL:125:PRO:HD2 | 2.02 | 0.40 |
| 12:AL:10:LEU:O | 12:AL:14:GLY:N | 2.54 | 0.40 |
| 12:AL:64:TYR:HD1 | 12:AL:64:TYR:H | 1.69 | 0.40 |
| 1:AA:1202:G:H1' | 14:AN:29:ARG:CD | 2.51 | 0.40 |
| 15:AO:39:LEU:CD2 | 15:AO:43:LEU:HG | 2.51 | 0.40 |
| 15:AO:65:ARG:NH1 | 15:AO:65:ARG:HG2 | 2.36 | 0.40 |
| 22:AV:18:G:C2 | 22:AV:58:A:C6 | 3.09 | 0.40 |
| 22:AW:9:A:N6 | 22:AW:23:A:C8 | 2.90 | 0.40 |
| 25:AZ:271:GLU:HA | 25:AZ:277:LEU:H | 1.86 | 0.40 |
| 25:AZ:282:ALA:C | 25:AZ:284:ASP:H | 2.24 | 0.40 |
| 25:AZ:38:GLU:O | 25:AZ:38:GLU:CD | 2.59 | 0.40 |
| 29:B3:15:TYR:HD2 | 29:B3:19:GLN:HE22 | 1.69 | 0.40 |
| 29:B3:3:ARG:HB2 | 29:B3:59:VAL:C | 2.41 | 0.40 |
| 30:B4:35:VAL:CG1 | 30:B4:36:CYS:N | 2.84 | 0.40 |
| 36:BA:1018:C:O2' | 36:BA:1019:U:H5' | 2.21 | 0.40 |
| 36:BA:1190:G:H5' | 48:BP:35:HIS:H | 1.86 | 0.40 |
| 36:BA:585:G:H2' | 36:BA:1251:C:H42 | 1.85 | 0.40 |
| 36:BA:1309:G:O2' | 36:BA:1310:G:H5' | 2.22 | 0.40 |
| 36:BA:1389:G:H2' | 36:BA:1390:U:H6 | 1.86 | 0.40 |
| 36:BA:2038:G:H2' | 36:BA:2039:C:O4' | 2.20 | 0.40 |
| 36:BA:2101:G:C2' | 36:BA:2102:U:C5' | 2.93 | 0.40 |
| 36:BA:2505:G:O6 | 36:BA:2576:G:H2' | 2.21 | 0.40 |
| 36:BA:2592:G:H2' | 36:BA:2593:U:O4' | 2.21 | 0.40 |
| 36:BA:2661:G:C6 | 36:BA:2662:A:C2 | 3.09 | 0.40 |
| 36:BA:270:A:H2' | 36:BA:271:A:C5' | 2.51 | 0.40 |
| 36:BA:2627:G:O2' | 36:BA:2781:A:N1 | 2.45 | 0.40 |
| 36:BA:2810:A:C2' | 40:BE:61:ARG:HH21 | 2.34 | 0.40 |
| 36:BA:314:A:H2' | 36:BA:315:G:H8 | 1.85 | 0.40 |
| 36:BA:572:A:H5'' | 54:BV:78:LYS:HZ1 | 1.85 | 0.40 |
| 36:BA:645:C:C3' | 36:BA:645:C:O2 | 2.69 | 0.40 |
| 36:BA:997:G:C2 | 36:BA:1159:U:O2 | 2.75 | 0.40 |
| 39:BD:146:GLU:HG2 | 39:BD:153:ALA:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BD:197:GLY:O | 39:BD:198:ASN:C | 2.59 | 0.40 |
| 39:BD:74:GLY:O | 39:BD:76:PRO:HD3 | 2.22 | 0.40 |
| 40:BE:127:ASP:HA | 40:BE:135:HIS:CD2 | 2.57 | 0.40 |
| 41:BF:192:LEU:HD23 | 41:BF:192:LEU:O | 2.21 | 0.40 |
| 42:BG:47:LYS:NZ | 42:BG:81:LYS:HG3 | 2.37 | 0.40 |
| 43:BH:136:ILE:CD1 | 43:BH:136:ILE:N | 2.84 | 0.40 |
| 43:BH:84:SER:O | 43:BH:85:LYS:HB3 | 2.20 | 0.40 |
| 46:BN:1:MET:C | 46:BN:2:LYS:HD2 | 2.42 | 0.40 |
| 48:BP:22:GLY:HA2 | 48:BP:23:PRO:HD3 | 1.86 | 0.40 |
| 51:BS:54:LEU:HD22 | 51:BS:58:LEU:C | 2.42 | 0.40 |
| 52:BT:129:ARG:HG3 | 52:BT:129:ARG:NH1 | 2.37 | 0.40 |
| 52:BT:29:ARG:HG2 | 52:BT:86:ILE:HG22 | 2.03 | 0.40 |
| 52:BT:79:HIS:O | 52:BT:80:SER:CB | 2.69 | 0.40 |
| 53:BU:97:ASP:O | 53:BU:98:LEU:C | 2.59 | 0.40 |
| 53:BU:90:VAL:HG21 | 54:BV:47:VAL:HG23 | 2.02 | 0.40 |
| 57:BY:50:ARG:HG3 | 57:BY:53:PRO:HA | 2.03 | 0.40 |
| 57:BY:50:ARG:CB | 57:BY:53:PRO:HG3 | 2.47 | 0.40 |
| 57:BY:73:ARG:HA | 57:BY:74:PRO:HD2 | 1.91 | 0.40 |
| 1:AA:1058:G:H2' | 1:AA:1059:C:C6 | 2.57 | 0.40 |
| 1:AA:109:A:C6 | 1:AA:326:G:C5 | 3.09 | 0.40 |
| 1:AA:261:U:OP2 | 20:AT:79:ARG:NH2 | 2.53 | 0.40 |
| 1:AA:49:U:H5 | 1:AA:365:U:O4 | 2.05 | 0.40 |
| 1:AA:495:A:H4' | 1:AA:496:A:O5' | 2.21 | 0.40 |
| 1:AA:828:A:H4' | 1:AA:828:A:OP1 | 2.21 | 0.40 |
| 1:AA:862:C:C2' | 1:AA:863:U:H5' | 2.51 | 0.40 |
| 4:AD:190:ASP:HB3 | 4:AD:193:ASP:OD2 | 2.21 | 0.40 |
| 6:AF:22:GLU:C | 6:AF:24:GLU:H | 2.25 | 0.40 |
| 7:AG:111:ARG:NH1 | 7:AG:113:GLU:OE2 | 2.54 | 0.40 |
| 11:AK:126:ARG:O | 11:AK:127:LYS:C | 2.60 | 0.40 |
| 16:AP:21:VAL:O | 16:AP:21:VAL:HG13 | 2.22 | 0.40 |
| 17:AQ:16:GLN:HB2 | 17:AQ:16:GLN:HE21 | 1.63 | 0.40 |
| 1:AA:1318:A:O2' | 19:AS:10:PHE:HD2 | 2.04 | 0.40 |
| 24:AY:36:A:C4 | 24:AY:37:MIA:C8 | 3.04 | 0.40 |
| 28:B2:17:SER:CB | 28:B2:18:PRO:CD | 2.90 | 0.40 |
| 28:B2:29:LYS:O | 28:B2:32:LEU:HB3 | 2.21 | 0.40 |
| 30:B4:15:ILE:HD13 | 30:B4:21:VAL:HG13 | 2.03 | 0.40 |
| 31:B5:47:PRO:C | 31:B5:49:CYS:N | 2.73 | 0.40 |
| 35:B9:29:ASN:HD21 | 35:B9:32:HIS:CE1 | 2.40 | 0.40 |
| 35:B9:16:VAL:HG11 | 36:BA:1032:A:O3' | 2.21 | 0.40 |
| 36:BA:86:C:H1' | 36:BA:103:A:H2 | 1.86 | 0.40 |
| 36:BA:1204:A:N1 | 36:BA:1241:A:C2 | 2.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BA:1535:A:O5' | 36:BA:1535:A:H8 | 2.03 | 0.40 |
| 36:BA:1542:A:C6 | 36:BA:1544:A:C8 | 3.09 | 0.40 |
| 36:BA:1682:G:H2' | 36:BA:1683:C:H6 | 1.84 | 0.40 |
| 36:BA:1800:C:OP1 | 39:BD:264:LYS:HE2 | 2.22 | 0.40 |
| 36:BA:1996:C:H5 | 47:BO:32:TYR:HH | 1.68 | 0.40 |
| 36:BA:2001:A:H2' | 36:BA:2002:G:C8 | 2.57 | 0.40 |
| 27:B1:35:THR:HG21 | 36:BA:2080:G:OP1 | 2.21 | 0.40 |
| 36:BA:246:C:H5' | 48:BP:71:VAL:HG23 | 2.03 | 0.40 |
| 36:BA:2517:C:O2' | 36:BA:2542:A:C2 | 2.65 | 0.40 |
| 36:BA:1638:C:H5'' | 36:BA:2710:C:O2' | 2.20 | 0.40 |
| 36:BA:271(R):G:O2' | 36:BA:271(S):G:H5' | 2.21 | 0.40 |
| 36:BA:271(X):G:C2 | 36:BA:271(Y):U:O4 | 2.74 | 0.40 |
| 36:BA:2870:C:C2' | 36:BA:2871:C:H5' | 2.51 | 0.40 |
| 36:BA:718:A:H3' | 36:BA:719:C:H6 | 1.86 | 0.40 |
| 36:BA:814:C:O2' | 36:BA:815:C:H5' | 2.21 | 0.40 |
| 36:BA:947:G:H2' | 36:BA:948:G:C8 | 2.57 | 0.40 |
| 38:BC:46:LYS:HD2 | 38:BC:47:LEU:N | 2.37 | 0.40 |
| 38:BC:54:SER:C | 38:BC:56:GLN:H | 2.25 | 0.40 |
| 40:BE:1:MET:O | 40:BE:2:LYS:C | 2.60 | 0.40 |
| 36:BA:321:G:N2 | 41:BF:165:ARG:HE | 2.19 | 0.40 |
| 42:BG:64:THR:HG23 | 42:BG:65:GLY:N | 2.37 | 0.40 |
| 48:BP:123:LEU:HD23 | 48:BP:123:LEU:N | 2.35 | 0.40 |
| 49:BQ:65:PHE:CZ | 58:BZ:118:GLN:OE1 | 2.75 | 0.40 |
| 50:BR:55:ALA:HB2 | 50:BR:79:LEU:HD13 | 2.02 | 0.40 |
| 50:BR:63:ARG:HA | 50:BR:80:PHE:CE2 | 2.56 | 0.40 |
| 47:BO:71:ARG:HH12 | 52:BT:74:ARG:NH2 | 2.19 | 0.40 |
| 52:BT:50:ILE:HA | 52:BT:99:LEU:HD11 | 2.03 | 0.40 |
| 53:BU:13:LYS:HD2 | 53:BU:16:LYS:HZ2 | 1.86 | 0.40 |
| 36:BA:139(A):G:N2 | 56:BX:44:GLU:OE1 | 2.52 | 0.40 |
| 57:BY:27:VAL:CG1 | 57:BY:29:GLU:OE1 | 2.69 | 0.40 |
| 57:BY:74:PRO:O | 57:BY:79:CYS:O | 2.38 | 0.40 |
| 1:AA:272:C:O2' | 1:AA:273:A:H5' | 2.22 | 0.40 |
| 1:AA:342:C:O2' | 1:AA:343:U:H5' | 2.20 | 0.40 |
| 1:AA:355:C:N3 | 1:AA:356:A:N7 | 2.69 | 0.40 |
| 1:AA:518:C:H2' | 1:AA:530:G:N3 | 2.37 | 0.40 |
| 1:AA:636:U:O2' | 1:AA:637:G:H5' | 2.21 | 0.40 |
| 1:AA:956:U:O2 | 1:AA:1225:A:C2 | 2.74 | 0.40 |
| 1:AA:1190:G:OP1 | 3:AC:4:LYS:HA | 2.21 | 0.40 |
| 5:AE:12:LEU:CD2 | 5:AE:12:LEU:C | 2.90 | 0.40 |
| 8:AH:35:ILE:HG23 | 8:AH:111:ILE:HD13 | 2.03 | 0.40 |
| 10:AJ:40:LEU:HG | 10:AJ:69:ASN:HB2 | 2.01 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:27:LYS:HG3 | 13:AM:31:LYS:HE3 | 2.03 | 0.40 |
| 15:AO:82:ILE:CG2 | 15:AO:83:GLU:N | 2.84 | 0.40 |
| 16:AP:6:LEU:HB3 | 16:AP:17:TYR:CD2 | 2.56 | 0.40 |
| 18:AR:50:ILE:CD1 | 18:AR:70:ILE:HG21 | 2.50 | 0.40 |
| 20:AT:30:LYS:NZ | 20:AT:72:LEU:HD21 | 2.36 | 0.40 |
| 20:AT:49:ALA:O | 20:AT:52:ALA:HB3 | 2.21 | 0.40 |
| 22:AV:59:U:O2' | 22:AV:60:U:O5' | 2.39 | 0.40 |
| 25:AZ:216:ASP:C | 25:AZ:216:ASP:OD1 | 2.59 | 0.40 |
| 25:AZ:341:GLN:H | 25:AZ:341:GLN:NE2 | 2.20 | 0.40 |
| 26:B0:10:THR:HG22 | 26:B0:11:ARG:N | 2.37 | 0.40 |
| 26:B0:7:LEU:O | 26:B0:8:GLY:O | 2.40 | 0.40 |
| 32:B6:53:LYS:CD | 32:B6:54:ILE:N | 2.81 | 0.40 |
| 34:B8:54:GLU:O | 34:B8:58:ILE:HG12 | 2.22 | 0.40 |
| 35:B9:1:MET:CA | 35:B9:4:ARG:NH2 | 2.71 | 0.40 |
| 36:BA:1151:G:H2' | 36:BA:1152:C:H6 | 1.83 | 0.40 |
| 36:BA:1578:U:C2' | 36:BA:1579:A:H5'' | 2.51 | 0.40 |
| 36:BA:1708:C:H2' | 36:BA:1709:U:H6 | 1.87 | 0.40 |
| 36:BA:1748:G:H5' | 36:BA:1748:G:H8 | 1.87 | 0.40 |
| 36:BA:1773:A:H2' | 36:BA:1774:C:C5' | 2.50 | 0.40 |
| 36:BA:2176:A:H2 | 38:BC:172:HIS:HE2 | 1.68 | 0.40 |
| 36:BA:2400:G:N2 | 36:BA:2417:C:C2 | 2.90 | 0.40 |
| 36:BA:2839:G:H5'' | 50:BR:46:GLY:HA2 | 2.03 | 0.40 |
| 36:BA:614(A):U:H4' | 36:BA:614(B):G:OP1 | 2.21 | 0.40 |
| 36:BA:607:U:O2 | 36:BA:621:A:N1 | 2.55 | 0.40 |
| 36:BA:673:C:C3' | 36:BA:673:C:C6 | 3.04 | 0.40 |
| 36:BA:714:U:H2' | 36:BA:716:A:OP2 | 2.21 | 0.40 |
| 36:BA:764:A:N1 | 36:BA:1789:A:O2' | 2.48 | 0.40 |
| 38:BC:171:ILE:HG12 | 38:BC:196:LEU:CD2 | 2.51 | 0.40 |
| 36:BA:2203:U:O2' | 39:BD:151:LYS:HG2 | 2.21 | 0.40 |
| 39:BD:226:MET:HB3 | 39:BD:230:ASP:CB | 2.47 | 0.40 |
| 41:BF:47:GLY:O | 41:BF:94:PRO:HA | 2.22 | 0.40 |
| 46:BN:129:PRO:O | 46:BN:130:HIS:CB | 2.69 | 0.40 |
| 46:BN:18:ALA:C | 46:BN:20:GLY:N | 2.73 | 0.40 |
| 47:BO:35:VAL:CG2 | 47:BO:65:THR:HG23 | 2.50 | 0.40 |
| 36:BA:671:C:C5 | 48:BP:42:SER:HA | 2.57 | 0.40 |
| 49:BQ:26:TYR:HA | 49:BQ:137:TYR:CD1 | 2.56 | 0.40 |
| 51:BS:15:ARG:NH1 | 51:BS:15:ARG:CB | 2.80 | 0.40 |
| 51:BS:48:LEU:HD12 | 51:BS:48:LEU:N | 2.36 | 0.40 |
| 51:BS:89:ARG:NH1 | 51:BS:91:PRO:O | 2.55 | 0.40 |
| 52:BT:50:ILE:CD1 | 52:BT:64:ARG:HB2 | 2.50 | 0.40 |
| 54:BV:57:VAL:HG23 | 54:BV:98:GLU:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:BW:70:TYR:O | 55:BW:72:LYS:N | 2.54 | 0.40 |
| 55:BW:84:ARG:HA | 55:BW:84:ARG:HD3 | 1.93 | 0.40 |
| 55:BW:96:ILE:O | 55:BW:96:ILE:CG2 | 2.69 | 0.40 |
| 57:BY:27:VAL:CG1 | 57:BY:28:LYS:N | 2.84 | 0.40 |
| 57:BY:96:ILE:CD1 | 57:BY:99:CYS:HB3 | 2.51 | 0.40 |
| 58:BZ:46:LYS:O | 58:BZ:50:GLN:HG3 | 2.21 | 0.40 |
| 1:AA:1044:A:C5 | 1:AA:1045:C:H1' | 2.57 | 0.40 |
| 1:AA:1191:A:H2' | 1:AA:1192:C:C6 | 2.56 | 0.40 |
| 1:AA:1201:A:H4' | 1:AA:1202:G:C5' | 2.51 | 0.40 |
| 1:AA:1314:C:H2' | 1:AA:1315:U:C6 | 2.56 | 0.40 |
| 1:AA:368:U:C5 | 25:AZ:234:ARG:CZ | 3.05 | 0.40 |
| 1:AA:495:A:O2' | 1:AA:496:A:P | 2.79 | 0.40 |
| 1:AA:621:A:C6 | 1:AA:622:A:C6 | 3.10 | 0.40 |
| 1:AA:787:A:N1 | 1:AA:795:C:N4 | 2.70 | 0.40 |
| 1:AA:982:U:O2' | 1:AA:983:A:OP2 | 2.35 | 0.40 |
| 2:AB:116:GLU:O | 2:AB:118:LEU:N | 2.54 | 0.40 |
| 2:AB:34:ALA:O | 2:AB:41:ILE:HB | 2.21 | 0.40 |
| 3:AC:65:ALA:O | 3:AC:66:VAL:C | 2.59 | 0.40 |
| 4:AD:18:LYS:HA | 4:AD:33:MET:HE3 | 2.04 | 0.40 |
| 5:AE:83:GLU:HG2 | 5:AE:88:LYS:HG3 | 2.02 | 0.40 |
| 7:AG:66:VAL:HG12 | 7:AG:67:GLU:N | 2.36 | 0.40 |
| 1:AA:590:C:OP1 | 8:AH:30:ARG:HB2 | 2.21 | 0.40 |
| 9:AI:28:VAL:O | 9:AI:29:ASN:HB2 | 2.22 | 0.40 |
| 10:AJ:28:ARG:HG2 | 10:AJ:28:ARG:NH1 | 2.36 | 0.40 |
| 10:AJ:74:ILE:HG13 | 10:AJ:74:ILE:O | 2.22 | 0.40 |
| 12:AL:102:ARG:NH1 | 12:AL:102:ARG:CG | 2.81 | 0.40 |
| 13:AM:15:VAL:HG23 | 13:AM:16:ASP:H | 1.84 | 0.40 |
| 14:AN:33:VAL:HA | 14:AN:40:CYS:HA | 2.03 | 0.40 |
| 15:AO:31:LEU:HD12 | 15:AO:31:LEU:HA | 1.92 | 0.40 |
| 16:AP:80:PHE:CD1 | 16:AP:80:PHE:N | 2.89 | 0.40 |
| 19:AS:9:VAL:HG12 | 19:AS:11:VAL:HG12 | 2.04 | 0.40 |
| 21:AU:3:LYS:HD3 | 21:AU:14:TRP:HD1 | 1.85 | 0.40 |
| 25:AZ:117:ARG:HB2 | 25:AZ:117:ARG:NH1 | 2.37 | 0.40 |
| 25:AZ:124:ARG:CD | 25:AZ:161:TYR:O | 2.70 | 0.40 |
| 30:B4:10:VAL:CG2 | 30:B4:11:PRO:CD | 2.96 | 0.40 |
| 32:B6:26:ASN:ND2 | 32:B6:32:ASN:CG | 2.75 | 0.40 |
| 34:B8:4:MET:HE1 | 36:BA:592:G:H21 | 1.86 | 0.40 |
| 36:BA:1342:A:O2' | 36:BA:1344:G:OP2 | 2.34 | 0.40 |
| 36:BA:139:G:N1 | 36:BA:143:G:N1 | 2.70 | 0.40 |
| 36:BA:1339:G:N2 | 36:BA:1603:A:H1' | 2.37 | 0.40 |
| 36:BA:1664:A:H1' | 36:BA:2726:U:C5 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BA:203:C:C3' | 36:BA:204:A:H5'' | 2.45 | 0.40 |
| 36:BA:2206:G:H3' | 36:BA:2206:G:N3 | 2.37 | 0.40 |
| 36:BA:2208:A:H1' | 36:BA:2219:G:N7 | 2.36 | 0.40 |
| 36:BA:2392:A:C2 | 36:BA:2424:C:N4 | 2.87 | 0.40 |
| 36:BA:2531:A:H2' | 36:BA:2532:G:H8 | 1.87 | 0.40 |
| 36:BA:300:A:H2' | 36:BA:334:C:O2' | 2.22 | 0.40 |
| 36:BA:503:A:C6 | 36:BA:506:G:C6 | 3.10 | 0.40 |
| 36:BA:553:G:H2' | 36:BA:554:U:O4' | 2.21 | 0.40 |
| 36:BA:652:C:HO2' | 36:BA:653:A:P | 2.44 | 0.40 |
| 36:BA:903:C:H2' | 36:BA:904:C:C6 | 2.57 | 0.40 |
| 39:BD:257:LEU:CD2 | 39:BD:257:LEU:C | 2.90 | 0.40 |
| 36:BA:2048:G:N2 | 40:BE:113:PHE:CZ | 2.88 | 0.40 |
| 40:BE:132:HIS:CG | 40:BE:135:HIS:HE1 | 2.39 | 0.40 |
| 40:BE:167:VAL:HG12 | 40:BE:189:PRO:CD | 2.52 | 0.40 |
| 40:BE:199:ARG:HB2 | 40:BE:199:ARG:CZ | 2.50 | 0.40 |
| 41:BF:84:VAL:CG1 | 41:BF:85:GLY:N | 2.66 | 0.40 |
| 42:BG:63:ILE:HG22 | 42:BG:143:GLU:HG3 | 2.04 | 0.40 |
| 42:BG:95:ARG:NH1 | 42:BG:95:ARG:HG2 | 2.37 | 0.40 |
| 47:BO:25:LEU:HB2 | 47:BO:38:VAL:O | 2.22 | 0.40 |
| 49:BQ:135:ASP:C | 49:BQ:137:TYR:H | 2.25 | 0.40 |
| 52:BT:1:MET:HG3 | 52:BT:1:MET:O | 2.21 | 0.40 |
| 57:BY:19:LYS:HB2 | 57:BY:20:TYR:CE1 | 2.56 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------------------|--------------------------|-------------------|
| 1:AA:1267:C:O5' | 36:BA:654(I):C:O4'[2_746] | 1.83 | 0.37 |
| 1:AA:1266:G:O3' | 36:BA:654(I):C:O4'[2_746] | 2.16 | 0.04 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 2 | AB | 232/256 (91%) | 163 (70%) | 41 (18%) | 28 (12%) | 0 | 1 |
| 3 | AC | 204/239 (85%) | 155 (76%) | 33 (16%) | 16 (8%) | 1 | 5 |
| 4 | AD | 206/209 (99%) | 157 (76%) | 34 (16%) | 15 (7%) | 1 | 6 |
| 5 | AE | 148/162 (91%) | 125 (84%) | 16 (11%) | 7 (5%) | 2 | 14 |
| 6 | AF | 99/101 (98%) | 81 (82%) | 11 (11%) | 7 (7%) | 1 | 6 |
| 7 | AG | 153/156 (98%) | 118 (77%) | 25 (16%) | 10 (6%) | 1 | 8 |
| 8 | AH | 136/138 (99%) | 118 (87%) | 16 (12%) | 2 (2%) | 10 | 39 |
| 9 | AI | 125/128 (98%) | 83 (66%) | 29 (23%) | 13 (10%) | 0 | 3 |
| 10 | AJ | 96/105 (91%) | 67 (70%) | 17 (18%) | 12 (12%) | 0 | 1 |
| 11 | AK | 117/129 (91%) | 94 (80%) | 19 (16%) | 4 (3%) | 3 | 21 |
| 12 | AL | 122/135 (90%) | 89 (73%) | 20 (16%) | 13 (11%) | 0 | 2 |
| 13 | AM | 122/126 (97%) | 74 (61%) | 27 (22%) | 21 (17%) | 0 | 0 |
| 14 | AN | 58/61 (95%) | 37 (64%) | 11 (19%) | 10 (17%) | 0 | 0 |
| 15 | AO | 86/89 (97%) | 65 (76%) | 17 (20%) | 4 (5%) | 2 | 14 |
| 16 | AP | 81/88 (92%) | 62 (76%) | 14 (17%) | 5 (6%) | 1 | 9 |
| 17 | AQ | 97/105 (92%) | 74 (76%) | 18 (19%) | 5 (5%) | 2 | 12 |
| 18 | AR | 68/88 (77%) | 49 (72%) | 14 (21%) | 5 (7%) | 1 | 6 |
| 19 | AS | 76/93 (82%) | 41 (54%) | 21 (28%) | 14 (18%) | 0 | 0 |
| 20 | AT | 97/106 (92%) | 63 (65%) | 26 (27%) | 8 (8%) | 1 | 5 |
| 21 | AU | 22/27 (82%) | 17 (77%) | 4 (18%) | 1 (4%) | 2 | 15 |
| 25 | AZ | 403/405 (100%) | 285 (71%) | 83 (21%) | 35 (9%) | 1 | 4 |
| 26 | B0 | 82/85 (96%) | 65 (79%) | 12 (15%) | 5 (6%) | 1 | 9 |
| 27 | B1 | 91/98 (93%) | 73 (80%) | 9 (10%) | 9 (10%) | 0 | 3 |
| 28 | B2 | 69/72 (96%) | 46 (67%) | 15 (22%) | 8 (12%) | 0 | 2 |
| 29 | B3 | 57/60 (95%) | 40 (70%) | 9 (16%) | 8 (14%) | 0 | 1 |
| 30 | B4 | 42/71 (59%) | 23 (55%) | 11 (26%) | 8 (19%) | 0 | 0 |
| 31 | B5 | 57/60 (95%) | 42 (74%) | 8 (14%) | 7 (12%) | 0 | 1 |
| 32 | B6 | 48/54 (89%) | 23 (48%) | 12 (25%) | 13 (27%) | 0 | 0 |
| 33 | B7 | 46/49 (94%) | 39 (85%) | 7 (15%) | 0 | 100 | 100 |
| 34 | B8 | 61/65 (94%) | 34 (56%) | 17 (28%) | 10 (16%) | 0 | 0 |
| 35 | B9 | 35/37 (95%) | 21 (60%) | 9 (26%) | 5 (14%) | 0 | 1 |
| 38 | BC | 226/229 (99%) | 161 (71%) | 46 (20%) | 19 (8%) | 1 | 5 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-----------|-------------|----|
| 39 | BD | 273/276 (99%) | 219 (80%) | 28 (10%) | 26 (10%) | 0 | 3 |
| 40 | BE | 202/206 (98%) | 116 (57%) | 53 (26%) | 33 (16%) | 0 | 0 |
| 41 | BF | 205/210 (98%) | 144 (70%) | 35 (17%) | 26 (13%) | 0 | 1 |
| 42 | BG | 179/182 (98%) | 107 (60%) | 47 (26%) | 25 (14%) | 0 | 1 |
| 43 | BH | 157/180 (87%) | 96 (61%) | 42 (27%) | 19 (12%) | 0 | 1 |
| 46 | BN | 136/140 (97%) | 93 (68%) | 21 (15%) | 22 (16%) | 0 | 0 |
| 47 | BO | 120/122 (98%) | 97 (81%) | 16 (13%) | 7 (6%) | 1 | 10 |
| 48 | BP | 144/150 (96%) | 74 (51%) | 36 (25%) | 34 (24%) | 0 | 0 |
| 49 | BQ | 139/141 (99%) | 108 (78%) | 24 (17%) | 7 (5%) | 2 | 13 |
| 50 | BR | 115/118 (98%) | 72 (63%) | 28 (24%) | 15 (13%) | 0 | 1 |
| 51 | BS | 96/112 (86%) | 37 (38%) | 37 (38%) | 22 (23%) | 0 | 0 |
| 52 | BT | 135/146 (92%) | 85 (63%) | 27 (20%) | 23 (17%) | 0 | 0 |
| 53 | BU | 115/118 (98%) | 72 (63%) | 34 (30%) | 9 (8%) | 1 | 5 |
| 54 | BV | 99/101 (98%) | 69 (70%) | 13 (13%) | 17 (17%) | 0 | 0 |
| 55 | BW | 111/113 (98%) | 81 (73%) | 21 (19%) | 9 (8%) | 1 | 5 |
| 56 | BX | 90/96 (94%) | 67 (74%) | 15 (17%) | 8 (9%) | 1 | 4 |
| 57 | BY | 98/110 (89%) | 45 (46%) | 26 (26%) | 27 (28%) | 0 | 0 |
| 58 | BZ | 174/206 (84%) | 108 (62%) | 39 (22%) | 27 (16%) | 0 | 0 |
| All | All | 6150/6553 (94%) | 4274 (70%) | 1193 (19%) | 683 (11%) | 0 | 2 |

All (683) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 191 | ASP |
| 2 | AB | 194 | PRO |
| 2 | AB | 195 | ASP |
| 3 | AC | 146 | ALA |
| 4 | AD | 4 | TYR |
| 4 | AD | 24 | GLU |
| 4 | AD | 30 | LYS |
| 4 | AD | 44 | GLY |
| 4 | AD | 125 | HIS |
| 5 | AE | 64 | ARG |
| 6 | AF | 64 | GLN |
| 7 | AG | 53 | LYS |
| 8 | AH | 109 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AI | 41 | VAL |
| 9 | AI | 58 | ARG |
| 9 | AI | 89 | ASN |
| 10 | AJ | 36 | GLY |
| 10 | AJ | 55 | LYS |
| 10 | AJ | 83 | GLU |
| 10 | AJ | 86 | MET |
| 12 | AL | 18 | VAL |
| 12 | AL | 27 | LEU |
| 12 | AL | 28 | LYS |
| 12 | AL | 47 | LYS |
| 12 | AL | 92 | ASP |
| 12 | AL | 122 | THR |
| 13 | AM | 12 | ASN |
| 13 | AM | 14 | ARG |
| 13 | AM | 53 | VAL |
| 13 | AM | 83 | ASP |
| 13 | AM | 91 | ARG |
| 13 | AM | 117 | VAL |
| 13 | AM | 124 | PRO |
| 14 | AN | 14 | PRO |
| 14 | AN | 15 | LYS |
| 14 | AN | 23 | ARG |
| 14 | AN | 56 | VAL |
| 14 | AN | 59 | ALA |
| 16 | AP | 17 | TYR |
| 16 | AP | 45 | THR |
| 17 | AQ | 27 | PHE |
| 19 | AS | 5 | LEU |
| 19 | AS | 10 | PHE |
| 19 | AS | 28 | LYS |
| 19 | AS | 61 | TYR |
| 19 | AS | 62 | ILE |
| 19 | AS | 80 | TYR |
| 20 | AT | 48 | LYS |
| 25 | AZ | 19 | HIS |
| 25 | AZ | 85 | HIS |
| 25 | AZ | 99 | MET |
| 25 | AZ | 141 | VAL |
| 25 | AZ | 188 | THR |
| 25 | AZ | 194 | GLU |
| 25 | AZ | 213 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | AZ | 220 | PRO |
| 25 | AZ | 276 | THR |
| 25 | AZ | 360 | GLU |
| 25 | AZ | 364 | PRO |
| 25 | AZ | 390 | GLU |
| 25 | AZ | 404 | LEU |
| 26 | B0 | 43 | THR |
| 27 | B1 | 83 | GLU |
| 27 | B1 | 85 | LEU |
| 28 | B2 | 17 | SER |
| 28 | B2 | 18 | PRO |
| 28 | B2 | 47 | ASN |
| 28 | B2 | 48 | HIS |
| 29 | B3 | 3 | ARG |
| 29 | B3 | 13 | ILE |
| 30 | B4 | 26 | SER |
| 31 | B5 | 4 | HIS |
| 31 | B5 | 24 | ALA |
| 31 | B5 | 49 | CYS |
| 32 | B6 | 17 | LYS |
| 32 | B6 | 18 | ARG |
| 32 | B6 | 20 | ASN |
| 32 | B6 | 27 | LYS |
| 32 | B6 | 28 | ARG |
| 32 | B6 | 31 | PRO |
| 32 | B6 | 33 | LYS |
| 32 | B6 | 46 | HIS |
| 32 | B6 | 52 | VAL |
| 34 | B8 | 33 | ASN |
| 34 | B8 | 34 | TRP |
| 34 | B8 | 35 | GLN |
| 34 | B8 | 46 | ARG |
| 35 | B9 | 11 | CYS |
| 35 | B9 | 36 | GLN |
| 38 | BC | 4 | GLY |
| 38 | BC | 78 | ALA |
| 38 | BC | 95 | GLY |
| 38 | BC | 109 | ASP |
| 38 | BC | 111 | ASP |
| 38 | BC | 126 | LYS |
| 38 | BC | 149 | ILE |
| 38 | BC | 217 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BD | 25 | THR |
| 39 | BD | 26 | LYS |
| 39 | BD | 27 | THR |
| 39 | BD | 36 | PRO |
| 39 | BD | 267 | SER |
| 40 | BE | 2 | LYS |
| 40 | BE | 4 | ILE |
| 40 | BE | 33 | VAL |
| 40 | BE | 35 | GLN |
| 40 | BE | 45 | THR |
| 40 | BE | 53 | PRO |
| 40 | BE | 66 | HIS |
| 40 | BE | 88 | GLY |
| 40 | BE | 90 | THR |
| 40 | BE | 178 | GLU |
| 40 | BE | 187 | ALA |
| 41 | BF | 10 | PRO |
| 41 | BF | 11 | VAL |
| 41 | BF | 14 | PRO |
| 41 | BF | 21 | ALA |
| 41 | BF | 84 | VAL |
| 41 | BF | 133 | ASN |
| 42 | BG | 3 | LEU |
| 42 | BG | 28 | VAL |
| 42 | BG | 79 | ASN |
| 42 | BG | 82 | LEU |
| 42 | BG | 84 | LYS |
| 42 | BG | 86 | MET |
| 42 | BG | 96 | ARG |
| 42 | BG | 126 | ASP |
| 42 | BG | 137 | GLU |
| 43 | BH | 41 | MET |
| 43 | BH | 84 | SER |
| 43 | BH | 92 | ILE |
| 43 | BH | 155 | SER |
| 43 | BH | 158 | HIS |
| 43 | BH | 159 | GLU |
| 46 | BN | 7 | LYS |
| 46 | BN | 8 | GLN |
| 46 | BN | 45 | ASN |
| 46 | BN | 46 | VAL |
| 46 | BN | 58 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 46 | BN | 63 | THR |
| 46 | BN | 129 | PRO |
| 46 | BN | 130 | HIS |
| 47 | BO | 48 | PRO |
| 47 | BO | 68 | GLU |
| 48 | BP | 9 | ASN |
| 48 | BP | 17 | LYS |
| 48 | BP | 21 | ARG |
| 48 | BP | 30 | THR |
| 48 | BP | 31 | ALA |
| 48 | BP | 33 | ARG |
| 48 | BP | 36 | LYS |
| 48 | BP | 40 | SER |
| 48 | BP | 47 | ASP |
| 48 | BP | 65 | ARG |
| 48 | BP | 67 | MET |
| 48 | BP | 70 | GLN |
| 48 | BP | 71 | VAL |
| 48 | BP | 103 | ALA |
| 48 | BP | 106 | LEU |
| 48 | BP | 108 | LYS |
| 48 | BP | 111 | ARG |
| 49 | BQ | 135 | ASP |
| 50 | BR | 6 | SER |
| 50 | BR | 8 | ARG |
| 50 | BR | 9 | LYS |
| 50 | BR | 58 | GLY |
| 50 | BR | 117 | VAL |
| 51 | BS | 23 | ARG |
| 51 | BS | 39 | ILE |
| 51 | BS | 62 | LYS |
| 51 | BS | 94 | TYR |
| 51 | BS | 97 | ARG |
| 51 | BS | 98 | VAL |
| 51 | BS | 103 | GLU |
| 51 | BS | 105 | ALA |
| 52 | BT | 24 | PRO |
| 52 | BT | 27 | THR |
| 52 | BT | 28 | VAL |
| 52 | BT | 32 | TYR |
| 52 | BT | 69 | GLY |
| 52 | BT | 80 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | BT | 83 | ILE |
| 52 | BT | 84 | GLN |
| 52 | BT | 88 | ILE |
| 52 | BT | 107 | ASP |
| 52 | BT | 135 | ALA |
| 53 | BU | 91 | ASP |
| 54 | BV | 16 | PRO |
| 54 | BV | 18 | LEU |
| 54 | BV | 24 | LYS |
| 54 | BV | 53 | GLU |
| 54 | BV | 97 | LYS |
| 55 | BW | 65 | LEU |
| 55 | BW | 92 | ARG |
| 56 | BX | 48 | LYS |
| 56 | BX | 87 | GLN |
| 57 | BY | 17 | SER |
| 57 | BY | 26 | LYS |
| 57 | BY | 46 | LYS |
| 57 | BY | 50 | ARG |
| 57 | BY | 53 | PRO |
| 57 | BY | 56 | PRO |
| 57 | BY | 57 | GLN |
| 57 | BY | 64 | GLU |
| 57 | BY | 65 | ALA |
| 57 | BY | 76 | CYS |
| 57 | BY | 77 | PRO |
| 57 | BY | 78 | ALA |
| 57 | BY | 79 | CYS |
| 57 | BY | 81 | LYS |
| 57 | BY | 82 | PRO |
| 58 | BZ | 34 | ASN |
| 58 | BZ | 38 | TYR |
| 58 | BZ | 77 | ASP |
| 58 | BZ | 141 | VAL |
| 58 | BZ | 163 | LEU |
| 58 | BZ | 177 | PRO |
| 2 | AB | 9 | GLU |
| 2 | AB | 14 | GLY |
| 2 | AB | 18 | GLY |
| 2 | AB | 44 | LEU |
| 2 | AB | 75 | LYS |
| 2 | AB | 150 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 153 | ARG |
| 2 | AB | 204 | ASN |
| 2 | AB | 224 | GLN |
| 2 | AB | 234 | PRO |
| 2 | AB | 236 | TYR |
| 3 | AC | 81 | GLY |
| 3 | AC | 160 | ALA |
| 3 | AC | 204 | LEU |
| 4 | AD | 13 | ARG |
| 4 | AD | 92 | VAL |
| 5 | AE | 22 | GLY |
| 5 | AE | 126 | ARG |
| 5 | AE | 153 | LYS |
| 6 | AF | 37 | VAL |
| 6 | AF | 54 | LYS |
| 7 | AG | 147 | ALA |
| 9 | AI | 12 | GLU |
| 9 | AI | 70 | LYS |
| 9 | AI | 94 | ALA |
| 9 | AI | 119 | ALA |
| 10 | AJ | 30 | SER |
| 10 | AJ | 59 | SER |
| 10 | AJ | 84 | GLN |
| 11 | AK | 127 | LYS |
| 12 | AL | 72 | GLY |
| 12 | AL | 87 | GLY |
| 13 | AM | 5 | ALA |
| 13 | AM | 33 | ALA |
| 13 | AM | 60 | VAL |
| 13 | AM | 114 | ARG |
| 13 | AM | 120 | LYS |
| 14 | AN | 16 | PHE |
| 14 | AN | 20 | ALA |
| 15 | AO | 71 | GLN |
| 16 | AP | 28 | ARG |
| 16 | AP | 43 | LYS |
| 16 | AP | 49 | LEU |
| 17 | AQ | 78 | GLU |
| 17 | AQ | 82 | MET |
| 18 | AR | 32 | ARG |
| 18 | AR | 47 | THR |
| 19 | AS | 9 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AS | 14 | HIS |
| 19 | AS | 17 | GLU |
| 19 | AS | 25 | LYS |
| 19 | AS | 30 | LEU |
| 20 | AT | 98 | PRO |
| 25 | AZ | 67 | HIS |
| 25 | AZ | 139 | ASP |
| 25 | AZ | 209 | TYR |
| 25 | AZ | 211 | PRO |
| 25 | AZ | 212 | THR |
| 25 | AZ | 260 | PRO |
| 26 | B0 | 8 | GLY |
| 26 | B0 | 42 | GLY |
| 29 | B3 | 30 | ARG |
| 29 | B3 | 57 | GLU |
| 30 | B4 | 8 | LYS |
| 30 | B4 | 43 | TYR |
| 31 | B5 | 35 | GLU |
| 31 | B5 | 48 | GLU |
| 31 | B5 | 55 | ARG |
| 32 | B6 | 16 | CYS |
| 32 | B6 | 34 | LEU |
| 34 | B8 | 31 | HIS |
| 34 | B8 | 50 | LEU |
| 34 | B8 | 61 | LEU |
| 35 | B9 | 10 | ILE |
| 35 | B9 | 33 | LYS |
| 38 | BC | 45 | ALA |
| 38 | BC | 59 | ARG |
| 38 | BC | 105 | ASP |
| 38 | BC | 202 | GLU |
| 38 | BC | 221 | SER |
| 39 | BD | 3 | VAL |
| 39 | BD | 41 | GLY |
| 39 | BD | 42 | GLY |
| 39 | BD | 127 | VAL |
| 39 | BD | 225 | ALA |
| 40 | BE | 69 | LYS |
| 40 | BE | 77 | ILE |
| 40 | BE | 82 | ARG |
| 40 | BE | 83 | ASP |
| 40 | BE | 117 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 41 | BF | 91 | GLY |
| 41 | BF | 134 | GLY |
| 42 | BG | 43 | LEU |
| 42 | BG | 87 | PRO |
| 42 | BG | 110 | ALA |
| 42 | BG | 129 | GLY |
| 42 | BG | 138 | GLN |
| 43 | BH | 45 | VAL |
| 43 | BH | 52 | VAL |
| 43 | BH | 160 | LYS |
| 46 | BN | 64 | GLY |
| 46 | BN | 76 | SER |
| 46 | BN | 102 | ALA |
| 46 | BN | 133 | GLN |
| 47 | BO | 5 | GLN |
| 47 | BO | 49 | ARG |
| 48 | BP | 11 | GLY |
| 48 | BP | 20 | GLY |
| 48 | BP | 32 | THR |
| 48 | BP | 39 | LYS |
| 48 | BP | 104 | GLY |
| 48 | BP | 110 | TYR |
| 49 | BQ | 2 | LEU |
| 49 | BQ | 21 | THR |
| 49 | BQ | 88 | GLY |
| 50 | BR | 4 | LEU |
| 50 | BR | 14 | SER |
| 50 | BR | 70 | LEU |
| 50 | BR | 82 | GLU |
| 50 | BR | 93 | GLY |
| 50 | BR | 103 | ARG |
| 50 | BR | 107 | ASP |
| 51 | BS | 14 | VAL |
| 51 | BS | 24 | LEU |
| 51 | BS | 50 | SER |
| 51 | BS | 90 | GLY |
| 51 | BS | 102 | ALA |
| 52 | BT | 4 | GLY |
| 52 | BT | 33 | LYS |
| 52 | BT | 41 | ARG |
| 52 | BT | 129 | ARG |
| 53 | BU | 46 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 53 | BU | 58 | ARG |
| 53 | BU | 83 | LEU |
| 53 | BU | 90 | VAL |
| 53 | BU | 93 | LYS |
| 53 | BU | 102 | GLU |
| 54 | BV | 19 | LYS |
| 54 | BV | 40 | LEU |
| 54 | BV | 50 | PRO |
| 55 | BW | 11 | ARG |
| 55 | BW | 22 | ASP |
| 55 | BW | 63 | ASP |
| 55 | BW | 71 | VAL |
| 56 | BX | 19 | ALA |
| 56 | BX | 62 | LYS |
| 56 | BX | 93 | GLU |
| 57 | BY | 3 | VAL |
| 57 | BY | 7 | VAL |
| 57 | BY | 38 | ILE |
| 57 | BY | 39 | VAL |
| 57 | BY | 51 | VAL |
| 58 | BZ | 31 | ARG |
| 58 | BZ | 80 | ARG |
| 58 | BZ | 113 | ALA |
| 58 | BZ | 140 | ASP |
| 58 | BZ | 142 | SER |
| 58 | BZ | 147 | GLY |
| 58 | BZ | 150 | LEU |
| 58 | BZ | 152 | ALA |
| 2 | AB | 19 | HIS |
| 2 | AB | 130 | ARG |
| 2 | AB | 139 | LYS |
| 2 | AB | 190 | THR |
| 2 | AB | 225 | ALA |
| 2 | AB | 235 | SER |
| 2 | AB | 238 | LEU |
| 3 | AC | 4 | LYS |
| 3 | AC | 15 | THR |
| 3 | AC | 66 | VAL |
| 3 | AC | 129 | ALA |
| 3 | AC | 181 | ASN |
| 4 | AD | 3 | ARG |
| 4 | AD | 14 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AD | 159 | ARG |
| 4 | AD | 172 | PRO |
| 5 | AE | 125 | SER |
| 6 | AF | 16 | GLN |
| 6 | AF | 23 | LYS |
| 7 | AG | 80 | VAL |
| 7 | AG | 100 | ALA |
| 8 | AH | 2 | LEU |
| 9 | AI | 44 | VAL |
| 9 | AI | 54 | ASP |
| 9 | AI | 82 | ALA |
| 9 | AI | 95 | LYS |
| 10 | AJ | 21 | GLN |
| 10 | AJ | 27 | ALA |
| 10 | AJ | 88 | LEU |
| 11 | AK | 50 | TYR |
| 11 | AK | 123 | LYS |
| 12 | AL | 29 | GLY |
| 12 | AL | 91 | LYS |
| 12 | AL | 115 | LYS |
| 13 | AM | 43 | THR |
| 13 | AM | 75 | ALA |
| 14 | AN | 22 | THR |
| 15 | AO | 25 | THR |
| 17 | AQ | 68 | ARG |
| 18 | AR | 45 | SER |
| 19 | AS | 72 | GLY |
| 20 | AT | 25 | ARG |
| 20 | AT | 49 | ALA |
| 25 | AZ | 40 | PRO |
| 25 | AZ | 43 | GLU |
| 25 | AZ | 66 | ALA |
| 25 | AZ | 97 | ALA |
| 25 | AZ | 130 | TYR |
| 25 | AZ | 142 | ASP |
| 25 | AZ | 186 | PRO |
| 25 | AZ | 332 | THR |
| 25 | AZ | 366 | ASP |
| 26 | B0 | 75 | LEU |
| 28 | B2 | 26 | ARG |
| 28 | B2 | 68 | ARG |
| 29 | B3 | 51 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | B4 | 9 | LEU |
| 30 | B4 | 20 | ASN |
| 31 | B5 | 57 | VAL |
| 34 | B8 | 37 | SER |
| 38 | BC | 68 | LEU |
| 39 | BD | 87 | ASN |
| 39 | BD | 196 | VAL |
| 39 | BD | 215 | LEU |
| 39 | BD | 273 | ARG |
| 40 | BE | 46 | ALA |
| 40 | BE | 56 | PRO |
| 40 | BE | 60 | ASN |
| 40 | BE | 71 | GLY |
| 41 | BF | 3 | GLU |
| 41 | BF | 24 | LEU |
| 41 | BF | 43 | LYS |
| 41 | BF | 58 | ALA |
| 41 | BF | 62 | ARG |
| 41 | BF | 98 | SER |
| 41 | BF | 171 | PRO |
| 42 | BG | 97 | ASP |
| 42 | BG | 112 | PRO |
| 42 | BG | 115 | ARG |
| 42 | BG | 127 | GLY |
| 42 | BG | 144 | ILE |
| 43 | BH | 69 | ARG |
| 43 | BH | 77 | LYS |
| 43 | BH | 151 | ILE |
| 46 | BN | 44 | PRO |
| 46 | BN | 59 | LYS |
| 46 | BN | 68 | GLU |
| 48 | BP | 6 | LEU |
| 48 | BP | 23 | PRO |
| 48 | BP | 25 | SER |
| 48 | BP | 34 | GLY |
| 48 | BP | 46 | LYS |
| 49 | BQ | 28 | ALA |
| 50 | BR | 45 | ARG |
| 51 | BS | 13 | ARG |
| 51 | BS | 55 | ALA |
| 51 | BS | 57 | LYS |
| 52 | BT | 45 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | BU | 60 | LEU |
| 54 | BV | 27 | ALA |
| 54 | BV | 36 | PRO |
| 54 | BV | 46 | VAL |
| 54 | BV | 48 | GLY |
| 57 | BY | 91 | GLU |
| 57 | BY | 99 | CYS |
| 58 | BZ | 63 | ASP |
| 58 | BZ | 78 | LYS |
| 58 | BZ | 151 | HIS |
| 58 | BZ | 166 | SER |
| 2 | AB | 78 | GLN |
| 2 | AB | 83 | MET |
| 3 | AC | 51 | GLY |
| 3 | AC | 206 | GLU |
| 4 | AD | 118 | ARG |
| 7 | AG | 8 | GLU |
| 7 | AG | 19 | GLY |
| 7 | AG | 52 | GLU |
| 9 | AI | 83 | ARG |
| 10 | AJ | 90 | LEU |
| 11 | AK | 48 | ILE |
| 13 | AM | 10 | PRO |
| 13 | AM | 42 | ALA |
| 14 | AN | 24 | CYS |
| 15 | AO | 70 | LEU |
| 19 | AS | 6 | LYS |
| 20 | AT | 71 | THR |
| 20 | AT | 74 | LYS |
| 20 | AT | 82 | SER |
| 20 | AT | 99 | LEU |
| 21 | AU | 24 | ARG |
| 25 | AZ | 38 | GLU |
| 25 | AZ | 367 | ASN |
| 26 | B0 | 64 | ASP |
| 27 | B1 | 52 | ARG |
| 27 | B1 | 53 | VAL |
| 27 | B1 | 91 | LYS |
| 27 | B1 | 94 | LEU |
| 28 | B2 | 70 | GLN |
| 30 | B4 | 28 | LYS |
| 32 | B6 | 23 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | B6 | 44 | ARG |
| 34 | B8 | 49 | VAL |
| 35 | B9 | 13 | LYS |
| 38 | BC | 97 | GLU |
| 39 | BD | 156 | ALA |
| 39 | BD | 211 | ARG |
| 39 | BD | 242 | ARG |
| 39 | BD | 244 | ARG |
| 40 | BE | 52 | LEU |
| 40 | BE | 54 | GLN |
| 40 | BE | 129 | HIS |
| 40 | BE | 185 | LYS |
| 41 | BF | 25 | PRO |
| 41 | BF | 164 | ARG |
| 41 | BF | 172 | TRP |
| 42 | BG | 143 | GLU |
| 46 | BN | 5 | VAL |
| 46 | BN | 40 | PRO |
| 46 | BN | 47 | ALA |
| 46 | BN | 57 | ALA |
| 47 | BO | 18 | LYS |
| 48 | BP | 12 | ALA |
| 48 | BP | 35 | HIS |
| 48 | BP | 132 | LYS |
| 50 | BR | 11 | ASN |
| 51 | BS | 18 | ILE |
| 51 | BS | 79 | ALA |
| 51 | BS | 88 | ASP |
| 52 | BT | 38 | ASN |
| 52 | BT | 39 | ARG |
| 52 | BT | 68 | TYR |
| 52 | BT | 91 | ARG |
| 55 | BW | 6 | ILE |
| 55 | BW | 35 | ILE |
| 56 | BX | 14 | SER |
| 56 | BX | 24 | GLY |
| 58 | BZ | 14 | LYS |
| 58 | BZ | 22 | GLY |
| 58 | BZ | 41 | LEU |
| 2 | AB | 216 | SER |
| 3 | AC | 12 | LEU |
| 3 | AC | 55 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AD | 5 | ILE |
| 4 | AD | 102 | ASP |
| 5 | AE | 8 | GLU |
| 6 | AF | 51 | PRO |
| 9 | AI | 101 | PHE |
| 12 | AL | 94 | PRO |
| 13 | AM | 3 | ARG |
| 14 | AN | 60 | SER |
| 17 | AQ | 14 | LYS |
| 19 | AS | 63 | THR |
| 25 | AZ | 117 | ARG |
| 25 | AZ | 310 | ILE |
| 25 | AZ | 345 | ARG |
| 27 | B1 | 66 | HIS |
| 27 | B1 | 81 | LYS |
| 28 | B2 | 58 | ALA |
| 29 | B3 | 32 | GLN |
| 30 | B4 | 10 | VAL |
| 38 | BC | 164 | ARG |
| 39 | BD | 9 | TYR |
| 39 | BD | 12 | SER |
| 39 | BD | 246 | PRO |
| 40 | BE | 29 | GLY |
| 40 | BE | 58 | ARG |
| 40 | BE | 72 | VAL |
| 41 | BF | 54 | ARG |
| 41 | BF | 82 | ILE |
| 41 | BF | 83 | PHE |
| 41 | BF | 96 | ASP |
| 41 | BF | 168 | ARG |
| 42 | BG | 19 | LEU |
| 42 | BG | 42 | GLY |
| 42 | BG | 74 | LYS |
| 43 | BH | 20 | ALA |
| 43 | BH | 76 | VAL |
| 47 | BO | 91 | LEU |
| 48 | BP | 10 | PRO |
| 48 | BP | 141 | ALA |
| 49 | BQ | 137 | TYR |
| 50 | BR | 60 | LEU |
| 51 | BS | 61 | ASN |
| 51 | BS | 107 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | BT | 26 | ASP |
| 52 | BT | 132 | LYS |
| 53 | BU | 92 | ARG |
| 54 | BV | 23 | GLU |
| 54 | BV | 79 | VAL |
| 55 | BW | 57 | ASN |
| 56 | BX | 4 | ALA |
| 57 | BY | 42 | VAL |
| 58 | BZ | 143 | GLY |
| 2 | AB | 15 | VAL |
| 2 | AB | 26 | PRO |
| 3 | AC | 154 | SER |
| 4 | AD | 23 | GLY |
| 5 | AE | 70 | PRO |
| 6 | AF | 40 | VAL |
| 7 | AG | 79 | ARG |
| 7 | AG | 81 | GLY |
| 13 | AM | 6 | GLY |
| 18 | AR | 41 | LYS |
| 18 | AR | 56 | THR |
| 25 | AZ | 245 | GLY |
| 39 | BD | 44 | ASN |
| 39 | BD | 245 | PRO |
| 39 | BD | 268 | ARG |
| 40 | BE | 43 | GLY |
| 40 | BE | 44 | TYR |
| 40 | BE | 55 | ASN |
| 40 | BE | 189 | PRO |
| 41 | BF | 7 | TYR |
| 41 | BF | 132 | VAL |
| 43 | BH | 15 | VAL |
| 43 | BH | 85 | LYS |
| 47 | BO | 35 | VAL |
| 52 | BT | 93 | ARG |
| 57 | BY | 37 | VAL |
| 57 | BY | 96 | ILE |
| 58 | BZ | 139 | VAL |
| 10 | AJ | 77 | PRO |
| 12 | AL | 71 | PRO |
| 30 | B4 | 19 | GLY |
| 38 | BC | 51 | PRO |
| 38 | BC | 224 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | BE | 197 | ILE |
| 41 | BF | 159 | GLY |
| 43 | BH | 21 | PRO |
| 46 | BN | 108 | PRO |
| 46 | BN | 135 | PRO |
| 54 | BV | 47 | VAL |
| 58 | BZ | 12 | GLY |
| 58 | BZ | 37 | VAL |
| 58 | BZ | 53 | ILE |
| 3 | AC | 77 | ILE |
| 13 | AM | 4 | ILE |
| 13 | AM | 7 | VAL |
| 13 | AM | 74 | VAL |
| 25 | AZ | 164 | PRO |
| 29 | B3 | 2 | PRO |
| 29 | B3 | 16 | PRO |
| 34 | B8 | 58 | ILE |
| 39 | BD | 24 | ILE |
| 42 | BG | 114 | ILE |
| 43 | BH | 55 | PRO |
| 46 | BN | 110 | GLY |
| 49 | BQ | 15 | GLY |
| 51 | BS | 85 | VAL |
| 54 | BV | 67 | GLY |
| 57 | BY | 31 | LEU |
| 57 | BY | 66 | PRO |
| 2 | AB | 93 | VAL |
| 3 | AC | 153 | VAL |
| 38 | BC | 161 | ILE |
| 39 | BD | 74 | GLY |
| 43 | BH | 43 | VAL |
| 54 | BV | 51 | VAL |
| 2 | AB | 227 | GLY |
| 15 | AO | 87 | ILE |
| 27 | B1 | 30 | VAL |
| 40 | BE | 73 | GLU |
| 48 | BP | 146 | VAL |
| 7 | AG | 88 | PRO |
| 42 | BG | 111 | LEU |
| 58 | BZ | 146 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AB | 202/220 (92%) | 171 (85%) | 31 (15%) | 2 | 12 |
| 3 | AC | 160/188 (85%) | 139 (87%) | 21 (13%) | 4 | 17 |
| 4 | AD | 180/181 (99%) | 159 (88%) | 21 (12%) | 5 | 22 |
| 5 | AE | 115/123 (94%) | 96 (84%) | 19 (16%) | 2 | 10 |
| 6 | AF | 90/90 (100%) | 79 (88%) | 11 (12%) | 5 | 19 |
| 7 | AG | 126/127 (99%) | 118 (94%) | 8 (6%) | 18 | 48 |
| 8 | AH | 119/119 (100%) | 104 (87%) | 15 (13%) | 4 | 18 |
| 9 | AI | 98/99 (99%) | 85 (87%) | 13 (13%) | 4 | 16 |
| 10 | AJ | 88/92 (96%) | 75 (85%) | 13 (15%) | 3 | 13 |
| 11 | AK | 90/99 (91%) | 80 (89%) | 10 (11%) | 6 | 24 |
| 12 | AL | 104/111 (94%) | 88 (85%) | 16 (15%) | 2 | 11 |
| 13 | AM | 99/101 (98%) | 85 (86%) | 14 (14%) | 3 | 15 |
| 14 | AN | 49/50 (98%) | 39 (80%) | 10 (20%) | 1 | 5 |
| 15 | AO | 79/80 (99%) | 73 (92%) | 6 (8%) | 13 | 41 |
| 16 | AP | 72/74 (97%) | 64 (89%) | 8 (11%) | 6 | 24 |
| 17 | AQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 42 |
| 18 | AR | 61/77 (79%) | 55 (90%) | 6 (10%) | 8 | 29 |
| 19 | AS | 69/80 (86%) | 54 (78%) | 15 (22%) | 1 | 4 |
| 20 | AT | 76/82 (93%) | 66 (87%) | 10 (13%) | 4 | 17 |
| 21 | AU | 19/22 (86%) | 18 (95%) | 1 (5%) | 22 | 54 |
| 25 | AZ | 339/339 (100%) | 289 (85%) | 50 (15%) | 3 | 13 |
| 26 | B0 | 66/67 (98%) | 55 (83%) | 11 (17%) | 2 | 9 |
| 27 | B1 | 78/83 (94%) | 65 (83%) | 13 (17%) | 2 | 9 |
| 28 | B2 | 66/67 (98%) | 61 (92%) | 5 (8%) | 13 | 41 |
| 29 | B3 | 51/52 (98%) | 48 (94%) | 3 (6%) | 19 | 50 |
| 30 | B4 | 39/63 (62%) | 30 (77%) | 9 (23%) | 1 | 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 31 | B5 | 51/52 (98%) | 46 (90%) | 5 (10%) | 8 | 29 |
| 32 | B6 | 49/52 (94%) | 39 (80%) | 10 (20%) | 1 | 5 |
| 33 | B7 | 41/42 (98%) | 35 (85%) | 6 (15%) | 3 | 13 |
| 34 | B8 | 53/55 (96%) | 43 (81%) | 10 (19%) | 1 | 6 |
| 35 | B9 | 34/34 (100%) | 27 (79%) | 7 (21%) | 1 | 5 |
| 38 | BC | 180/181 (99%) | 159 (88%) | 21 (12%) | 5 | 22 |
| 39 | BD | 217/218 (100%) | 175 (81%) | 42 (19%) | 1 | 6 |
| 40 | BE | 165/166 (99%) | 142 (86%) | 23 (14%) | 3 | 15 |
| 41 | BF | 165/166 (99%) | 149 (90%) | 16 (10%) | 8 | 30 |
| 42 | BG | 155/156 (99%) | 132 (85%) | 23 (15%) | 3 | 13 |
| 43 | BH | 132/148 (89%) | 124 (94%) | 8 (6%) | 18 | 49 |
| 46 | BN | 117/119 (98%) | 102 (87%) | 15 (13%) | 4 | 18 |
| 47 | BO | 100/100 (100%) | 92 (92%) | 8 (8%) | 12 | 40 |
| 48 | BP | 112/116 (97%) | 87 (78%) | 25 (22%) | 1 | 3 |
| 49 | BQ | 111/111 (100%) | 97 (87%) | 14 (13%) | 4 | 18 |
| 50 | BR | 100/101 (99%) | 81 (81%) | 19 (19%) | 1 | 6 |
| 51 | BS | 77/88 (88%) | 66 (86%) | 11 (14%) | 3 | 14 |
| 52 | BT | 120/127 (94%) | 96 (80%) | 24 (20%) | 1 | 5 |
| 53 | BU | 92/94 (98%) | 81 (88%) | 11 (12%) | 5 | 20 |
| 54 | BV | 82/82 (100%) | 72 (88%) | 10 (12%) | 5 | 19 |
| 55 | BW | 91/92 (99%) | 80 (88%) | 11 (12%) | 5 | 20 |
| 56 | BX | 74/78 (95%) | 68 (92%) | 6 (8%) | 11 | 39 |
| 57 | BY | 84/91 (92%) | 71 (84%) | 13 (16%) | 2 | 11 |
| 58 | BZ | 155/179 (87%) | 129 (83%) | 26 (17%) | 2 | 9 |
| All | All | 5186/5431 (96%) | 4476 (86%) | 710 (14%) | 3 | 16 |

All (710) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 16 | HIS |
| 2 | AB | 17 | PHE |
| 2 | AB | 24 | TRP |
| 2 | AB | 26 | PRO |
| 2 | AB | 36 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 69 | LEU |
| 2 | AB | 79 | ASP |
| 2 | AB | 83 | MET |
| 2 | AB | 93 | VAL |
| 2 | AB | 106 | LYS |
| 2 | AB | 116 | GLU |
| 2 | AB | 130 | ARG |
| 2 | AB | 137 | ARG |
| 2 | AB | 140 | HIS |
| 2 | AB | 145 | LEU |
| 2 | AB | 146 | GLN |
| 2 | AB | 162 | ILE |
| 2 | AB | 178 | ARG |
| 2 | AB | 187 | LEU |
| 2 | AB | 189 | ASP |
| 2 | AB | 193 | ASP |
| 2 | AB | 196 | LEU |
| 2 | AB | 200 | ILE |
| 2 | AB | 204 | ASN |
| 2 | AB | 213 | LEU |
| 2 | AB | 217 | ARG |
| 2 | AB | 221 | LEU |
| 2 | AB | 222 | ILE |
| 2 | AB | 226 | ARG |
| 2 | AB | 236 | TYR |
| 2 | AB | 238 | LEU |
| 3 | AC | 5 | ILE |
| 3 | AC | 14 | ILE |
| 3 | AC | 16 | ARG |
| 3 | AC | 21 | ARG |
| 3 | AC | 26 | LYS |
| 3 | AC | 37 | GLN |
| 3 | AC | 38 | ARG |
| 3 | AC | 59 | ARG |
| 3 | AC | 62 | ASP |
| 3 | AC | 82 | GLU |
| 3 | AC | 85 | ARG |
| 3 | AC | 94 | LEU |
| 3 | AC | 107 | GLN |
| 3 | AC | 154 | SER |
| 3 | AC | 165 | THR |
| 3 | AC | 167 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 178 | LEU |
| 3 | AC | 179 | ARG |
| 3 | AC | 188 | LEU |
| 3 | AC | 191 | THR |
| 3 | AC | 192 | THR |
| 4 | AD | 3 | ARG |
| 4 | AD | 8 | VAL |
| 4 | AD | 10 | ARG |
| 4 | AD | 15 | GLU |
| 4 | AD | 19 | LEU |
| 4 | AD | 25 | ARG |
| 4 | AD | 49 | ARG |
| 4 | AD | 50 | ARG |
| 4 | AD | 78 | LEU |
| 4 | AD | 108 | LEU |
| 4 | AD | 122 | ARG |
| 4 | AD | 131 | ARG |
| 4 | AD | 132 | ARG |
| 4 | AD | 135 | LEU |
| 4 | AD | 150 | GLU |
| 4 | AD | 162 | LEU |
| 4 | AD | 181 | MET |
| 4 | AD | 190 | ASP |
| 4 | AD | 198 | VAL |
| 4 | AD | 201 | GLN |
| 4 | AD | 209 | ARG |
| 5 | AE | 10 | MET |
| 5 | AE | 12 | LEU |
| 5 | AE | 13 | ILE |
| 5 | AE | 20 | GLN |
| 5 | AE | 31 | LEU |
| 5 | AE | 40 | ARG |
| 5 | AE | 41 | VAL |
| 5 | AE | 52 | PRO |
| 5 | AE | 53 | LEU |
| 5 | AE | 73 | ASN |
| 5 | AE | 75 | THR |
| 5 | AE | 76 | ILE |
| 5 | AE | 79 | GLU |
| 5 | AE | 80 | ILE |
| 5 | AE | 91 | LEU |
| 5 | AE | 107 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 128 | PRO |
| 5 | AE | 140 | ARG |
| 5 | AE | 147 | ASP |
| 6 | AF | 14 | LEU |
| 6 | AF | 21 | LEU |
| 6 | AF | 25 | ILE |
| 6 | AF | 43 | LEU |
| 6 | AF | 47 | ARG |
| 6 | AF | 55 | ASP |
| 6 | AF | 57 | GLN |
| 6 | AF | 61 | LEU |
| 6 | AF | 69 | GLU |
| 6 | AF | 83 | ASP |
| 6 | AF | 98 | LEU |
| 7 | AG | 66 | VAL |
| 7 | AG | 78 | ARG |
| 7 | AG | 89 | MET |
| 7 | AG | 104 | LEU |
| 7 | AG | 113 | GLU |
| 7 | AG | 114 | ARG |
| 7 | AG | 124 | LEU |
| 7 | AG | 156 | TRP |
| 8 | AH | 1 | MET |
| 8 | AH | 2 | LEU |
| 8 | AH | 18 | ARG |
| 8 | AH | 22 | GLU |
| 8 | AH | 26 | VAL |
| 8 | AH | 27 | PRO |
| 8 | AH | 29 | SER |
| 8 | AH | 30 | ARG |
| 8 | AH | 39 | LEU |
| 8 | AH | 52 | ASP |
| 8 | AH | 91 | ARG |
| 8 | AH | 102 | ARG |
| 8 | AH | 104 | ARG |
| 8 | AH | 109 | ILE |
| 8 | AH | 127 | LEU |
| 9 | AI | 3 | GLN |
| 9 | AI | 10 | ARG |
| 9 | AI | 53 | VAL |
| 9 | AI | 85 | LEU |
| 9 | AI | 93 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AI | 95 | LYS |
| 9 | AI | 102 | LEU |
| 9 | AI | 104 | ARG |
| 9 | AI | 105 | ASP |
| 9 | AI | 112 | LYS |
| 9 | AI | 114 | TYR |
| 9 | AI | 121 | ARG |
| 9 | AI | 128 | ARG |
| 10 | AJ | 17 | ASP |
| 10 | AJ | 40 | LEU |
| 10 | AJ | 49 | VAL |
| 10 | AJ | 50 | ILE |
| 10 | AJ | 54 | PHE |
| 10 | AJ | 55 | LYS |
| 10 | AJ | 57 | LYS |
| 10 | AJ | 59 | SER |
| 10 | AJ | 67 | THR |
| 10 | AJ | 73 | ASP |
| 10 | AJ | 78 | ASN |
| 10 | AJ | 83 | GLU |
| 10 | AJ | 96 | ILE |
| 11 | AK | 29 | ILE |
| 11 | AK | 31 | THR |
| 11 | AK | 51 | LYS |
| 11 | AK | 57 | THR |
| 11 | AK | 62 | GLN |
| 11 | AK | 93 | GLN |
| 11 | AK | 104 | GLN |
| 11 | AK | 114 | VAL |
| 11 | AK | 117 | ASN |
| 11 | AK | 126 | ARG |
| 12 | AL | 7 | ILE |
| 12 | AL | 20 | LYS |
| 12 | AL | 27 | LEU |
| 12 | AL | 33 | ARG |
| 12 | AL | 36 | VAL |
| 12 | AL | 47 | LYS |
| 12 | AL | 48 | PRO |
| 12 | AL | 50 | SER |
| 12 | AL | 53 | ARG |
| 12 | AL | 64 | TYR |
| 12 | AL | 83 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | AL | 84 | LEU |
| 12 | AL | 85 | ILE |
| 12 | AL | 89 | ARG |
| 12 | AL | 102 | ARG |
| 12 | AL | 122 | THR |
| 13 | AM | 12 | ASN |
| 13 | AM | 23 | TYR |
| 13 | AM | 36 | LYS |
| 13 | AM | 47 | ASP |
| 13 | AM | 64 | TRP |
| 13 | AM | 66 | LEU |
| 13 | AM | 67 | GLU |
| 13 | AM | 73 | GLU |
| 13 | AM | 82 | MET |
| 13 | AM | 93 | ARG |
| 13 | AM | 101 | GLN |
| 13 | AM | 108 | ARG |
| 13 | AM | 115 | LYS |
| 13 | AM | 120 | LYS |
| 14 | AN | 4 | LYS |
| 14 | AN | 14 | PRO |
| 14 | AN | 16 | PHE |
| 14 | AN | 17 | LYS |
| 14 | AN | 18 | VAL |
| 14 | AN | 23 | ARG |
| 14 | AN | 29 | ARG |
| 14 | AN | 41 | ARG |
| 14 | AN | 45 | ARG |
| 14 | AN | 57 | ARG |
| 15 | AO | 10 | LYS |
| 15 | AO | 24 | SER |
| 15 | AO | 38 | ARG |
| 15 | AO | 66 | LEU |
| 15 | AO | 81 | LEU |
| 15 | AO | 82 | ILE |
| 16 | AP | 1 | MET |
| 16 | AP | 2 | VAL |
| 16 | AP | 16 | HIS |
| 16 | AP | 22 | THR |
| 16 | AP | 27 | LYS |
| 16 | AP | 44 | THR |
| 16 | AP | 62 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | AP | 69 | THR |
| 17 | AQ | 25 | ARG |
| 17 | AQ | 36 | ILE |
| 17 | AQ | 49 | GLU |
| 17 | AQ | 52 | LYS |
| 17 | AQ | 64 | PRO |
| 17 | AQ | 74 | LEU |
| 17 | AQ | 87 | LYS |
| 18 | AR | 29 | PHE |
| 18 | AR | 31 | LEU |
| 18 | AR | 36 | ASN |
| 18 | AR | 38 | GLU |
| 18 | AR | 44 | LEU |
| 18 | AR | 84 | LYS |
| 19 | AS | 5 | LEU |
| 19 | AS | 6 | LYS |
| 19 | AS | 7 | LYS |
| 19 | AS | 10 | PHE |
| 19 | AS | 15 | LEU |
| 19 | AS | 27 | GLU |
| 19 | AS | 29 | ARG |
| 19 | AS | 37 | ARG |
| 19 | AS | 40 | ILE |
| 19 | AS | 41 | VAL |
| 19 | AS | 42 | PRO |
| 19 | AS | 44 | MET |
| 19 | AS | 49 | ILE |
| 19 | AS | 65 | ASN |
| 19 | AS | 77 | THR |
| 20 | AT | 13 | LEU |
| 20 | AT | 23 | ARG |
| 20 | AT | 26 | ASN |
| 20 | AT | 27 | LYS |
| 20 | AT | 36 | LEU |
| 20 | AT | 41 | ILE |
| 20 | AT | 45 | GLN |
| 20 | AT | 73 | HIS |
| 20 | AT | 74 | LYS |
| 20 | AT | 93 | GLU |
| 21 | AU | 12 | LYS |
| 25 | AZ | 16 | THR |
| 25 | AZ | 20 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | AZ | 26 | THR |
| 25 | AZ | 39 | ASN |
| 25 | AZ | 52 | LYS |
| 25 | AZ | 65 | THR |
| 25 | AZ | 78 | SER |
| 25 | AZ | 92 | MET |
| 25 | AZ | 107 | SER |
| 25 | AZ | 110 | ASP |
| 25 | AZ | 138 | VAL |
| 25 | AZ | 141 | VAL |
| 25 | AZ | 145 | GLU |
| 25 | AZ | 152 | MET |
| 25 | AZ | 182 | MET |
| 25 | AZ | 188 | THR |
| 25 | AZ | 197 | ASP |
| 25 | AZ | 198 | LYS |
| 25 | AZ | 203 | LEU |
| 25 | AZ | 208 | GLU |
| 25 | AZ | 210 | ILE |
| 25 | AZ | 212 | THR |
| 25 | AZ | 216 | ASP |
| 25 | AZ | 218 | ASP |
| 25 | AZ | 220 | PRO |
| 25 | AZ | 234 | ARG |
| 25 | AZ | 241 | ARG |
| 25 | AZ | 243 | GLU |
| 25 | AZ | 244 | ARG |
| 25 | AZ | 248 | LYS |
| 25 | AZ | 252 | GLU |
| 25 | AZ | 265 | THR |
| 25 | AZ | 274 | ARG |
| 25 | AZ | 277 | LEU |
| 25 | AZ | 278 | GLN |
| 25 | AZ | 284 | ASP |
| 25 | AZ | 291 | ARG |
| 25 | AZ | 299 | GLU |
| 25 | AZ | 311 | THR |
| 25 | AZ | 317 | GLU |
| 25 | AZ | 324 | LYS |
| 25 | AZ | 325 | LYS |
| 25 | AZ | 332 | THR |
| 25 | AZ | 341 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | AZ | 355 | LEU |
| 25 | AZ | 356 | PRO |
| 25 | AZ | 364 | PRO |
| 25 | AZ | 378 | VAL |
| 25 | AZ | 403 | ILE |
| 25 | AZ | 404 | LEU |
| 26 | B0 | 12 | ASN |
| 26 | B0 | 14 | ARG |
| 26 | B0 | 16 | SER |
| 26 | B0 | 20 | ARG |
| 26 | B0 | 26 | TYR |
| 26 | B0 | 27 | GLU |
| 26 | B0 | 30 | VAL |
| 26 | B0 | 37 | LEU |
| 26 | B0 | 62 | LEU |
| 26 | B0 | 75 | LEU |
| 26 | B0 | 84 | LEU |
| 27 | B1 | 13 | ILE |
| 27 | B1 | 21 | ARG |
| 27 | B1 | 26 | ARG |
| 27 | B1 | 38 | SER |
| 27 | B1 | 39 | LYS |
| 27 | B1 | 43 | TYR |
| 27 | B1 | 49 | VAL |
| 27 | B1 | 52 | ARG |
| 27 | B1 | 56 | GLN |
| 27 | B1 | 73 | LEU |
| 27 | B1 | 83 | GLU |
| 27 | B1 | 92 | LYS |
| 27 | B1 | 93 | GLU |
| 28 | B2 | 3 | LEU |
| 28 | B2 | 7 | ARG |
| 28 | B2 | 33 | MET |
| 28 | B2 | 59 | ARG |
| 28 | B2 | 68 | ARG |
| 29 | B3 | 28 | LEU |
| 29 | B3 | 35 | ARG |
| 29 | B3 | 46 | ASN |
| 30 | B4 | 5 | ILE |
| 30 | B4 | 6 | HIS |
| 30 | B4 | 9 | LEU |
| 30 | B4 | 20 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | B4 | 22 | ILE |
| 30 | B4 | 27 | THR |
| 30 | B4 | 32 | TYR |
| 30 | B4 | 34 | GLU |
| 30 | B4 | 47 | GLN |
| 31 | B5 | 3 | LYS |
| 31 | B5 | 4 | HIS |
| 31 | B5 | 21 | SER |
| 31 | B5 | 26 | THR |
| 31 | B5 | 51 | TYR |
| 32 | B6 | 11 | LEU |
| 32 | B6 | 14 | THR |
| 32 | B6 | 17 | LYS |
| 32 | B6 | 18 | ARG |
| 32 | B6 | 19 | ARG |
| 32 | B6 | 31 | PRO |
| 32 | B6 | 42 | TRP |
| 32 | B6 | 44 | ARG |
| 32 | B6 | 45 | LYS |
| 32 | B6 | 53 | LYS |
| 33 | B7 | 4 | THR |
| 33 | B7 | 8 | ASN |
| 33 | B7 | 19 | ARG |
| 33 | B7 | 44 | PRO |
| 33 | B7 | 47 | ARG |
| 33 | B7 | 48 | LYS |
| 34 | B8 | 30 | ARG |
| 34 | B8 | 31 | HIS |
| 34 | B8 | 32 | LEU |
| 34 | B8 | 34 | TRP |
| 34 | B8 | 35 | GLN |
| 34 | B8 | 41 | ILE |
| 34 | B8 | 44 | LYS |
| 34 | B8 | 47 | LYS |
| 34 | B8 | 61 | LEU |
| 34 | B8 | 64 | TYR |
| 35 | B9 | 1 | MET |
| 35 | B9 | 2 | LYS |
| 35 | B9 | 11 | CYS |
| 35 | B9 | 18 | ARG |
| 35 | B9 | 20 | HIS |
| 35 | B9 | 28 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | B9 | 29 | ASN |
| 38 | BC | 3 | HIS |
| 38 | BC | 28 | LEU |
| 38 | BC | 30 | LYS |
| 38 | BC | 38 | ASP |
| 38 | BC | 52 | ARG |
| 38 | BC | 55 | ASP |
| 38 | BC | 58 | VAL |
| 38 | BC | 101 | GLN |
| 38 | BC | 104 | LEU |
| 38 | BC | 108 | MET |
| 38 | BC | 111 | ASP |
| 38 | BC | 134 | ARG |
| 38 | BC | 139 | ASN |
| 38 | BC | 147 | PHE |
| 38 | BC | 162 | GLU |
| 38 | BC | 182 | PRO |
| 38 | BC | 183 | GLU |
| 38 | BC | 184 | LYS |
| 38 | BC | 209 | LEU |
| 38 | BC | 215 | THR |
| 38 | BC | 225 | ASN |
| 39 | BD | 5 | LYS |
| 39 | BD | 10 | THR |
| 39 | BD | 14 | ARG |
| 39 | BD | 18 | VAL |
| 39 | BD | 20 | ASP |
| 39 | BD | 24 | ILE |
| 39 | BD | 26 | LYS |
| 39 | BD | 27 | THR |
| 39 | BD | 35 | LYS |
| 39 | BD | 37 | LEU |
| 39 | BD | 43 | ARG |
| 39 | BD | 46 | GLN |
| 39 | BD | 49 | ILE |
| 39 | BD | 61 | LEU |
| 39 | BD | 64 | ILE |
| 39 | BD | 65 | ILE |
| 39 | BD | 69 | ARG |
| 39 | BD | 71 | ASP |
| 39 | BD | 75 | ILE |
| 39 | BD | 88 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | BD | 92 | ILE |
| 39 | BD | 111 | LEU |
| 39 | BD | 117 | VAL |
| 39 | BD | 131 | LEU |
| 39 | BD | 134 | ARG |
| 39 | BD | 138 | VAL |
| 39 | BD | 157 | ARG |
| 39 | BD | 166 | GLN |
| 39 | BD | 176 | ARG |
| 39 | BD | 188 | GLU |
| 39 | BD | 192 | THR |
| 39 | BD | 211 | ARG |
| 39 | BD | 212 | SER |
| 39 | BD | 221 | VAL |
| 39 | BD | 229 | VAL |
| 39 | BD | 239 | ARG |
| 39 | BD | 254 | THR |
| 39 | BD | 257 | LEU |
| 39 | BD | 259 | THR |
| 39 | BD | 268 | ARG |
| 39 | BD | 270 | ILE |
| 39 | BD | 275 | LYS |
| 40 | BE | 18 | ASP |
| 40 | BE | 21 | VAL |
| 40 | BE | 33 | VAL |
| 40 | BE | 36 | ARG |
| 40 | BE | 53 | PRO |
| 40 | BE | 54 | GLN |
| 40 | BE | 55 | ASN |
| 40 | BE | 57 | LYS |
| 40 | BE | 58 | ARG |
| 40 | BE | 61 | ARG |
| 40 | BE | 67 | PHE |
| 40 | BE | 76 | ARG |
| 40 | BE | 78 | LEU |
| 40 | BE | 82 | ARG |
| 40 | BE | 111 | ARG |
| 40 | BE | 121 | ASN |
| 40 | BE | 146 | THR |
| 40 | BE | 154 | LYS |
| 40 | BE | 169 | ASN |
| 40 | BE | 171 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | BE | 197 | ILE |
| 40 | BE | 202 | LYS |
| 40 | BE | 203 | LYS |
| 41 | BF | 19 | GLU |
| 41 | BF | 23 | ASP |
| 41 | BF | 28 | ILE |
| 41 | BF | 62 | ARG |
| 41 | BF | 65 | TRP |
| 41 | BF | 67 | GLN |
| 41 | BF | 70 | THR |
| 41 | BF | 78 | ILE |
| 41 | BF | 83 | PHE |
| 41 | BF | 122 | LYS |
| 41 | BF | 125 | LEU |
| 41 | BF | 160 | ASN |
| 41 | BF | 170 | LEU |
| 41 | BF | 172 | TRP |
| 41 | BF | 179 | GLU |
| 41 | BF | 192 | LEU |
| 42 | BG | 10 | LYS |
| 42 | BG | 21 | ARG |
| 42 | BG | 22 | ARG |
| 42 | BG | 26 | GLN |
| 42 | BG | 33 | ARG |
| 42 | BG | 36 | LYS |
| 42 | BG | 39 | ILE |
| 42 | BG | 40 | ASN |
| 42 | BG | 52 | ILE |
| 42 | BG | 58 | GLN |
| 42 | BG | 67 | LYS |
| 42 | BG | 72 | ARG |
| 42 | BG | 80 | PHE |
| 42 | BG | 82 | LEU |
| 42 | BG | 84 | LYS |
| 42 | BG | 88 | ILE |
| 42 | BG | 104 | GLU |
| 42 | BG | 111 | LEU |
| 42 | BG | 125 | PHE |
| 42 | BG | 143 | GLU |
| 42 | BG | 146 | TYR |
| 42 | BG | 152 | LEU |
| 42 | BG | 153 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | BH | 41 | MET |
| 43 | BH | 43 | VAL |
| 43 | BH | 53 | GLU |
| 43 | BH | 54 | ARG |
| 43 | BH | 85 | LYS |
| 43 | BH | 143 | GLN |
| 43 | BH | 153 | LYS |
| 43 | BH | 170 | ARG |
| 46 | BN | 1 | MET |
| 46 | BN | 12 | ARG |
| 46 | BN | 19 | GLU |
| 46 | BN | 25 | ARG |
| 46 | BN | 34 | LEU |
| 46 | BN | 45 | ASN |
| 46 | BN | 48 | MET |
| 46 | BN | 56 | ASN |
| 46 | BN | 63 | THR |
| 46 | BN | 65 | LYS |
| 46 | BN | 76 | SER |
| 46 | BN | 78 | TYR |
| 46 | BN | 99 | LEU |
| 46 | BN | 123 | TYR |
| 46 | BN | 127 | ASP |
| 47 | BO | 8 | LEU |
| 47 | BO | 34 | THR |
| 47 | BO | 47 | ILE |
| 47 | BO | 48 | PRO |
| 47 | BO | 49 | ARG |
| 47 | BO | 80 | ASP |
| 47 | BO | 94 | ARG |
| 47 | BO | 98 | VAL |
| 48 | BP | 6 | LEU |
| 48 | BP | 10 | PRO |
| 48 | BP | 16 | ARG |
| 48 | BP | 18 | ARG |
| 48 | BP | 21 | ARG |
| 48 | BP | 32 | THR |
| 48 | BP | 39 | LYS |
| 48 | BP | 42 | SER |
| 48 | BP | 45 | LEU |
| 48 | BP | 47 | ASP |
| 48 | BP | 48 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | BP | 55 | ARG |
| 48 | BP | 57 | THR |
| 48 | BP | 61 | ARG |
| 48 | BP | 65 | ARG |
| 48 | BP | 67 | MET |
| 48 | BP | 75 | ILE |
| 48 | BP | 77 | ARG |
| 48 | BP | 85 | LEU |
| 48 | BP | 90 | ARG |
| 48 | BP | 91 | PHE |
| 48 | BP | 110 | TYR |
| 48 | BP | 111 | ARG |
| 48 | BP | 112 | LEU |
| 48 | BP | 136 | GLU |
| 49 | BQ | 1 | MET |
| 49 | BQ | 25 | ASP |
| 49 | BQ | 45 | GLN |
| 49 | BQ | 46 | GLN |
| 49 | BQ | 51 | ARG |
| 49 | BQ | 54 | MET |
| 49 | BQ | 55 | VAL |
| 49 | BQ | 58 | PHE |
| 49 | BQ | 59 | ARG |
| 49 | BQ | 74 | TYR |
| 49 | BQ | 81 | VAL |
| 49 | BQ | 89 | ASN |
| 49 | BQ | 110 | THR |
| 49 | BQ | 133 | ARG |
| 50 | BR | 2 | ARG |
| 50 | BR | 4 | LEU |
| 50 | BR | 5 | LYS |
| 50 | BR | 8 | ARG |
| 50 | BR | 21 | TYR |
| 50 | BR | 29 | LEU |
| 50 | BR | 35 | THR |
| 50 | BR | 37 | THR |
| 50 | BR | 63 | ARG |
| 50 | BR | 67 | LEU |
| 50 | BR | 68 | ARG |
| 50 | BR | 75 | LEU |
| 50 | BR | 82 | GLU |
| 50 | BR | 89 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | BR | 94 | TYR |
| 50 | BR | 97 | VAL |
| 50 | BR | 99 | LYS |
| 50 | BR | 100 | LEU |
| 50 | BR | 117 | VAL |
| 51 | BS | 11 | LYS |
| 51 | BS | 12 | PHE |
| 51 | BS | 15 | ARG |
| 51 | BS | 26 | LEU |
| 51 | BS | 29 | PHE |
| 51 | BS | 36 | TYR |
| 51 | BS | 54 | LEU |
| 51 | BS | 67 | ARG |
| 51 | BS | 73 | LEU |
| 51 | BS | 97 | ARG |
| 51 | BS | 106 | ARG |
| 52 | BT | 11 | GLU |
| 52 | BT | 13 | ARG |
| 52 | BT | 16 | ARG |
| 52 | BT | 24 | PRO |
| 52 | BT | 27 | THR |
| 52 | BT | 29 | ARG |
| 52 | BT | 32 | TYR |
| 52 | BT | 38 | ASN |
| 52 | BT | 41 | ARG |
| 52 | BT | 51 | ARG |
| 52 | BT | 58 | ASN |
| 52 | BT | 61 | PHE |
| 52 | BT | 65 | LYS |
| 52 | BT | 67 | SER |
| 52 | BT | 78 | LEU |
| 52 | BT | 82 | LEU |
| 52 | BT | 83 | ILE |
| 52 | BT | 90 | GLN |
| 52 | BT | 99 | LEU |
| 52 | BT | 100 | TYR |
| 52 | BT | 105 | LEU |
| 52 | BT | 121 | ILE |
| 52 | BT | 124 | ASP |
| 52 | BT | 128 | GLU |
| 53 | BU | 9 | VAL |
| 53 | BU | 14 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | BU | 20 | LEU |
| 53 | BU | 47 | TYR |
| 53 | BU | 66 | ASN |
| 53 | BU | 72 | HIS |
| 53 | BU | 74 | LEU |
| 53 | BU | 81 | HIS |
| 53 | BU | 103 | PRO |
| 53 | BU | 108 | GLU |
| 53 | BU | 114 | LYS |
| 54 | BV | 16 | PRO |
| 54 | BV | 18 | LEU |
| 54 | BV | 19 | LYS |
| 54 | BV | 21 | ARG |
| 54 | BV | 39 | LEU |
| 54 | BV | 51 | VAL |
| 54 | BV | 72 | VAL |
| 54 | BV | 82 | ARG |
| 54 | BV | 89 | GLN |
| 54 | BV | 99 | ILE |
| 55 | BW | 11 | ARG |
| 55 | BW | 51 | LEU |
| 55 | BW | 52 | GLU |
| 55 | BW | 63 | ASP |
| 55 | BW | 71 | VAL |
| 55 | BW | 75 | TYR |
| 55 | BW | 85 | VAL |
| 55 | BW | 88 | ARG |
| 55 | BW | 102 | HIS |
| 55 | BW | 103 | ILE |
| 55 | BW | 107 | LEU |
| 56 | BX | 15 | GLU |
| 56 | BX | 28 | PHE |
| 56 | BX | 35 | THR |
| 56 | BX | 57 | LEU |
| 56 | BX | 68 | ARG |
| 56 | BX | 76 | ARG |
| 57 | BY | 2 | ARG |
| 57 | BY | 6 | HIS |
| 57 | BY | 9 | LYS |
| 57 | BY | 13 | VAL |
| 57 | BY | 29 | GLU |
| 57 | BY | 50 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57 | BY | 56 | PRO |
| 57 | BY | 57 | GLN |
| 57 | BY | 62 | GLU |
| 57 | BY | 68 | HIS |
| 57 | BY | 76 | CYS |
| 57 | BY | 77 | PRO |
| 57 | BY | 99 | CYS |
| 58 | BZ | 3 | TYR |
| 58 | BZ | 6 | LYS |
| 58 | BZ | 11 | GLU |
| 58 | BZ | 20 | ARG |
| 58 | BZ | 24 | LEU |
| 58 | BZ | 28 | MET |
| 58 | BZ | 35 | ARG |
| 58 | BZ | 38 | TYR |
| 58 | BZ | 48 | PHE |
| 58 | BZ | 70 | LEU |
| 58 | BZ | 73 | GLN |
| 58 | BZ | 76 | LEU |
| 58 | BZ | 86 | VAL |
| 58 | BZ | 87 | ASP |
| 58 | BZ | 93 | ASP |
| 58 | BZ | 97 | GLU |
| 58 | BZ | 99 | TYR |
| 58 | BZ | 103 | ARG |
| 58 | BZ | 104 | PHE |
| 58 | BZ | 119 | GLU |
| 58 | BZ | 123 | ASP |
| 58 | BZ | 127 | LYS |
| 58 | BZ | 150 | LEU |
| 58 | BZ | 155 | LEU |
| 58 | BZ | 163 | LEU |
| 58 | BZ | 175 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 45 | GLN |
| 2 | AB | 78 | GLN |
| 2 | AB | 146 | GLN |
| 2 | AB | 204 | ASN |
| 2 | AB | 212 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 224 | GLN |
| 3 | AC | 6 | HIS |
| 3 | AC | 28 | GLN |
| 3 | AC | 118 | GLN |
| 3 | AC | 170 | GLN |
| 3 | AC | 176 | HIS |
| 3 | AC | 181 | ASN |
| 4 | AD | 62 | GLN |
| 4 | AD | 74 | GLN |
| 4 | AD | 129 | ASN |
| 5 | AE | 20 | GLN |
| 5 | AE | 73 | ASN |
| 5 | AE | 141 | GLN |
| 6 | AF | 7 | ASN |
| 6 | AF | 27 | GLN |
| 6 | AF | 84 | ASN |
| 6 | AF | 100 | ASN |
| 7 | AG | 13 | GLN |
| 7 | AG | 37 | ASN |
| 7 | AG | 68 | ASN |
| 7 | AG | 86 | GLN |
| 7 | AG | 96 | GLN |
| 8 | AH | 82 | HIS |
| 9 | AI | 3 | GLN |
| 9 | AI | 73 | GLN |
| 9 | AI | 89 | ASN |
| 9 | AI | 124 | GLN |
| 10 | AJ | 13 | HIS |
| 10 | AJ | 56 | HIS |
| 10 | AJ | 68 | HIS |
| 10 | AJ | 78 | ASN |
| 10 | AJ | 84 | GLN |
| 11 | AK | 38 | ASN |
| 11 | AK | 99 | GLN |
| 11 | AK | 117 | ASN |
| 12 | AL | 8 | ASN |
| 12 | AL | 9 | GLN |
| 12 | AL | 49 | ASN |
| 12 | AL | 75 | HIS |
| 13 | AM | 12 | ASN |
| 13 | AM | 40 | ASN |
| 13 | AM | 77 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | AM | 92 | HIS |
| 13 | AM | 101 | GLN |
| 15 | AO | 9 | GLN |
| 15 | AO | 37 | ASN |
| 15 | AO | 46 | HIS |
| 15 | AO | 62 | GLN |
| 16 | AP | 65 | GLN |
| 16 | AP | 76 | GLN |
| 17 | AQ | 16 | GLN |
| 19 | AS | 14 | HIS |
| 19 | AS | 47 | HIS |
| 20 | AT | 16 | HIS |
| 20 | AT | 26 | ASN |
| 20 | AT | 42 | GLN |
| 20 | AT | 75 | ASN |
| 25 | AZ | 39 | ASN |
| 25 | AZ | 67 | HIS |
| 25 | AZ | 98 | GLN |
| 25 | AZ | 115 | GLN |
| 25 | AZ | 125 | GLN |
| 25 | AZ | 159 | ASN |
| 25 | AZ | 183 | HIS |
| 25 | AZ | 193 | ASN |
| 25 | AZ | 341 | GLN |
| 25 | AZ | 367 | ASN |
| 26 | B0 | 29 | GLN |
| 26 | B0 | 35 | ASN |
| 26 | B0 | 50 | ASN |
| 26 | B0 | 70 | GLN |
| 27 | B1 | 45 | ASN |
| 28 | B2 | 43 | GLN |
| 28 | B2 | 47 | ASN |
| 28 | B2 | 65 | ASN |
| 29 | B3 | 19 | GLN |
| 29 | B3 | 32 | GLN |
| 29 | B3 | 46 | ASN |
| 29 | B3 | 52 | HIS |
| 30 | B4 | 20 | ASN |
| 30 | B4 | 40 | HIS |
| 30 | B4 | 47 | GLN |
| 31 | B5 | 43 | HIS |
| 32 | B6 | 26 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | B6 | 29 | ASN |
| 33 | B7 | 8 | ASN |
| 34 | B8 | 35 | GLN |
| 35 | B9 | 29 | ASN |
| 35 | B9 | 32 | HIS |
| 38 | BC | 57 | ASN |
| 38 | BC | 66 | HIS |
| 38 | BC | 188 | ASN |
| 38 | BC | 225 | ASN |
| 39 | BD | 58 | HIS |
| 39 | BD | 96 | HIS |
| 39 | BD | 115 | GLN |
| 39 | BD | 126 | GLN |
| 39 | BD | 166 | GLN |
| 39 | BD | 186 | HIS |
| 39 | BD | 198 | ASN |
| 40 | BE | 48 | GLN |
| 40 | BE | 54 | GLN |
| 40 | BE | 55 | ASN |
| 40 | BE | 121 | ASN |
| 40 | BE | 135 | HIS |
| 40 | BE | 143 | ASN |
| 41 | BF | 29 | ASN |
| 41 | BF | 40 | GLN |
| 41 | BF | 69 | HIS |
| 41 | BF | 75 | HIS |
| 41 | BF | 133 | ASN |
| 41 | BF | 160 | ASN |
| 41 | BF | 169 | ASN |
| 41 | BF | 203 | GLN |
| 42 | BG | 121 | ASN |
| 42 | BG | 123 | ASN |
| 43 | BH | 61 | HIS |
| 43 | BH | 74 | ASN |
| 43 | BH | 143 | GLN |
| 43 | BH | 147 | ASN |
| 46 | BN | 45 | ASN |
| 46 | BN | 56 | ASN |
| 46 | BN | 131 | GLN |
| 48 | BP | 35 | HIS |
| 48 | BP | 70 | GLN |
| 48 | BP | 81 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | BP | 84 | ASN |
| 48 | BP | 128 | HIS |
| 49 | BQ | 45 | GLN |
| 50 | BR | 3 | HIS |
| 50 | BR | 13 | HIS |
| 50 | BR | 23 | ASN |
| 50 | BR | 53 | HIS |
| 50 | BR | 61 | HIS |
| 50 | BR | 71 | GLN |
| 51 | BS | 95 | HIS |
| 52 | BT | 43 | GLN |
| 52 | BT | 58 | ASN |
| 52 | BT | 79 | HIS |
| 52 | BT | 123 | GLN |
| 53 | BU | 49 | HIS |
| 53 | BU | 66 | ASN |
| 53 | BU | 94 | ASN |
| 53 | BU | 117 | GLN |
| 54 | BV | 11 | GLN |
| 54 | BV | 80 | GLN |
| 55 | BW | 57 | ASN |
| 55 | BW | 60 | ASN |
| 55 | BW | 62 | HIS |
| 56 | BX | 31 | HIS |
| 56 | BX | 41 | ASN |
| 56 | BX | 55 | ASN |
| 57 | BY | 6 | HIS |
| 57 | BY | 43 | ASN |
| 57 | BY | 68 | HIS |
| 58 | BZ | 55 | HIS |
| 58 | BZ | 85 | HIS |
| 58 | BZ | 118 | GLN |
| 58 | BZ | 151 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1503/1522 (98%) | 247 (16%) | 56 (3%) |
| 22 | AV | 75/76 (98%) | 22 (29%) | 0 |
| 22 | AW | 75/76 (98%) | 17 (22%) | 0 |
| 23 | AX | 13/14 (92%) | 2 (15%) | 1 (7%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 24 | AY | 74/77 (96%) | 23 (31%) | 2 (2%) |
| 36 | BA | 2900/2915 (99%) | 547 (18%) | 52 (1%) |
| 37 | BB | 118/122 (96%) | 24 (20%) | 2 (1%) |
| All | All | 4758/4802 (99%) | 882 (18%) | 113 (2%) |

All (882) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 31 | G |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 51 | A |
| 1 | AA | 61 | G |
| 1 | AA | 65 | U |
| 1 | AA | 79 | G |
| 1 | AA | 80 | G |
| 1 | AA | 81 | U |
| 1 | AA | 82 | U |
| 1 | AA | 89 | C |
| 1 | AA | 90 | U |
| 1 | AA | 109 | A |
| 1 | AA | 110 | C |
| 1 | AA | 116 | A |
| 1 | AA | 120 | A |
| 1 | AA | 121 | C |
| 1 | AA | 122 | G |
| 1 | AA | 131 | C |
| 1 | AA | 144 | G |
| 1 | AA | 146 | G |
| 1 | AA | 147 | G |
| 1 | AA | 189(G) | G |
| 1 | AA | 189(H) | G |
| 1 | AA | 189(I) | G |
| 1 | AA | 195 | A |
| 1 | AA | 197 | A |
| 1 | AA | 198 | G |
| 1 | AA | 199 | G |
| 1 | AA | 202 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 203 | U |
| 1 | AA | 216 | G |
| 1 | AA | 244 | U |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 252 | U |
| 1 | AA | 267 | C |
| 1 | AA | 274 | A |
| 1 | AA | 275 | G |
| 1 | AA | 289 | G |
| 1 | AA | 321 | A |
| 1 | AA | 328 | C |
| 1 | AA | 330 | C |
| 1 | AA | 332 | G |
| 1 | AA | 344 | A |
| 1 | AA | 345 | C |
| 1 | AA | 346 | G |
| 1 | AA | 347 | G |
| 1 | AA | 348 | G |
| 1 | AA | 352 | C |
| 1 | AA | 353 | A |
| 1 | AA | 354 | G |
| 1 | AA | 367 | U |
| 1 | AA | 368 | U |
| 1 | AA | 369 | C |
| 1 | AA | 370 | C |
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 389 | A |
| 1 | AA | 397 | A |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 414 | A |
| 1 | AA | 421 | U |
| 1 | AA | 422 | C |
| 1 | AA | 428 | G |
| 1 | AA | 429 | U |
| 1 | AA | 430 | A |
| 1 | AA | 435 | C |
| 1 | AA | 439 | A |
| 1 | AA | 442 | C |
| 1 | AA | 452 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 453 | A |
| 1 | AA | 454 | C |
| 1 | AA | 461 | A |
| 1 | AA | 470 | C |
| 1 | AA | 484 | G |
| 1 | AA | 485 | G |
| 1 | AA | 495 | A |
| 1 | AA | 496 | A |
| 1 | AA | 498 | U |
| 1 | AA | 499 | A |
| 1 | AA | 508 | C |
| 1 | AA | 509 | A |
| 1 | AA | 518 | C |
| 1 | AA | 527 | G |
| 1 | AA | 531 | U |
| 1 | AA | 532 | A |
| 1 | AA | 533 | A |
| 1 | AA | 534 | U |
| 1 | AA | 548 | G |
| 1 | AA | 559 | A |
| 1 | AA | 561 | U |
| 1 | AA | 562 | C |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 576 | G |
| 1 | AA | 577 | G |
| 1 | AA | 632 | A |
| 1 | AA | 653 | A |
| 1 | AA | 665 | A |
| 1 | AA | 688 | G |
| 1 | AA | 701 | C |
| 1 | AA | 702 | A |
| 1 | AA | 721 | G |
| 1 | AA | 722 | A |
| 1 | AA | 723 | U |
| 1 | AA | 731 | G |
| 1 | AA | 734 | G |
| 1 | AA | 749 | C |
| 1 | AA | 755 | G |
| 1 | AA | 777 | A |
| 1 | AA | 792 | A |
| 1 | AA | 793 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 794 | A |
| 1 | AA | 816 | A |
| 1 | AA | 817 | C |
| 1 | AA | 827 | U |
| 1 | AA | 828 | A |
| 1 | AA | 839 | U |
| 1 | AA | 840 | C |
| 1 | AA | 841 | U |
| 1 | AA | 848 | C |
| 1 | AA | 858 | G |
| 1 | AA | 859 | A |
| 1 | AA | 872 | A |
| 1 | AA | 914 | A |
| 1 | AA | 927 | G |
| 1 | AA | 934 | C |
| 1 | AA | 935 | A |
| 1 | AA | 960 | U |
| 1 | AA | 962 | C |
| 1 | AA | 966 | G |
| 1 | AA | 967 | C |
| 1 | AA | 968 | A |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 974 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 978 | A |
| 1 | AA | 980 | C |
| 1 | AA | 981 | U |
| 1 | AA | 982 | U |
| 1 | AA | 983 | A |
| 1 | AA | 991 | U |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 996 | A |
| 1 | AA | 1004 | A |
| 1 | AA | 1026 | G |
| 1 | AA | 1030 | C |
| 1 | AA | 1050 | G |
| 1 | AA | 1051 | C |
| 1 | AA | 1054 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1066 | C |
| 1 | AA | 1087 | G |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1101 | A |
| 1 | AA | 1102 | A |
| 1 | AA | 1117 | G |
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1126 | U |
| 1 | AA | 1127 | G |
| 1 | AA | 1129 | C |
| 1 | AA | 1130 | A |
| 1 | AA | 1131 | G |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1140 | C |
| 1 | AA | 1141 | C |
| 1 | AA | 1145 | C |
| 1 | AA | 1152 | A |
| 1 | AA | 1154 | G |
| 1 | AA | 1158 | C |
| 1 | AA | 1159 | U |
| 1 | AA | 1184 | G |
| 1 | AA | 1190 | G |
| 1 | AA | 1191 | A |
| 1 | AA | 1196 | U |
| 1 | AA | 1197 | G |
| 1 | AA | 1199 | U |
| 1 | AA | 1200 | C |
| 1 | AA | 1201 | A |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | U |
| 1 | AA | 1267 | C |
| 1 | AA | 1268 | A |
| 1 | AA | 1273 | G |
| 1 | AA | 1281 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1284 | C |
| 1 | AA | 1285 | A |
| 1 | AA | 1286 | A |
| 1 | AA | 1287 | A |
| 1 | AA | 1299 | A |
| 1 | AA | 1300 | G |
| 1 | AA | 1302 | U |
| 1 | AA | 1303 | C |
| 1 | AA | 1305 | G |
| 1 | AA | 1317 | C |
| 1 | AA | 1320 | C |
| 1 | AA | 1321 | C |
| 1 | AA | 1322 | C |
| 1 | AA | 1327 | C |
| 1 | AA | 1331 | G |
| 1 | AA | 1335 | C |
| 1 | AA | 1346 | A |
| 1 | AA | 1347 | G |
| 1 | AA | 1353 | G |
| 1 | AA | 1363 | C |
| 1 | AA | 1364 | U |
| 1 | AA | 1379 | G |
| 1 | AA | 1387 | G |
| 1 | AA | 1394 | A |
| 1 | AA | 1397 | C |
| 1 | AA | 1398 | A |
| 1 | AA | 1400 | C |
| 1 | AA | 1419 | G |
| 1 | AA | 1422 | G |
| 1 | AA | 1442(A) | G |
| 1 | AA | 1442(B) | A |
| 1 | AA | 1452 | C |
| 1 | AA | 1456 | G |
| 1 | AA | 1487 | G |
| 1 | AA | 1492 | A |
| 1 | AA | 1499 | A |
| 1 | AA | 1503 | A |
| 1 | AA | 1504 | G |
| 1 | AA | 1505 | G |
| 1 | AA | 1506 | U |
| 1 | AA | 1517 | G |
| 1 | AA | 1519 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1520 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 22 | AV | 4 | C |
| 22 | AV | 5 | G |
| 22 | AV | 7 | A |
| 22 | AV | 8 | U |
| 22 | AV | 17 | C |
| 22 | AV | 18 | G |
| 22 | AV | 19 | G |
| 22 | AV | 20 | U |
| 22 | AV | 22 | G |
| 22 | AV | 37 | A |
| 22 | AV | 44 | G |
| 22 | AV | 45 | U |
| 22 | AV | 46 | G |
| 22 | AV | 47 | U |
| 22 | AV | 48 | C |
| 22 | AV | 60 | U |
| 22 | AV | 61 | C |
| 22 | AV | 62 | C |
| 22 | AV | 69 | G |
| 22 | AV | 73 | A |
| 22 | AV | 75 | C |
| 22 | AV | 76 | A |
| 22 | AW | 6 | G |
| 22 | AW | 9 | A |
| 22 | AW | 18 | G |
| 22 | AW | 19 | G |
| 22 | AW | 20 | U |
| 22 | AW | 21 | A |
| 22 | AW | 34 | G |
| 22 | AW | 39 | U |
| 22 | AW | 43 | C |
| 22 | AW | 44 | G |
| 22 | AW | 45 | U |
| 22 | AW | 47 | U |
| 22 | AW | 48 | C |
| 22 | AW | 50 | U |
| 22 | AW | 59 | U |
| 22 | AW | 61 | C |
| 22 | AW | 65 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | AX | 17 | U |
| 23 | AX | 27 | A |
| 24 | AY | 5 | G |
| 24 | AY | 8 | 4SU |
| 24 | AY | 9 | A |
| 24 | AY | 10 | G |
| 24 | AY | 16 | H2U |
| 24 | AY | 17 | H2U |
| 24 | AY | 18 | G |
| 24 | AY | 19 | G |
| 24 | AY | 20 | H2U |
| 24 | AY | 21 | A |
| 24 | AY | 22 | G |
| 24 | AY | 36 | A |
| 24 | AY | 38 | A |
| 24 | AY | 44 | G |
| 24 | AY | 45 | U |
| 24 | AY | 46 | 7MG |
| 24 | AY | 58 | A |
| 24 | AY | 59 | G |
| 24 | AY | 61 | C |
| 24 | AY | 62 | U |
| 24 | AY | 73 | G |
| 24 | AY | 75 | C |
| 24 | AY | 76 | A |
| 36 | BA | 10 | G |
| 36 | BA | 15 | G |
| 36 | BA | 45 | C |
| 36 | BA | 50 | U |
| 36 | BA | 71 | A |
| 36 | BA | 72 | U |
| 36 | BA | 74 | A |
| 36 | BA | 75 | G |
| 36 | BA | 84 | A |
| 36 | BA | 85 | G |
| 36 | BA | 88 | G |
| 36 | BA | 90 | U |
| 36 | BA | 92 | A |
| 36 | BA | 94 | C |
| 36 | BA | 95 | G |
| 36 | BA | 100 | G |
| 36 | BA | 102 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 36 | BA | 118 | A |
| 36 | BA | 119 | A |
| 36 | BA | 120 | U |
| 36 | BA | 129 | C |
| 36 | BA | 139(A) | G |
| 36 | BA | 141 | A |
| 36 | BA | 146 | G |
| 36 | BA | 149 | A |
| 36 | BA | 155 | U |
| 36 | BA | 156 | U |
| 36 | BA | 181 | A |
| 36 | BA | 196 | A |
| 36 | BA | 197 | A |
| 36 | BA | 199 | A |
| 36 | BA | 204 | A |
| 36 | BA | 205 | G |
| 36 | BA | 221 | A |
| 36 | BA | 222 | A |
| 36 | BA | 228 | A |
| 36 | BA | 229 | A |
| 36 | BA | 233 | A |
| 36 | BA | 245 | G |
| 36 | BA | 248 | G |
| 36 | BA | 252 | G |
| 36 | BA | 267 | C |
| 36 | BA | 271(I) | G |
| 36 | BA | 271(K) | U |
| 36 | BA | 271(L) | U |
| 36 | BA | 271(M) | G |
| 36 | BA | 271(O) | C |
| 36 | BA | 271(P) | C |
| 36 | BA | 271(R) | G |
| 36 | BA | 271(Y) | U |
| 36 | BA | 272(A) | U |
| 36 | BA | 272(B) | G |
| 36 | BA | 272(I) | U |
| 36 | BA | 276 | A |
| 36 | BA | 284 | U |
| 36 | BA | 288 | C |
| 36 | BA | 294 | A |
| 36 | BA | 311 | A |
| 36 | BA | 329 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BA | 330 | A |
| 36 | BA | 332 | A |
| 36 | BA | 333 | G |
| 36 | BA | 343 | C |
| 36 | BA | 349 | G |
| 36 | BA | 352 | G |
| 36 | BA | 353 | G |
| 36 | BA | 356 | G |
| 36 | BA | 358 | U |
| 36 | BA | 362 | U |
| 36 | BA | 363 | G |
| 36 | BA | 363(E) | U |
| 36 | BA | 363(F) | A |
| 36 | BA | 386 | G |
| 36 | BA | 387 | U |
| 36 | BA | 388 | G |
| 36 | BA | 405 | U |
| 36 | BA | 406 | G |
| 36 | BA | 411 | G |
| 36 | BA | 428 | A |
| 36 | BA | 444 | C |
| 36 | BA | 448 | U |
| 36 | BA | 451 | C |
| 36 | BA | 456 | C |
| 36 | BA | 457 | A |
| 36 | BA | 470 | A |
| 36 | BA | 472 | A |
| 36 | BA | 473 | G |
| 36 | BA | 481 | G |
| 36 | BA | 482 | A |
| 36 | BA | 494 | G |
| 36 | BA | 505 | A |
| 36 | BA | 508 | G |
| 36 | BA | 509 | C |
| 36 | BA | 512 | G |
| 36 | BA | 528 | A |
| 36 | BA | 530 | G |
| 36 | BA | 531 | C |
| 36 | BA | 532 | A |
| 36 | BA | 533 | G |
| 36 | BA | 537 | C |
| 36 | BA | 563 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BA | 573 | G |
| 36 | BA | 575 | A |
| 36 | BA | 586 | A |
| 36 | BA | 588 | U |
| 36 | BA | 603 | A |
| 36 | BA | 604 | G |
| 36 | BA | 607 | U |
| 36 | BA | 613 | G |
| 36 | BA | 614(B) | G |
| 36 | BA | 614(C) | A |
| 36 | BA | 615 | G |
| 36 | BA | 622 | G |
| 36 | BA | 627 | A |
| 36 | BA | 629 | G |
| 36 | BA | 637 | A |
| 36 | BA | 645 | C |
| 36 | BA | 646 | A |
| 36 | BA | 651 | G |
| 36 | BA | 653 | A |
| 36 | BA | 654 | A |
| 36 | BA | 654(D) | G |
| 36 | BA | 654(J) | A |
| 36 | BA | 654(K) | C |
| 36 | BA | 654(L) | G |
| 36 | BA | 654(M) | C |
| 36 | BA | 656 | G |
| 36 | BA | 669 | G |
| 36 | BA | 670 | A |
| 36 | BA | 673 | C |
| 36 | BA | 686 | G |
| 36 | BA | 708 | C |
| 36 | BA | 722 | A |
| 36 | BA | 730 | C |
| 36 | BA | 753 | C |
| 36 | BA | 761 | A |
| 36 | BA | 764 | A |
| 36 | BA | 765 | G |
| 36 | BA | 776 | G |
| 36 | BA | 782 | A |
| 36 | BA | 784 | A |
| 36 | BA | 785 | G |
| 36 | BA | 790 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 36 | BA | 791 | C |
| 36 | BA | 792 | G |
| 36 | BA | 805 | G |
| 36 | BA | 812 | C |
| 36 | BA | 819 | A |
| 36 | BA | 827 | U |
| 36 | BA | 828 | U |
| 36 | BA | 830 | G |
| 36 | BA | 848 | G |
| 36 | BA | 856 | C |
| 36 | BA | 857 | C |
| 36 | BA | 859 | G |
| 36 | BA | 866 | A |
| 36 | BA | 878 | A |
| 36 | BA | 885 | C |
| 36 | BA | 890 | A |
| 36 | BA | 896 | A |
| 36 | BA | 897 | C |
| 36 | BA | 910 | A |
| 36 | BA | 917 | A |
| 36 | BA | 926 | A |
| 36 | BA | 932 | G |
| 36 | BA | 941 | A |
| 36 | BA | 945 | A |
| 36 | BA | 946 | G |
| 36 | BA | 958 | U |
| 36 | BA | 959 | A |
| 36 | BA | 961 | C |
| 36 | BA | 964 | C |
| 36 | BA | 965 | C |
| 36 | BA | 973 | A |
| 36 | BA | 974 | G |
| 36 | BA | 975 | C |
| 36 | BA | 983 | A |
| 36 | BA | 991 | C |
| 36 | BA | 996 | A |
| 36 | BA | 1005 | C |
| 36 | BA | 1011 | G |
| 36 | BA | 1012 | U |
| 36 | BA | 1013 | C |
| 36 | BA | 1022 | G |
| 36 | BA | 1025 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BA | 1026 | U |
| 36 | BA | 1039 | G |
| 36 | BA | 1045 | A |
| 36 | BA | 1046 | A |
| 36 | BA | 1047 | G |
| 36 | BA | 1048 | A |
| 36 | BA | 1051 | G |
| 36 | BA | 1053 | C |
| 36 | BA | 1059 | G |
| 36 | BA | 1061 | U |
| 36 | BA | 1062 | G |
| 36 | BA | 1065 | U |
| 36 | BA | 1067 | A |
| 36 | BA | 1068 | G |
| 36 | BA | 1069 | A |
| 36 | BA | 1070 | A |
| 36 | BA | 1071 | G |
| 36 | BA | 1072 | C |
| 36 | BA | 1073 | A |
| 36 | BA | 1075 | C |
| 36 | BA | 1079 | C |
| 36 | BA | 1087 | G |
| 36 | BA | 1088 | A |
| 36 | BA | 1090 | U |
| 36 | BA | 1103 | A |
| 36 | BA | 1107 | G |
| 36 | BA | 1108 | U |
| 36 | BA | 1111 | A |
| 36 | BA | 1112 | G |
| 36 | BA | 1114 | G |
| 36 | BA | 1130 | U |
| 36 | BA | 1135 | C |
| 36 | BA | 1136 | G |
| 36 | BA | 1142 | U |
| 36 | BA | 1142(A) | A |
| 36 | BA | 1143 | A |
| 36 | BA | 1155 | A |
| 36 | BA | 1167 | U |
| 36 | BA | 1171 | G |
| 36 | BA | 1174 | A |
| 36 | BA | 1175 | U |
| 36 | BA | 1176 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BA | 1178 | C |
| 36 | BA | 1195 | G |
| 36 | BA | 1204 | A |
| 36 | BA | 1205 | U |
| 36 | BA | 1210 | A |
| 36 | BA | 1211 | U |
| 36 | BA | 1212 | G |
| 36 | BA | 1221 | C |
| 36 | BA | 1223 | G |
| 36 | BA | 1244 | G |
| 36 | BA | 1247 | A |
| 36 | BA | 1248 | G |
| 36 | BA | 1253 | A |
| 36 | BA | 1256 | G |
| 36 | BA | 1265 | A |
| 36 | BA | 1271 | G |
| 36 | BA | 1272 | A |
| 36 | BA | 1273 | U |
| 36 | BA | 1292 | U |
| 36 | BA | 1300 | U |
| 36 | BA | 1301 | A |
| 36 | BA | 1302 | A |
| 36 | BA | 1314 | C |
| 36 | BA | 1319 | G |
| 36 | BA | 1321 | A |
| 36 | BA | 1332 | G |
| 36 | BA | 1349 | A |
| 36 | BA | 1359 | A |
| 36 | BA | 1360 | A |
| 36 | BA | 1365 | A |
| 36 | BA | 1379 | A |
| 36 | BA | 1380 | G |
| 36 | BA | 1384 | A |
| 36 | BA | 1385 | G |
| 36 | BA | 1386 | C |
| 36 | BA | 1396 | U |
| 36 | BA | 1404 | C |
| 36 | BA | 1407 | C |
| 36 | BA | 1416 | G |
| 36 | BA | 1419 | A |
| 36 | BA | 1420 | U |
| 36 | BA | 1421 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 36 | BA | 1427 | A |
| 36 | BA | 1428 | C |
| 36 | BA | 1437 | C |
| 36 | BA | 1445 | A |
| 36 | BA | 1449 | A |
| 36 | BA | 1450 | G |
| 36 | BA | 1452 | A |
| 36 | BA | 1455 | G |
| 36 | BA | 1460 | A |
| 36 | BA | 1461 | G |
| 36 | BA | 1467 | C |
| 36 | BA | 1471 | A |
| 36 | BA | 1475 | G |
| 36 | BA | 1478 | G |
| 36 | BA | 1482 | G |
| 36 | BA | 1485 | G |
| 36 | BA | 1490 | A |
| 36 | BA | 1493 | C |
| 36 | BA | 1494 | A |
| 36 | BA | 1495 | A |
| 36 | BA | 1496 | A |
| 36 | BA | 1497 | U |
| 36 | BA | 1499 | C |
| 36 | BA | 1502 | C |
| 36 | BA | 1505 | C |
| 36 | BA | 1509 | C |
| 36 | BA | 1509(A) | A |
| 36 | BA | 1517 | G |
| 36 | BA | 1528(A) | A |
| 36 | BA | 1537 | G |
| 36 | BA | 1541 | G |
| 36 | BA | 1542 | A |
| 36 | BA | 1544 | A |
| 36 | BA | 1554 | A |
| 36 | BA | 1558 | A |
| 36 | BA | 1559 | G |
| 36 | BA | 1569 | A |
| 36 | BA | 1575 | C |
| 36 | BA | 1578 | U |
| 36 | BA | 1579 | A |
| 36 | BA | 1580 | A |
| 36 | BA | 1584 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 36 | BA | 1586 | A |
| 36 | BA | 1588 | C |
| 36 | BA | 1591 | G |
| 36 | BA | 1598 | C |
| 36 | BA | 1603 | A |
| 36 | BA | 1608 | A |
| 36 | BA | 1610 | A |
| 36 | BA | 1615 | C |
| 36 | BA | 1616 | A |
| 36 | BA | 1617 | C |
| 36 | BA | 1618 | A |
| 36 | BA | 1640 | C |
| 36 | BA | 1648 | C |
| 36 | BA | 1654 | A |
| 36 | BA | 1666 | G |
| 36 | BA | 1674 | G |
| 36 | BA | 1696 | G |
| 36 | BA | 1698 | A |
| 36 | BA | 1718 | G |
| 36 | BA | 1721 | G |
| 36 | BA | 1722 | A |
| 36 | BA | 1739 | U |
| 36 | BA | 1740 | G |
| 36 | BA | 1742 | G |
| 36 | BA | 1744 | C |
| 36 | BA | 1748 | G |
| 36 | BA | 1756 | G |
| 36 | BA | 1763 | G |
| 36 | BA | 1764 | G |
| 36 | BA | 1773 | A |
| 36 | BA | 1780 | A |
| 36 | BA | 1781 | C |
| 36 | BA | 1791 | A |
| 36 | BA | 1799 | G |
| 36 | BA | 1800 | C |
| 36 | BA | 1801 | G |
| 36 | BA | 1816 | G |
| 36 | BA | 1820 | U |
| 36 | BA | 1835 | G |
| 36 | BA | 1847 | A |
| 36 | BA | 1853 | A |
| 36 | BA | 1858 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BA | 1866 | C |
| 36 | BA | 1878 | G |
| 36 | BA | 1881 | C |
| 36 | BA | 1882 | C |
| 36 | BA | 1885 | A |
| 36 | BA | 1888 | G |
| 36 | BA | 1889 | A |
| 36 | BA | 1900 | A |
| 36 | BA | 1903 | G |
| 36 | BA | 1906 | G |
| 36 | BA | 1912 | A |
| 36 | BA | 1913 | A |
| 36 | BA | 1929 | G |
| 36 | BA | 1936 | A |
| 36 | BA | 1937 | A |
| 36 | BA | 1938 | A |
| 36 | BA | 1948 | G |
| 36 | BA | 1955 | U |
| 36 | BA | 1963 | U |
| 36 | BA | 1967 | C |
| 36 | BA | 1970 | A |
| 36 | BA | 1971 | A |
| 36 | BA | 1972 | A |
| 36 | BA | 1982 | C |
| 36 | BA | 1987 | G |
| 36 | BA | 1992 | G |
| 36 | BA | 1993 | U |
| 36 | BA | 1997 | G |
| 36 | BA | 2023 | G |
| 36 | BA | 2031 | A |
| 36 | BA | 2033 | A |
| 36 | BA | 2034 | U |
| 36 | BA | 2036 | C |
| 36 | BA | 2043 | C |
| 36 | BA | 2055 | C |
| 36 | BA | 2056 | G |
| 36 | BA | 2060 | A |
| 36 | BA | 2061 | G |
| 36 | BA | 2062 | A |
| 36 | BA | 2069 | G |
| 36 | BA | 2093 | G |
| 36 | BA | 2096 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BA | 2100 | G |
| 36 | BA | 2102 | U |
| 36 | BA | 2103 | C |
| 36 | BA | 2104 | G |
| 36 | BA | 2105 | C |
| 36 | BA | 2107 | C |
| 36 | BA | 2108 | C |
| 36 | BA | 2109 | U |
| 36 | BA | 2111 | C |
| 36 | BA | 2112 | G |
| 36 | BA | 2113 | U |
| 36 | BA | 2115 | G |
| 36 | BA | 2116 | G |
| 36 | BA | 2117 | A |
| 36 | BA | 2118 | U |
| 36 | BA | 2127 | G |
| 36 | BA | 2129 | C |
| 36 | BA | 2131 | G |
| 36 | BA | 2132 | U |
| 36 | BA | 2133 | G |
| 36 | BA | 2146 | C |
| 36 | BA | 2147 | G |
| 36 | BA | 2157 | G |
| 36 | BA | 2159 | G |
| 36 | BA | 2160 | G |
| 36 | BA | 2169 | A |
| 36 | BA | 2172 | U |
| 36 | BA | 2173 | A |
| 36 | BA | 2174 | C |
| 36 | BA | 2178 | C |
| 36 | BA | 2179 | C |
| 36 | BA | 2180 | U |
| 36 | BA | 2185 | C |
| 36 | BA | 2186 | G |
| 36 | BA | 2187 | G |
| 36 | BA | 2189 | U |
| 36 | BA | 2190 | G |
| 36 | BA | 2193 | G |
| 36 | BA | 2198 | A |
| 36 | BA | 2199 | A |
| 36 | BA | 2200 | C |
| 36 | BA | 2207 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 36 | BA | 2208 | A |
| 36 | BA | 2218 | U |
| 36 | BA | 2219 | G |
| 36 | BA | 2221 | G |
| 36 | BA | 2225 | A |
| 36 | BA | 2238 | G |
| 36 | BA | 2239 | G |
| 36 | BA | 2268 | A |
| 36 | BA | 2275 | C |
| 36 | BA | 2279 | G |
| 36 | BA | 2283 | C |
| 36 | BA | 2287 | A |
| 36 | BA | 2288 | A |
| 36 | BA | 2305 | A |
| 36 | BA | 2307 | G |
| 36 | BA | 2308 | G |
| 36 | BA | 2309 | A |
| 36 | BA | 2311 | A |
| 36 | BA | 2313 | C |
| 36 | BA | 2319 | G |
| 36 | BA | 2320 | A |
| 36 | BA | 2327 | A |
| 36 | BA | 2336 | A |
| 36 | BA | 2343 | C |
| 36 | BA | 2345 | G |
| 36 | BA | 2347 | C |
| 36 | BA | 2361 | A |
| 36 | BA | 2383 | G |
| 36 | BA | 2385 | C |
| 36 | BA | 2392 | A |
| 36 | BA | 2399 | G |
| 36 | BA | 2402 | C |
| 36 | BA | 2406 | U |
| 36 | BA | 2423 | U |
| 36 | BA | 2424 | C |
| 36 | BA | 2425 | A |
| 36 | BA | 2429 | G |
| 36 | BA | 2430 | A |
| 36 | BA | 2439 | A |
| 36 | BA | 2441 | C |
| 36 | BA | 2448 | A |
| 36 | BA | 2465 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 36 | BA | 2469 | A |
| 36 | BA | 2470 | G |
| 36 | BA | 2476 | A |
| 36 | BA | 2477 | C |
| 36 | BA | 2478 | A |
| 36 | BA | 2482 | G |
| 36 | BA | 2484 | G |
| 36 | BA | 2494 | G |
| 36 | BA | 2502 | G |
| 36 | BA | 2505 | G |
| 36 | BA | 2518 | A |
| 36 | BA | 2524 | G |
| 36 | BA | 2529 | G |
| 36 | BA | 2543 | G |
| 36 | BA | 2554 | U |
| 36 | BA | 2566 | A |
| 36 | BA | 2567 | G |
| 36 | BA | 2573 | C |
| 36 | BA | 2578 | G |
| 36 | BA | 2602 | A |
| 36 | BA | 2610 | C |
| 36 | BA | 2611 | U |
| 36 | BA | 2612 | C |
| 36 | BA | 2615 | U |
| 36 | BA | 2630 | G |
| 36 | BA | 2641 | G |
| 36 | BA | 2646 | C |
| 36 | BA | 2654 | A |
| 36 | BA | 2657 | A |
| 36 | BA | 2673 | G |
| 36 | BA | 2690 | C |
| 36 | BA | 2691 | C |
| 36 | BA | 2712 | U |
| 36 | BA | 2712(A) | A |
| 36 | BA | 2713 | A |
| 36 | BA | 2720 | U |
| 36 | BA | 2726 | U |
| 36 | BA | 2750 | A |
| 36 | BA | 2751 | G |
| 36 | BA | 2752 | C |
| 36 | BA | 2757 | A |
| 36 | BA | 2759 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | BA | 2761 | G |
| 36 | BA | 2762 | G |
| 36 | BA | 2765 | A |
| 36 | BA | 2766 | G |
| 36 | BA | 2778 | A |
| 36 | BA | 2779 | U |
| 36 | BA | 2780 | G |
| 36 | BA | 2781 | A |
| 36 | BA | 2787 | C |
| 36 | BA | 2789 | C |
| 36 | BA | 2790 | A |
| 36 | BA | 2791 | C |
| 36 | BA | 2794 | C |
| 36 | BA | 2801 | A |
| 36 | BA | 2802 | G |
| 36 | BA | 2803 | C |
| 36 | BA | 2808 | U |
| 36 | BA | 2818 | G |
| 36 | BA | 2820 | A |
| 36 | BA | 2821 | A |
| 36 | BA | 2823 | A |
| 36 | BA | 2830 | G |
| 36 | BA | 2833 | G |
| 36 | BA | 2834 | G |
| 36 | BA | 2849 | U |
| 36 | BA | 2872 | G |
| 37 | BB | 2 | C |
| 37 | BB | 8 | U |
| 37 | BB | 13 | A |
| 37 | BB | 15 | A |
| 37 | BB | 16 | G |
| 37 | BB | 17 | C |
| 37 | BB | 21 | G |
| 37 | BB | 25 | A |
| 37 | BB | 27 | C |
| 37 | BB | 35 | U |
| 37 | BB | 40 | U |
| 37 | BB | 41 | U |
| 37 | BB | 42 | C |
| 37 | BB | 43 | C |
| 37 | BB | 45 | A |
| 37 | BB | 53 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | BB | 57 | A |
| 37 | BB | 68 | C |
| 37 | BB | 73 | A |
| 37 | BB | 75 | G |
| 37 | BB | 81 | G |
| 37 | BB | 82 | G |
| 37 | BB | 88 | C |
| 37 | BB | 110 | G |

All (113) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 30 | U |
| 1 | AA | 60 | A |
| 1 | AA | 79 | G |
| 1 | AA | 109 | A |
| 1 | AA | 115 | G |
| 1 | AA | 119 | A |
| 1 | AA | 197 | A |
| 1 | AA | 202 | U |
| 1 | AA | 243 | A |
| 1 | AA | 250 | A |
| 1 | AA | 251 | G |
| 1 | AA | 266 | G |
| 1 | AA | 274 | A |
| 1 | AA | 344 | A |
| 1 | AA | 347 | G |
| 1 | AA | 351 | G |
| 1 | AA | 353 | A |
| 1 | AA | 368 | U |
| 1 | AA | 369 | C |
| 1 | AA | 388 | G |
| 1 | AA | 412 | A |
| 1 | AA | 428 | G |
| 1 | AA | 429 | U |
| 1 | AA | 484 | G |
| 1 | AA | 495 | A |
| 1 | AA | 508 | C |
| 1 | AA | 534 | U |
| 1 | AA | 547 | A |
| 1 | AA | 560 | U |
| 1 | AA | 573 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 575 | G |
| 1 | AA | 687 | A |
| 1 | AA | 748 | C |
| 1 | AA | 792 | A |
| 1 | AA | 966 | G |
| 1 | AA | 968 | A |
| 1 | AA | 980 | C |
| 1 | AA | 982 | U |
| 1 | AA | 992 | U |
| 1 | AA | 1049 | U |
| 1 | AA | 1050 | G |
| 1 | AA | 1053 | G |
| 1 | AA | 1101 | A |
| 1 | AA | 1124 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1157 | A |
| 1 | AA | 1200 | C |
| 1 | AA | 1239 | A |
| 1 | AA | 1267 | C |
| 1 | AA | 1269 | A |
| 1 | AA | 1285 | A |
| 1 | AA | 1319 | A |
| 1 | AA | 1399 | C |
| 1 | AA | 1452 | C |
| 1 | AA | 1498 | U |
| 1 | AA | 1504 | G |
| 23 | AX | 26 | A |
| 24 | AY | 18 | G |
| 24 | AY | 75 | C |
| 36 | BA | 49 | A |
| 36 | BA | 71 | A |
| 36 | BA | 74 | A |
| 36 | BA | 197 | A |
| 36 | BA | 221 | A |
| 36 | BA | 331 | A |
| 36 | BA | 332 | A |
| 36 | BA | 387 | U |
| 36 | BA | 472 | A |
| 36 | BA | 481 | G |
| 36 | BA | 587 | C |
| 36 | BA | 603 | A |
| 36 | BA | 614(C) | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 36 | BA | 654(I) | C |
| 36 | BA | 654(K) | C |
| 36 | BA | 669 | G |
| 36 | BA | 752 | A |
| 36 | BA | 764 | A |
| 36 | BA | 790 | C |
| 36 | BA | 856 | C |
| 36 | BA | 1052 | C |
| 36 | BA | 1060 | U |
| 36 | BA | 1068 | G |
| 36 | BA | 1069 | A |
| 36 | BA | 1210 | A |
| 36 | BA | 1300 | U |
| 36 | BA | 1301 | A |
| 36 | BA | 1378 | A |
| 36 | BA | 1395 | A |
| 36 | BA | 1427 | A |
| 36 | BA | 1541 | G |
| 36 | BA | 1558 | A |
| 36 | BA | 1653 | G |
| 36 | BA | 1799 | G |
| 36 | BA | 1819 | A |
| 36 | BA | 1912 | A |
| 36 | BA | 1970 | A |
| 36 | BA | 1992 | G |
| 36 | BA | 2033 | A |
| 36 | BA | 2110 | G |
| 36 | BA | 2126 | A |
| 36 | BA | 2131 | G |
| 36 | BA | 2179 | C |
| 36 | BA | 2282 | G |
| 36 | BA | 2422 | A |
| 36 | BA | 2439 | A |
| 36 | BA | 2481 | G |
| 36 | BA | 2610 | C |
| 36 | BA | 2689 | U |
| 36 | BA | 2750 | A |
| 36 | BA | 2756 | U |
| 36 | BA | 2762 | G |
| 37 | BB | 34 | U |
| 37 | BB | 56 | G |

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | PSU | AY | 55 | 24 | 17,21,22 | 1.20 | 2 (11%) | 20,30,33 | 3.37 | 7 (35%) |
| 24 | H2U | AY | 17 | 24 | 18,21,22 | 0.91 | 1 (5%) | 21,30,33 | 1.77 | 4 (19%) |
| 24 | MIA | AY | 37 | 24 | 24,31,32 | 1.02 | 1 (4%) | 26,44,47 | 1.74 | 4 (15%) |
| 24 | OMC | AY | 32 | 24 | 15,22,23 | 0.78 | 0 | 17,31,34 | 1.15 | 2 (11%) |
| 24 | 5MU | AY | 54 | 24 | 15,22,23 | 1.20 | 1 (6%) | 16,32,35 | 3.76 | 2 (12%) |
| 24 | H2U | AY | 20 | 24 | 18,21,22 | 0.87 | 0 | 21,30,33 | 1.93 | 6 (28%) |
| 24 | 7MG | AY | 46 | 24 | 22,26,27 | 1.21 | 2 (9%) | 28,39,42 | 2.31 | 5 (17%) |
| 24 | H2U | AY | 16 | 24 | 18,21,22 | 0.81 | 0 | 21,30,33 | 1.87 | 5 (23%) |
| 24 | 4SU | AY | 8 | 24 | 14,21,22 | 1.39 | 3 (21%) | 15,30,33 | 2.58 | 2 (13%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 24 | PSU | AY | 55 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | H2U | AY | 17 | 24 | - | 5/7/38/39 | 0/2/2/2 |
| 24 | MIA | AY | 37 | 24 | - | 3/11/33/34 | 0/3/3/3 |
| 24 | OMC | AY | 32 | 24 | - | 0/7/27/28 | 0/2/2/2 |
| 24 | 5MU | AY | 54 | 24 | - | 0/5/25/26 | 0/2/2/2 |
| 24 | H2U | AY | 20 | 24 | - | 4/7/38/39 | 0/2/2/2 |
| 24 | 7MG | AY | 46 | 24 | - | 6/7/37/38 | 0/3/3/3 |
| 24 | H2U | AY | 16 | 24 | - | 2/7/38/39 | 0/2/2/2 |
| 24 | 4SU | AY | 8 | 24 | - | 1/5/25/26 | 0/2/2/2 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 24 | AY | 46 | 7MG | C6-N1 | 3.81 | 1.39 | 1.33 |
| 24 | AY | 8 | 4SU | C5-C4 | 3.53 | 1.42 | 1.38 |
| 24 | AY | 54 | 5MU | C4-N3 | 3.46 | 1.39 | 1.33 |
| 24 | AY | 55 | PSU | C4-N3 | 3.20 | 1.38 | 1.33 |
| 24 | AY | 46 | 7MG | C8-N9 | -3.13 | 1.38 | 1.45 |
| 24 | AY | 55 | PSU | C6-N1 | 2.67 | 1.40 | 1.34 |
| 24 | AY | 8 | 4SU | C6-N1 | 2.26 | 1.38 | 1.35 |
| 24 | AY | 8 | 4SU | C6-C5 | -2.24 | 1.33 | 1.38 |
| 24 | AY | 17 | H2U | C2-N1 | 2.23 | 1.38 | 1.35 |
| 24 | AY | 37 | MIA | C8-N7 | -2.06 | 1.31 | 1.34 |

All (37) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 24 | AY | 54 | 5MU | C4-N3-C2 | 14.70 | 127.55 | 115.14 |
| 24 | AY | 55 | PSU | N1-C2-N3 | -10.53 | 120.06 | 128.43 |
| 24 | AY | 8 | 4SU | C2-N3-C4 | 7.83 | 126.50 | 115.15 |
| 24 | AY | 46 | 7MG | N7-C8-N9 | 6.89 | 113.23 | 103.38 |
| 24 | AY | 55 | PSU | C4-N3-C2 | 6.80 | 120.89 | 115.14 |
| 24 | AY | 8 | 4SU | C5-C4-N3 | -5.97 | 115.85 | 123.83 |
| 24 | AY | 46 | 7MG | C6-N1-C2 | 5.81 | 125.16 | 115.93 |
| 24 | AY | 46 | 7MG | C5-C6-N1 | -5.65 | 111.54 | 123.14 |
| 24 | AY | 37 | MIA | C11-S10-C2 | 4.91 | 105.94 | 102.27 |
| 24 | AY | 17 | H2U | C4-N3-C2 | -4.75 | 121.85 | 125.79 |
| 24 | AY | 16 | H2U | C4-N3-C2 | -4.56 | 122.01 | 125.79 |
| 24 | AY | 20 | H2U | C4-N3-C2 | -4.47 | 122.08 | 125.79 |
| 24 | AY | 55 | PSU | C5-C4-N3 | -4.47 | 119.61 | 125.36 |
| 24 | AY | 16 | H2U | N3-C2-N1 | 4.33 | 121.23 | 116.65 |
| 24 | AY | 37 | MIA | C5-C6-N1 | -4.16 | 117.36 | 120.81 |
| 24 | AY | 20 | H2U | N3-C2-N1 | 4.15 | 121.04 | 116.65 |
| 24 | AY | 17 | H2U | N3-C2-N1 | 4.07 | 120.96 | 116.65 |
| 24 | AY | 37 | MIA | C12-N6-C6 | 3.93 | 128.36 | 122.55 |
| 24 | AY | 16 | H2U | C5-C4-N3 | 3.65 | 120.75 | 116.65 |
| 24 | AY | 17 | H2U | C5-C4-N3 | 3.65 | 120.75 | 116.65 |
| 24 | AY | 32 | OMC | C2-N3-C4 | 3.59 | 119.98 | 116.34 |
| 24 | AY | 55 | PSU | C6-N1-C2 | 3.57 | 121.24 | 115.36 |
| 24 | AY | 20 | H2U | C5-C4-N3 | 3.52 | 120.60 | 116.65 |
| 24 | AY | 55 | PSU | C5-C6-N1 | -3.36 | 120.31 | 124.44 |
| 24 | AY | 20 | H2U | O4'-C1'-N1 | 3.31 | 113.81 | 109.30 |
| 24 | AY | 46 | 7MG | C6-C5-C4 | 3.27 | 118.71 | 115.20 |
| 24 | AY | 37 | MIA | C2-N3-C4 | -3.26 | 110.83 | 115.32 |
| 24 | AY | 55 | PSU | O3'-C3'-C2' | 3.06 | 121.72 | 111.82 |
| 24 | AY | 55 | PSU | O3'-C3'-C4' | 2.50 | 118.26 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | AY | 46 | 7MG | C4-C5-N7 | 2.46 | 110.74 | 106.98 |
| 24 | AY | 16 | H2U | O2-C2-N1 | -2.44 | 120.04 | 123.11 |
| 24 | AY | 32 | OMC | CM2-O2'-C2' | -2.33 | 108.41 | 114.52 |
| 24 | AY | 20 | H2U | O4'-C1'-C2' | -2.28 | 101.66 | 106.64 |
| 24 | AY | 16 | H2U | O4'-C1'-N1 | 2.21 | 112.31 | 109.30 |
| 24 | AY | 20 | H2U | O2-C2-N1 | -2.06 | 120.52 | 123.11 |
| 24 | AY | 17 | H2U | O2-C2-N1 | -2.05 | 120.53 | 123.11 |
| 24 | AY | 54 | 5MU | C5M-C5-C6 | 2.01 | 122.92 | 118.68 |

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | AY | 17 | H2U | O4'-C1'-N1-C6 |
| 24 | AY | 37 | MIA | C5-C6-N6-C12 |
| 24 | AY | 20 | H2U | O4'-C1'-N1-C6 |
| 24 | AY | 20 | H2U | O4'-C4'-C5'-O5' |
| 24 | AY | 46 | 7MG | O4'-C4'-C5'-O5' |
| 24 | AY | 20 | H2U | O4'-C1'-N1-C2 |
| 24 | AY | 37 | MIA | N1-C6-N6-C12 |
| 24 | AY | 46 | 7MG | C2'-C1'-N9-C8 |
| 24 | AY | 46 | 7MG | C2'-C1'-N9-C4 |
| 24 | AY | 46 | 7MG | C3'-C4'-C5'-O5' |
| 24 | AY | 16 | H2U | C4'-C5'-O5'-P |
| 24 | AY | 20 | H2U | C3'-C4'-C5'-O5' |
| 24 | AY | 17 | H2U | C4'-C5'-O5'-P |
| 24 | AY | 37 | MIA | N6-C12-C13-C14 |
| 24 | AY | 17 | H2U | O4'-C1'-N1-C2 |
| 24 | AY | 46 | 7MG | O4'-C1'-N9-C8 |
| 24 | AY | 46 | 7MG | C4'-C5'-O5'-P |
| 24 | AY | 17 | H2U | O4'-C4'-C5'-O5' |
| 24 | AY | 16 | H2U | O4'-C4'-C5'-O5' |
| 24 | AY | 8 | 4SU | O4'-C4'-C5'-O5' |
| 24 | AY | 17 | H2U | C2'-C1'-N1-C2 |

There are no ring outliers.

7 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | AY | 55 | PSU | 1 | 0 |
| 24 | AY | 17 | H2U | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | AY | 37 | MIA | 2 | 0 |
| 24 | AY | 54 | 5MU | 2 | 0 |
| 24 | AY | 20 | H2U | 3 | 0 |
| 24 | AY | 16 | H2U | 1 | 0 |
| 24 | AY | 8 | 4SU | 3 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 59 | PAR | AA | 1601 | - | 45,45,45 | 1.57 | 7 (15%) | 64,67,67 | 1.26 | 6 (9%) |
| 61 | GCP | AZ | 501 | 62 | 26,34,34 | 2.53 | 7 (26%) | 31,54,54 | 2.00 | 7 (22%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 59 | PAR | AA | 1601 | - | - | 4/18/94/94 | 0/4/4/4 |
| 61 | GCP | AZ | 501 | 62 | - | 14/18/38/38 | 0/3/3/3 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 61 | AZ | 501 | GCP | C6-N1 | 7.35 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 61 | AZ | 501 | GCP | C5-C6 | -5.81 | 1.42 | 1.52 |
| 61 | AZ | 501 | GCP | C4-N9 | -5.68 | 1.40 | 1.47 |
| 59 | AA | 1601 | PAR | C64-C54 | 5.14 | 1.59 | 1.52 |
| 61 | AZ | 501 | GCP | PG-O2G | -3.93 | 1.45 | 1.54 |
| 59 | AA | 1601 | PAR | C52-C42 | 3.44 | 1.59 | 1.52 |
| 59 | AA | 1601 | PAR | O54-C14 | 2.94 | 1.49 | 1.41 |
| 61 | AZ | 501 | GCP | C8-N9 | -2.49 | 1.37 | 1.45 |
| 61 | AZ | 501 | GCP | PG-O3G | -2.43 | 1.49 | 1.54 |
| 59 | AA | 1601 | PAR | O54-C54 | 2.39 | 1.50 | 1.44 |
| 59 | AA | 1601 | PAR | O51-C11 | 2.24 | 1.47 | 1.41 |
| 61 | AZ | 501 | GCP | C5-C4 | -2.23 | 1.39 | 1.53 |
| 59 | AA | 1601 | PAR | C14-C24 | 2.06 | 1.56 | 1.52 |
| 59 | AA | 1601 | PAR | C11-C21 | 2.02 | 1.56 | 1.52 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 61 | AZ | 501 | GCP | C4-C5-N7 | 7.75 | 112.74 | 102.46 |
| 59 | AA | 1601 | PAR | O33-C14-C24 | 4.78 | 116.45 | 108.22 |
| 59 | AA | 1601 | PAR | O54-C54-C64 | 3.88 | 113.23 | 106.01 |
| 61 | AZ | 501 | GCP | O6-C6-N1 | -3.59 | 117.86 | 122.69 |
| 59 | AA | 1601 | PAR | C14-O54-C54 | 3.57 | 120.69 | 113.69 |
| 61 | AZ | 501 | GCP | O3G-PG-O2G | 2.90 | 116.55 | 108.08 |
| 59 | AA | 1601 | PAR | O52-C13-C23 | 2.78 | 113.72 | 107.96 |
| 61 | AZ | 501 | GCP | O6-C6-C5 | 2.63 | 125.23 | 119.86 |
| 61 | AZ | 501 | GCP | O2G-PG-O1G | -2.51 | 105.75 | 112.39 |
| 61 | AZ | 501 | GCP | O3G-PG-O1G | -2.35 | 106.17 | 112.39 |
| 61 | AZ | 501 | GCP | O2'-C2'-C3' | 2.23 | 119.03 | 111.82 |
| 59 | AA | 1601 | PAR | O11-C11-C21 | 2.16 | 111.93 | 108.22 |
| 59 | AA | 1601 | PAR | C22-C32-C42 | 2.06 | 114.75 | 109.53 |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 59 | AA | 1601 | PAR | C44-C54-C64-N64 |
| 59 | AA | 1601 | PAR | O54-C54-C64-N64 |
| 61 | AZ | 501 | GCP | PB-C3B-PG-O1G |
| 61 | AZ | 501 | GCP | PB-C3B-PG-O2G |
| 61 | AZ | 501 | GCP | PG-C3B-PB-O1B |
| 61 | AZ | 501 | GCP | PG-C3B-PB-O2B |
| 61 | AZ | 501 | GCP | PG-C3B-PB-O3A |

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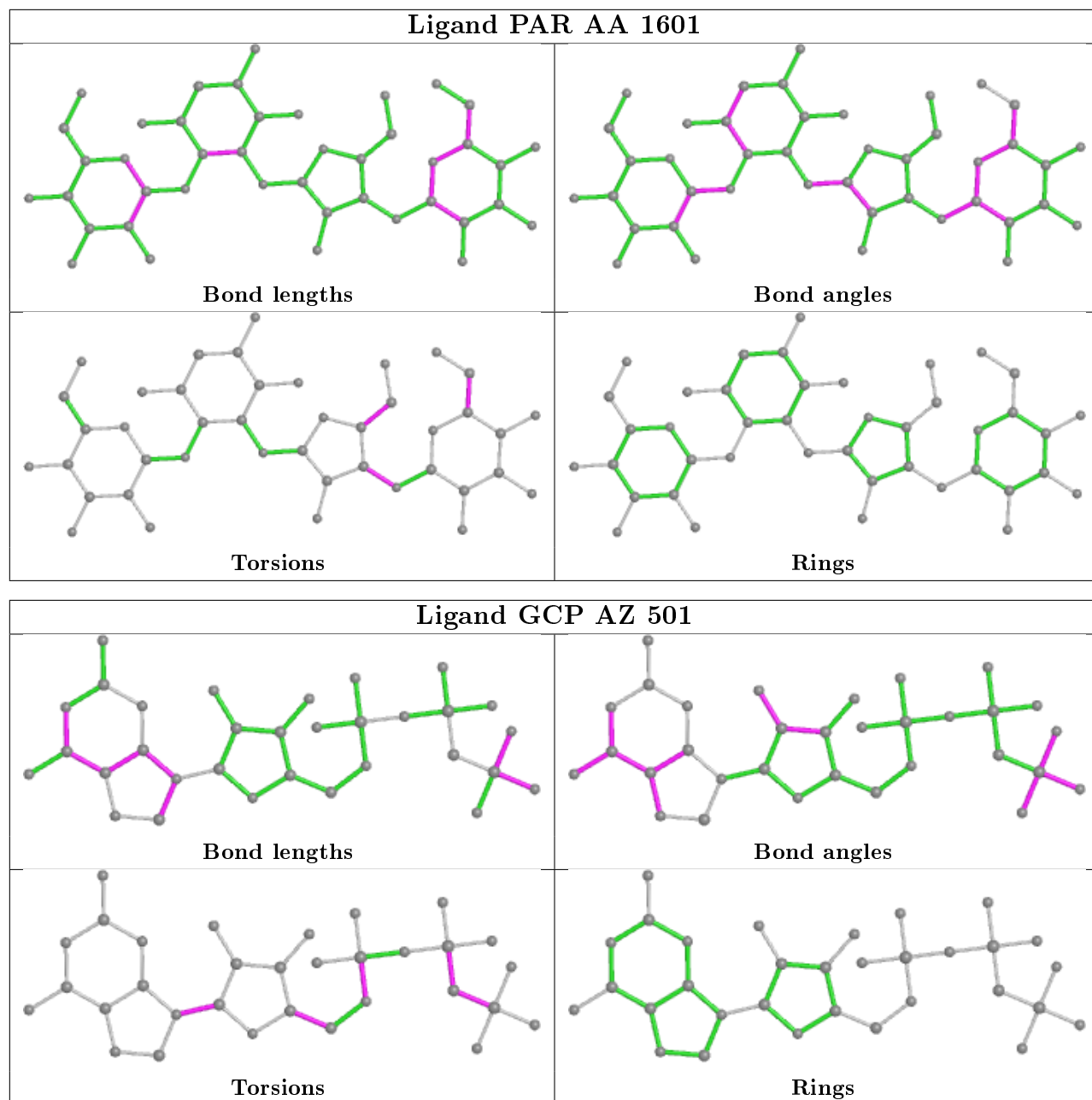
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 61 | AZ | 501 | GCP | C5'-O5'-PA-O1A |
| 61 | AZ | 501 | GCP | C5'-O5'-PA-O2A |
| 61 | AZ | 501 | GCP | O4'-C4'-C5'-O5' |
| 61 | AZ | 501 | GCP | O4'-C1'-N9-C4 |
| 61 | AZ | 501 | GCP | C2'-C1'-N9-C8 |
| 61 | AZ | 501 | GCP | C2'-C1'-N9-C4 |
| 61 | AZ | 501 | GCP | C3'-C4'-C5'-O5' |
| 59 | AA | 1601 | PAR | C33-C43-C53-O53 |
| 61 | AZ | 501 | GCP | PB-C3B-PG-O3G |
| 61 | AZ | 501 | GCP | C5'-O5'-PA-O3A |
| 59 | AA | 1601 | PAR | C43-C33-O33-C14 |

There are no ring outliers.

2 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 59 | AA | 1601 | PAR | 2 | 0 |
| 61 | AZ | 501 | GCP | 5 | 0 |

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1504/1522 (98%) | 0.03 | 34 (2%) 60 39 | 25, 58, 149, 200 | 0 |
| 2 | AB | 234/256 (91%) | 0.03 | 12 (5%) 28 13 | 35, 74, 133, 147 | 0 |
| 3 | AC | 206/239 (86%) | -0.35 | 1 (0%) 91 81 | 34, 57, 91, 103 | 0 |
| 4 | AD | 208/209 (99%) | -0.08 | 2 (0%) 82 67 | 44, 68, 96, 102 | 0 |
| 5 | AE | 150/162 (92%) | -0.34 | 0 100 100 | 33, 52, 82, 102 | 0 |
| 6 | AF | 101/101 (100%) | -0.12 | 1 (0%) 82 67 | 52, 74, 89, 100 | 0 |
| 7 | AG | 155/156 (99%) | -0.24 | 2 (1%) 77 59 | 46, 71, 96, 119 | 0 |
| 8 | AH | 138/138 (100%) | -0.19 | 1 (0%) 87 75 | 38, 58, 78, 87 | 0 |
| 9 | AI | 127/128 (99%) | 0.12 | 5 (3%) 39 20 | 41, 74, 103, 112 | 0 |
| 10 | AJ | 98/105 (93%) | 0.21 | 6 (6%) 21 9 | 35, 75, 111, 117 | 0 |
| 11 | AK | 119/129 (92%) | -0.09 | 4 (3%) 45 24 | 39, 59, 95, 117 | 0 |
| 12 | AL | 124/135 (91%) | -0.12 | 5 (4%) 38 19 | 36, 48, 77, 112 | 0 |
| 13 | AM | 124/126 (98%) | 0.39 | 8 (6%) 18 8 | 50, 80, 107, 132 | 0 |
| 14 | AN | 60/61 (98%) | -0.18 | 0 100 100 | 32, 48, 76, 83 | 0 |
| 15 | AO | 88/89 (98%) | -0.02 | 0 100 100 | 42, 64, 89, 93 | 0 |
| 16 | AP | 83/88 (94%) | 0.02 | 0 100 100 | 50, 65, 85, 114 | 0 |
| 17 | AQ | 99/105 (94%) | 0.10 | 0 100 100 | 45, 70, 95, 97 | 0 |
| 18 | AR | 70/88 (79%) | -0.02 | 1 (1%) 75 56 | 46, 65, 97, 111 | 0 |
| 19 | AS | 78/93 (83%) | 0.41 | 9 (11%) 4 2 | 58, 84, 115, 123 | 0 |
| 20 | AT | 99/106 (93%) | 0.73 | 11 (11%) 5 2 | 56, 86, 128, 131 | 0 |
| 21 | AU | 24/27 (88%) | 0.05 | 0 100 100 | 52, 64, 79, 91 | 0 |
| 22 | AV | 76/76 (100%) | 1.00 | 11 (14%) 2 1 | 35, 127, 168, 176 | 0 |
| 22 | AW | 76/76 (100%) | 2.16 | 37 (48%) 0 0 | 60, 175, 200, 200 | 0 |
| 23 | AX | 14/14 (100%) | 0.74 | 1 (7%) 16 6 | 35, 57, 98, 114 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 24 | AY | 68/77 (88%) | 0.40 | 3 (4%) 34 17 | 47, 110, 160, 196 | 0 |
| 25 | AZ | 405/405 (100%) | 0.22 | 19 (4%) 31 15 | 57, 100, 135, 143 | 0 |
| 26 | B0 | 84/85 (98%) | 0.75 | 9 (10%) 6 2 | 59, 75, 116, 136 | 0 |
| 27 | B1 | 93/98 (94%) | 0.25 | 4 (4%) 35 17 | 44, 65, 106, 114 | 0 |
| 28 | B2 | 71/72 (98%) | 0.71 | 7 (9%) 7 2 | 75, 108, 124, 146 | 0 |
| 29 | B3 | 59/60 (98%) | 0.79 | 7 (11%) 4 2 | 72, 93, 110, 135 | 0 |
| 30 | B4 | 44/71 (61%) | 0.52 | 2 (4%) 33 16 | 103, 134, 142, 149 | 0 |
| 31 | B5 | 59/60 (98%) | 0.54 | 4 (6%) 17 7 | 57, 89, 151, 155 | 0 |
| 32 | B6 | 50/54 (92%) | 0.93 | 6 (12%) 4 2 | 52, 81, 99, 108 | 0 |
| 33 | B7 | 48/49 (97%) | 0.27 | 1 (2%) 63 43 | 49, 59, 99, 117 | 0 |
| 34 | B8 | 63/65 (96%) | 0.35 | 2 (3%) 47 25 | 53, 73, 91, 106 | 0 |
| 35 | B9 | 37/37 (100%) | 0.97 | 6 (16%) 1 1 | 61, 82, 96, 97 | 0 |
| 36 | BA | 2901/2915 (99%) | 0.37 | 211 (7%) 15 6 | 28, 76, 190, 200 | 0 |
| 37 | BB | 119/122 (97%) | 0.14 | 4 (3%) 45 24 | 74, 103, 134, 150 | 0 |
| 38 | BC | 228/229 (99%) | 3.41 | 148 (64%) 0 0 | 125, 160, 177, 186 | 0 |
| 39 | BD | 275/276 (99%) | -0.20 | 4 (1%) 73 54 | 24, 45, 71, 93 | 0 |
| 40 | BE | 204/206 (99%) | 0.34 | 8 (3%) 39 20 | 50, 77, 128, 135 | 0 |
| 41 | BF | 207/210 (98%) | 0.66 | 22 (10%) 6 2 | 47, 97, 149, 155 | 0 |
| 42 | BG | 181/182 (99%) | 0.42 | 13 (7%) 15 6 | 79, 101, 126, 137 | 0 |
| 43 | BH | 159/180 (88%) | 0.86 | 27 (16%) 1 0 | 80, 119, 144, 150 | 0 |
| 44 | BJ | 0/130 | - | - | - | - |
| 45 | BK | 0/140 | - | - | - | - |
| 46 | BN | 138/140 (98%) | 0.42 | 5 (3%) 42 22 | 68, 93, 127, 132 | 0 |
| 47 | BO | 122/122 (100%) | -0.23 | 0 100 100 | 42, 59, 72, 83 | 0 |
| 48 | BP | 146/150 (97%) | 0.70 | 10 (6%) 17 7 | 55, 90, 121, 146 | 0 |
| 49 | BQ | 141/141 (100%) | 0.05 | 5 (3%) 44 23 | 50, 68, 100, 134 | 0 |
| 50 | BR | 117/118 (99%) | 0.29 | 3 (2%) 56 33 | 58, 81, 100, 105 | 0 |
| 51 | BS | 98/112 (87%) | 0.55 | 9 (9%) 9 3 | 70, 93, 121, 126 | 0 |
| 52 | BT | 137/146 (93%) | 0.35 | 10 (7%) 15 6 | 54, 80, 139, 161 | 0 |
| 53 | BU | 117/118 (99%) | 0.31 | 6 (5%) 28 13 | 68, 88, 113, 120 | 0 |
| 54 | BV | 101/101 (100%) | 0.96 | 13 (12%) 3 1 | 67, 117, 132, 137 | 0 |
| 55 | BW | 113/113 (100%) | 0.35 | 4 (3%) 44 23 | 65, 88, 115, 135 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------|------|-----------------------|-------|
| 56 | BX | 92/96 (95%) | 0.48 | 6 (6%) | 18 8 | 65, 85, 101, 107 | 0 |
| 57 | BY | 100/110 (90%) | 1.72 | 40 (40%) | 0 0 | 94, 125, 149, 158 | 0 |
| 58 | BZ | 176/206 (85%) | 0.60 | 15 (8%) | 10 4 | 69, 102, 125, 134 | 0 |
| All | All | 11008/11625 (94%) | 0.34 | 784 (7%) | 16 6 | 24, 77, 158, 200 | 0 |

All (784) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 38 | BC | 220 | PRO | 12.6 |
| 58 | BZ | 114 | GLY | 12.1 |
| 38 | BC | 111 | ASP | 11.3 |
| 38 | BC | 123 | VAL | 11.1 |
| 36 | BA | 654(P) | C | 11.0 |
| 38 | BC | 79 | LYS | 10.6 |
| 38 | BC | 109 | ASP | 10.5 |
| 38 | BC | 127 | LEU | 10.3 |
| 36 | BA | 654(Q) | C | 10.1 |
| 38 | BC | 88 | GLU | 10.0 |
| 38 | BC | 2 | LYS | 9.9 |
| 36 | BA | 654(O) | G | 9.8 |
| 38 | BC | 1 | PRO | 9.6 |
| 38 | BC | 62 | VAL | 9.6 |
| 36 | BA | 654(L) | G | 9.2 |
| 36 | BA | 1073 | A | 9.1 |
| 38 | BC | 131 | LEU | 9.0 |
| 38 | BC | 3 | HIS | 8.9 |
| 22 | AW | 17 | C | 8.8 |
| 22 | AW | 18 | G | 8.8 |
| 36 | BA | 654(H) | G | 8.7 |
| 38 | BC | 107 | TRP | 8.7 |
| 36 | BA | 654(M) | C | 8.6 |
| 36 | BA | 654(T) | C | 8.4 |
| 38 | BC | 133 | PRO | 8.4 |
| 36 | BA | 1074 | G | 8.3 |
| 48 | BP | 150 | ALA | 8.3 |
| 28 | B2 | 72 | ALA | 8.2 |
| 13 | AM | 124 | PRO | 8.2 |
| 38 | BC | 8 | ARG | 8.2 |
| 36 | BA | 654(N) | G | 8.1 |
| 49 | BQ | 140 | ALA | 8.0 |
| 26 | B0 | 2 | ALA | 8.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 36 | BA | 1075 | C | 7.9 |
| 36 | BA | 654(B) | C | 7.9 |
| 13 | AM | 123 | ALA | 7.8 |
| 36 | BA | 271(N) | U | 7.8 |
| 38 | BC | 29 | VAL | 7.8 |
| 38 | BC | 163 | PHE | 7.8 |
| 36 | BA | 1104 | C | 7.8 |
| 38 | BC | 144 | THR | 7.8 |
| 38 | BC | 146 | GLY | 7.7 |
| 38 | BC | 91 | ALA | 7.7 |
| 36 | BA | 1091 | G | 7.7 |
| 36 | BA | 1093 | G | 7.7 |
| 36 | BA | 1064 | C | 7.7 |
| 38 | BC | 39 | GLU | 7.7 |
| 36 | BA | 2802 | G | 7.6 |
| 36 | BA | 1090 | U | 7.5 |
| 36 | BA | 1534 | U | 7.5 |
| 36 | BA | 654(D) | G | 7.5 |
| 36 | BA | 1068 | G | 7.5 |
| 42 | BG | 49 | ASP | 7.4 |
| 54 | BV | 36 | PRO | 7.4 |
| 38 | BC | 90 | GLY | 7.4 |
| 36 | BA | 654(A) | G | 7.3 |
| 29 | B3 | 1 | MET | 7.3 |
| 38 | BC | 36 | LYS | 7.2 |
| 38 | BC | 93 | TYR | 7.1 |
| 38 | BC | 38 | ASP | 7.0 |
| 36 | BA | 1103 | A | 7.0 |
| 42 | BG | 48 | GLU | 7.0 |
| 36 | BA | 2897 | U | 6.9 |
| 36 | BA | 1535 | A | 6.9 |
| 38 | BC | 28 | LEU | 6.9 |
| 38 | BC | 105 | ASP | 6.9 |
| 22 | AW | 12 | U | 6.8 |
| 1 | AA | 81 | U | 6.7 |
| 38 | BC | 17 | ASN | 6.7 |
| 36 | BA | 654(E) | G | 6.7 |
| 36 | BA | 2795 | G | 6.7 |
| 38 | BC | 97 | GLU | 6.6 |
| 36 | BA | 654(J) | A | 6.6 |
| 38 | BC | 135 | GLY | 6.5 |
| 38 | BC | 89 | ALA | 6.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 43 | BH | 53 | GLU | 6.5 |
| 38 | BC | 27 | ARG | 6.5 |
| 38 | BC | 219 | GLY | 6.4 |
| 52 | BT | 135 | ALA | 6.4 |
| 36 | BA | 1094 | U | 6.4 |
| 13 | AM | 121 | LYS | 6.3 |
| 22 | AW | 15 | G | 6.3 |
| 36 | BA | 1080 | C | 6.3 |
| 38 | BC | 108 | MET | 6.3 |
| 22 | AV | 19 | G | 6.2 |
| 36 | BA | 654 | A | 6.2 |
| 36 | BA | 654(C) | G | 6.2 |
| 36 | BA | 1088 | A | 6.2 |
| 31 | B5 | 58 | LEU | 6.1 |
| 38 | BC | 31 | GLU | 6.1 |
| 38 | BC | 102 | LYS | 6.1 |
| 38 | BC | 104 | LEU | 6.1 |
| 38 | BC | 222 | VAL | 6.1 |
| 36 | BA | 1078 | U | 6.1 |
| 36 | BA | 1174 | A | 6.0 |
| 42 | BG | 50 | ALA | 6.0 |
| 38 | BC | 210 | ARG | 6.0 |
| 36 | BA | 1076 | C | 6.0 |
| 38 | BC | 106 | GLY | 5.9 |
| 22 | AW | 22 | G | 5.9 |
| 1 | AA | 89 | C | 5.9 |
| 38 | BC | 80 | GLY | 5.9 |
| 38 | BC | 143 | GLY | 5.9 |
| 36 | BA | 2161 | C | 5.9 |
| 36 | BA | 1087 | G | 5.8 |
| 41 | BF | 2 | LYS | 5.8 |
| 38 | BC | 126 | LYS | 5.8 |
| 22 | AW | 56 | C | 5.8 |
| 36 | BA | 654(U) | A | 5.8 |
| 36 | BA | 2799 | C | 5.8 |
| 38 | BC | 221 | SER | 5.8 |
| 38 | BC | 83 | ILE | 5.7 |
| 38 | BC | 112 | ALA | 5.7 |
| 36 | BA | 654(R) | C | 5.7 |
| 38 | BC | 223 | ARG | 5.7 |
| 38 | BC | 130 | ILE | 5.7 |
| 52 | BT | 1 | MET | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | AA | 88 | A | 5.6 |
| 26 | B0 | 5 | LYS | 5.6 |
| 57 | BY | 89 | PHE | 5.6 |
| 51 | BS | 108 | GLY | 5.6 |
| 36 | BA | 654(K) | C | 5.6 |
| 26 | B0 | 3 | HIS | 5.6 |
| 36 | BA | 2145 | C | 5.5 |
| 36 | BA | 1099 | G | 5.5 |
| 36 | BA | 2144 | U | 5.5 |
| 57 | BY | 55 | TYR | 5.5 |
| 35 | B9 | 1 | MET | 5.5 |
| 12 | AL | 128 | ALA | 5.5 |
| 38 | BC | 176 | GLY | 5.5 |
| 58 | BZ | 115 | GLY | 5.5 |
| 38 | BC | 175 | VAL | 5.5 |
| 38 | BC | 98 | GLU | 5.4 |
| 41 | BF | 25 | PRO | 5.4 |
| 30 | B4 | 42 | PHE | 5.4 |
| 38 | BC | 125 | SER | 5.4 |
| 38 | BC | 35 | ALA | 5.4 |
| 36 | BA | 1067 | A | 5.3 |
| 1 | AA | 80 | G | 5.3 |
| 54 | BV | 25 | LEU | 5.3 |
| 1 | AA | 82 | U | 5.3 |
| 38 | BC | 78 | ALA | 5.2 |
| 38 | BC | 4 | GLY | 5.2 |
| 40 | BE | 69 | LYS | 5.2 |
| 36 | BA | 2146 | C | 5.2 |
| 43 | BH | 13 | LYS | 5.2 |
| 57 | BY | 2 | ARG | 5.1 |
| 26 | B0 | 85 | ALA | 5.1 |
| 36 | BA | 654(S) | G | 5.1 |
| 38 | BC | 103 | ILE | 5.1 |
| 22 | AV | 17 | C | 5.1 |
| 36 | BA | 1509 | C | 5.1 |
| 36 | BA | 1095 | A | 5.1 |
| 38 | BC | 228 | SER | 5.1 |
| 22 | AW | 11 | C | 5.1 |
| 41 | BF | 18 | ARG | 5.1 |
| 58 | BZ | 162 | GLU | 5.0 |
| 36 | BA | 2133 | G | 5.0 |
| 36 | BA | 2125 | G | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 38 | BC | 73 | ARG | 4.9 |
| 36 | BA | 1066 | U | 4.9 |
| 36 | BA | 654(F) | C | 4.9 |
| 36 | BA | 1057 | A | 4.9 |
| 38 | BC | 50 | ASP | 4.8 |
| 2 | AB | 128 | GLU | 4.8 |
| 31 | B5 | 60 | VAL | 4.8 |
| 36 | BA | 896 | A | 4.8 |
| 36 | BA | 654(G) | C | 4.8 |
| 38 | BC | 92 | ASP | 4.7 |
| 49 | BQ | 141 | GLN | 4.7 |
| 38 | BC | 60 | GLY | 4.7 |
| 43 | BH | 83 | TYR | 4.7 |
| 38 | BC | 12 | GLU | 4.7 |
| 31 | B5 | 59 | GLU | 4.7 |
| 38 | BC | 48 | GLY | 4.7 |
| 22 | AW | 14 | A | 4.7 |
| 38 | BC | 136 | LEU | 4.6 |
| 38 | BC | 227 | HIS | 4.6 |
| 38 | BC | 71 | GLN | 4.6 |
| 36 | BA | 1079 | C | 4.6 |
| 41 | BF | 1 | MET | 4.6 |
| 55 | BW | 112 | GLY | 4.6 |
| 38 | BC | 224 | ILE | 4.5 |
| 36 | BA | 1089 | G | 4.5 |
| 38 | BC | 122 | ALA | 4.5 |
| 36 | BA | 2162 | G | 4.5 |
| 36 | BA | 1063 | G | 4.5 |
| 32 | B6 | 42 | TRP | 4.4 |
| 36 | BA | 1071 | G | 4.4 |
| 10 | AJ | 36 | GLY | 4.4 |
| 38 | BC | 7 | TYR | 4.4 |
| 35 | B9 | 37 | GLY | 4.4 |
| 38 | BC | 99 | ILE | 4.4 |
| 36 | BA | 2892 | A | 4.4 |
| 1 | AA | 83 | U | 4.4 |
| 38 | BC | 87 | GLU | 4.4 |
| 57 | BY | 28 | LYS | 4.4 |
| 38 | BC | 181 | PRO | 4.4 |
| 38 | BC | 16 | PRO | 4.4 |
| 36 | BA | 1065 | U | 4.4 |
| 36 | BA | 1097 | U | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | B5 | 2 | ALA | 4.4 |
| 38 | BC | 120 | MET | 4.4 |
| 22 | AW | 50 | U | 4.4 |
| 22 | AW | 55 | U | 4.4 |
| 40 | BE | 204 | ALA | 4.4 |
| 57 | BY | 71 | LYS | 4.4 |
| 38 | BC | 67 | GLY | 4.4 |
| 1 | AA | 470 | C | 4.3 |
| 36 | BA | 1059 | G | 4.3 |
| 41 | BF | 24 | LEU | 4.3 |
| 51 | BS | 81 | GLY | 4.3 |
| 22 | AW | 13 | C | 4.3 |
| 36 | BA | 2894 | G | 4.3 |
| 22 | AW | 44 | G | 4.3 |
| 38 | BC | 182 | PRO | 4.2 |
| 46 | BN | 53 | VAL | 4.2 |
| 13 | AM | 122 | LYS | 4.2 |
| 11 | AK | 129 | SER | 4.2 |
| 36 | BA | 508 | G | 4.2 |
| 1 | AA | 96 | U | 4.2 |
| 7 | AG | 156 | TRP | 4.2 |
| 36 | BA | 2143 | C | 4.2 |
| 36 | BA | 889 | C | 4.1 |
| 38 | BC | 110 | PHE | 4.1 |
| 36 | BA | 2796 | U | 4.1 |
| 43 | BH | 57 | ASP | 4.1 |
| 26 | B0 | 7 | LEU | 4.1 |
| 22 | AW | 46 | G | 4.1 |
| 36 | BA | 1533 | G | 4.1 |
| 36 | BA | 2789 | C | 4.1 |
| 54 | BV | 17 | GLY | 4.1 |
| 38 | BC | 70 | LYS | 4.1 |
| 38 | BC | 69 | GLY | 4.0 |
| 1 | AA | 84 | U | 4.0 |
| 38 | BC | 9 | ALA | 4.0 |
| 41 | BF | 19 | GLU | 4.0 |
| 22 | AW | 19 | G | 4.0 |
| 36 | BA | 1176 | G | 4.0 |
| 1 | AA | 1267 | C | 4.0 |
| 38 | BC | 18 | LYS | 4.0 |
| 22 | AW | 48 | C | 3.9 |
| 57 | BY | 45 | VAL | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 56 | BX | 68 | ARG | 3.9 |
| 36 | BA | 10 | G | 3.9 |
| 20 | AT | 106 | ALA | 3.9 |
| 46 | BN | 133 | GLN | 3.9 |
| 38 | BC | 119 | VAL | 3.9 |
| 36 | BA | 275 | G | 3.9 |
| 36 | BA | 2131 | G | 3.9 |
| 38 | BC | 124 | GLY | 3.9 |
| 25 | AZ | 330 | ARG | 3.8 |
| 43 | BH | 169 | VAL | 3.8 |
| 36 | BA | 157 | U | 3.8 |
| 36 | BA | 2165 | G | 3.8 |
| 22 | AW | 7 | A | 3.8 |
| 22 | AW | 9 | A | 3.8 |
| 36 | BA | 6 | A | 3.8 |
| 36 | BA | 1098 | A | 3.8 |
| 36 | BA | 2132 | U | 3.8 |
| 57 | BY | 26 | LYS | 3.8 |
| 26 | B0 | 6 | GLY | 3.8 |
| 36 | BA | 883 | G | 3.8 |
| 38 | BC | 196 | LEU | 3.8 |
| 38 | BC | 19 | VAL | 3.8 |
| 36 | BA | 2801(A) | A | 3.8 |
| 38 | BC | 37 | PHE | 3.8 |
| 57 | BY | 32 | PRO | 3.8 |
| 22 | AV | 20 | U | 3.8 |
| 36 | BA | 7 | G | 3.8 |
| 57 | BY | 56 | PRO | 3.8 |
| 36 | BA | 2117 | A | 3.8 |
| 1 | AA | 163 | C | 3.8 |
| 36 | BA | 884 | C | 3.8 |
| 36 | BA | 2166 | G | 3.7 |
| 26 | B0 | 4 | LYS | 3.7 |
| 1 | AA | 162 | A | 3.7 |
| 41 | BF | 12 | LEU | 3.7 |
| 36 | BA | 2187 | G | 3.7 |
| 29 | B3 | 2 | PRO | 3.7 |
| 6 | AF | 101 | ALA | 3.7 |
| 38 | BC | 225 | ASN | 3.7 |
| 36 | BA | 2142 | C | 3.7 |
| 36 | BA | 2186 | G | 3.7 |
| 22 | AW | 45 | U | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | AB | 131 | PRO | 3.7 |
| 20 | AT | 99 | LEU | 3.7 |
| 36 | BA | 1173 | G | 3.7 |
| 38 | BC | 134 | ARG | 3.7 |
| 41 | BF | 134 | GLY | 3.7 |
| 1 | AA | 91 | C | 3.7 |
| 9 | AI | 87 | GLN | 3.7 |
| 36 | BA | 1092 | C | 3.6 |
| 9 | AI | 88 | TYR | 3.6 |
| 54 | BV | 18 | LEU | 3.6 |
| 38 | BC | 202 | GLU | 3.6 |
| 22 | AV | 1 | G | 3.6 |
| 32 | B6 | 54 | ILE | 3.6 |
| 57 | BY | 39 | VAL | 3.6 |
| 20 | AT | 101 | GLY | 3.6 |
| 36 | BA | 2140 | C | 3.6 |
| 53 | BU | 117 | GLN | 3.6 |
| 58 | BZ | 113 | ALA | 3.6 |
| 38 | BC | 59 | ARG | 3.6 |
| 27 | B1 | 85 | LEU | 3.6 |
| 43 | BH | 170 | ARG | 3.6 |
| 38 | BC | 139 | ASN | 3.5 |
| 38 | BC | 153 | ILE | 3.5 |
| 38 | BC | 100 | ILE | 3.5 |
| 22 | AW | 21 | A | 3.5 |
| 36 | BA | 2801 | A | 3.5 |
| 22 | AW | 47 | U | 3.5 |
| 36 | BA | 2896 | C | 3.5 |
| 1 | AA | 1030(C) | G | 3.5 |
| 1 | AA | 1030(B) | C | 3.5 |
| 53 | BU | 9 | VAL | 3.5 |
| 36 | BA | 2139 | C | 3.5 |
| 38 | BC | 11 | LEU | 3.5 |
| 38 | BC | 41 | VAL | 3.5 |
| 57 | BY | 37 | VAL | 3.5 |
| 22 | AW | 10 | G | 3.5 |
| 25 | AZ | 334 | PHE | 3.5 |
| 36 | BA | 277 | C | 3.5 |
| 38 | BC | 68 | LEU | 3.5 |
| 36 | BA | 1100 | C | 3.5 |
| 43 | BH | 51 | ARG | 3.5 |
| 13 | AM | 7 | VAL | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | AM | 125 | ARG | 3.5 |
| 43 | BH | 100 | GLY | 3.4 |
| 57 | BY | 72 | VAL | 3.4 |
| 19 | AS | 10 | PHE | 3.4 |
| 28 | B2 | 38 | GLN | 3.4 |
| 1 | AA | 1031 | G | 3.4 |
| 36 | BA | 2141 | G | 3.4 |
| 38 | BC | 154 | ARG | 3.4 |
| 36 | BA | 1053 | C | 3.4 |
| 38 | BC | 86 | ALA | 3.4 |
| 38 | BC | 216 | THR | 3.4 |
| 36 | BA | 1536 | C | 3.4 |
| 38 | BC | 118 | ASP | 3.4 |
| 42 | BG | 2 | PRO | 3.4 |
| 2 | AB | 136 | VAL | 3.4 |
| 36 | BA | 2118 | U | 3.4 |
| 58 | BZ | 167 | PRO | 3.4 |
| 24 | AY | 19 | G | 3.4 |
| 36 | BA | 1072 | C | 3.4 |
| 57 | BY | 41 | GLY | 3.4 |
| 36 | BA | 156 | U | 3.4 |
| 38 | BC | 53 | ARG | 3.4 |
| 36 | BA | 2803 | C | 3.4 |
| 52 | BT | 134 | GLU | 3.4 |
| 52 | BT | 91 | ARG | 3.4 |
| 38 | BC | 218 | MET | 3.4 |
| 38 | BC | 101 | GLN | 3.3 |
| 48 | BP | 15 | ARG | 3.3 |
| 20 | AT | 9 | ASN | 3.3 |
| 38 | BC | 32 | LEU | 3.3 |
| 11 | AK | 127 | LYS | 3.3 |
| 19 | AS | 81 | ARG | 3.3 |
| 36 | BA | 2893 | G | 3.3 |
| 55 | BW | 111 | HIS | 3.3 |
| 36 | BA | 2185 | C | 3.3 |
| 13 | AM | 120 | LYS | 3.3 |
| 36 | BA | 271(M) | G | 3.3 |
| 36 | BA | 2310 | A | 3.3 |
| 36 | BA | 2629 | A | 3.3 |
| 48 | BP | 119 | GLU | 3.3 |
| 38 | BC | 96 | GLY | 3.3 |
| 36 | BA | 2157 | G | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 38 | BC | 115 | ALA | 3.3 |
| 58 | BZ | 112 | ARG | 3.3 |
| 36 | BA | 1081 | U | 3.3 |
| 57 | BY | 59 | GLY | 3.3 |
| 38 | BC | 156 | ILE | 3.2 |
| 36 | BA | 1056 | G | 3.2 |
| 36 | BA | 2151 | G | 3.2 |
| 23 | AX | 14 | A | 3.2 |
| 53 | BU | 118 | GLY | 3.2 |
| 22 | AW | 60 | U | 3.2 |
| 36 | BA | 271(K) | U | 3.2 |
| 57 | BY | 54 | LYS | 3.2 |
| 1 | AA | 839 | U | 3.2 |
| 38 | BC | 213 | TYR | 3.2 |
| 22 | AW | 63 | G | 3.2 |
| 1 | AA | 1129 | C | 3.2 |
| 37 | BB | 88 | C | 3.2 |
| 36 | BA | 1061 | U | 3.2 |
| 34 | B8 | 48 | PHE | 3.2 |
| 51 | BS | 87 | PHE | 3.2 |
| 38 | BC | 204 | ALA | 3.2 |
| 38 | BC | 193 | ILE | 3.1 |
| 36 | BA | 2804 | C | 3.1 |
| 30 | B4 | 32 | TYR | 3.1 |
| 50 | BR | 105 | ARG | 3.1 |
| 43 | BH | 81 | GLU | 3.1 |
| 36 | BA | 2159 | G | 3.1 |
| 36 | BA | 881 | G | 3.1 |
| 48 | BP | 51 | PHE | 3.1 |
| 57 | BY | 60 | PHE | 3.1 |
| 57 | BY | 61 | ILE | 3.1 |
| 36 | BA | 654(I) | C | 3.1 |
| 36 | BA | 1085 | A | 3.1 |
| 1 | AA | 93 | G | 3.1 |
| 7 | AG | 2 | ALA | 3.1 |
| 28 | B2 | 71 | ASN | 3.1 |
| 36 | BA | 271(L) | U | 3.1 |
| 36 | BA | 1055 | G | 3.1 |
| 22 | AW | 61 | C | 3.1 |
| 36 | BA | 2155 | G | 3.1 |
| 38 | BC | 215 | THR | 3.0 |
| 19 | AS | 20 | LEU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 38 | BC | 214 | VAL | 3.0 |
| 36 | BA | 1102 | C | 3.0 |
| 38 | BC | 84 | LYS | 3.0 |
| 32 | B6 | 46 | HIS | 3.0 |
| 36 | BA | 2106 | G | 3.0 |
| 38 | BC | 211 | SER | 3.0 |
| 39 | BD | 276 | LYS | 3.0 |
| 54 | BV | 101 | GLY | 3.0 |
| 36 | BA | 34 | C | 3.0 |
| 57 | BY | 22 | GLY | 3.0 |
| 41 | BF | 156 | LEU | 3.0 |
| 20 | AT | 98 | PRO | 3.0 |
| 36 | BA | 1847 | A | 3.0 |
| 58 | BZ | 142 | SER | 3.0 |
| 36 | BA | 2175 | C | 3.0 |
| 57 | BY | 36 | ALA | 2.9 |
| 1 | AA | 723 | U | 2.9 |
| 51 | BS | 83 | LYS | 2.9 |
| 25 | AZ | 326 | GLU | 2.9 |
| 50 | BR | 3 | HIS | 2.9 |
| 1 | AA | 77 | G | 2.9 |
| 41 | BF | 8 | GLN | 2.9 |
| 56 | BX | 90 | GLU | 2.9 |
| 36 | BA | 2794 | C | 2.9 |
| 36 | BA | 353 | G | 2.9 |
| 25 | AZ | 1 | ALA | 2.9 |
| 37 | BB | 66 | A | 2.9 |
| 36 | BA | 2895 | U | 2.9 |
| 28 | B2 | 16 | LEU | 2.9 |
| 38 | BC | 192 | PHE | 2.9 |
| 1 | AA | 1001(A) | G | 2.9 |
| 36 | BA | 2129 | C | 2.9 |
| 36 | BA | 1177 | A | 2.9 |
| 54 | BV | 30 | GLY | 2.9 |
| 36 | BA | 11 | G | 2.9 |
| 42 | BG | 4 | ASP | 2.9 |
| 36 | BA | 1083 | U | 2.9 |
| 40 | BE | 75 | VAL | 2.9 |
| 46 | BN | 8 | GLN | 2.9 |
| 55 | BW | 5 | ALA | 2.9 |
| 57 | BY | 64 | GLU | 2.9 |
| 38 | BC | 161 | ILE | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 36 | BA | 2153 | G | 2.9 |
| 38 | BC | 189 | ILE | 2.8 |
| 36 | BA | 158 | U | 2.8 |
| 38 | BC | 116 | THR | 2.8 |
| 35 | B9 | 15 | LYS | 2.8 |
| 36 | BA | 1740 | G | 2.8 |
| 36 | BA | 2116 | G | 2.8 |
| 58 | BZ | 175 | VAL | 2.8 |
| 36 | BA | 2602 | A | 2.8 |
| 36 | BA | 894 | C | 2.8 |
| 36 | BA | 2104 | G | 2.8 |
| 54 | BV | 54 | GLY | 2.8 |
| 38 | BC | 207 | THR | 2.8 |
| 43 | BH | 34 | GLU | 2.8 |
| 35 | B9 | 36 | GLN | 2.8 |
| 10 | AJ | 100 | THR | 2.8 |
| 36 | BA | 1086 | A | 2.8 |
| 38 | BC | 169 | GLY | 2.8 |
| 57 | BY | 11 | ASP | 2.8 |
| 36 | BA | 2167 | U | 2.8 |
| 43 | BH | 52 | VAL | 2.8 |
| 57 | BY | 27 | VAL | 2.8 |
| 42 | BG | 51 | ARG | 2.8 |
| 36 | BA | 882 | G | 2.8 |
| 36 | BA | 2207 | G | 2.8 |
| 10 | AJ | 80 | LYS | 2.8 |
| 38 | BC | 147 | PHE | 2.8 |
| 22 | AW | 20 | U | 2.8 |
| 36 | BA | 1082 | U | 2.8 |
| 36 | BA | 1105 | U | 2.8 |
| 36 | BA | 654(V) | A | 2.8 |
| 36 | BA | 2791 | C | 2.8 |
| 43 | BH | 101 | ARG | 2.8 |
| 43 | BH | 85 | LYS | 2.7 |
| 57 | BY | 83 | THR | 2.7 |
| 38 | BC | 157 | LYS | 2.7 |
| 36 | BA | 2154 | G | 2.7 |
| 36 | BA | 2156 | G | 2.7 |
| 36 | BA | 2793 | G | 2.7 |
| 38 | BC | 212 | VAL | 2.7 |
| 58 | BZ | 165 | VAL | 2.7 |
| 36 | BA | 1762 | A | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 42 | BG | 146 | TYR | 2.7 |
| 36 | BA | 1537 | G | 2.7 |
| 36 | BA | 2160 | G | 2.7 |
| 36 | BA | 2402 | C | 2.7 |
| 9 | AI | 4 | TYR | 2.7 |
| 55 | BW | 113 | LYS | 2.7 |
| 57 | BY | 30 | VAL | 2.7 |
| 36 | BA | 2147 | G | 2.7 |
| 52 | BT | 136 | GLN | 2.7 |
| 57 | BY | 67 | LEU | 2.7 |
| 41 | BF | 131 | GLY | 2.7 |
| 54 | BV | 42 | GLY | 2.7 |
| 1 | AA | 1136 | U | 2.7 |
| 22 | AW | 34 | G | 2.7 |
| 11 | AK | 11 | LYS | 2.7 |
| 36 | BA | 271(O) | C | 2.7 |
| 51 | BS | 80 | LEU | 2.7 |
| 25 | AZ | 382 | GLU | 2.7 |
| 57 | BY | 17 | SER | 2.6 |
| 48 | BP | 93 | GLY | 2.6 |
| 57 | BY | 52 | SER | 2.6 |
| 22 | AW | 54 | U | 2.6 |
| 43 | BH | 54 | ARG | 2.6 |
| 52 | BT | 3 | ARG | 2.6 |
| 22 | AW | 49 | C | 2.6 |
| 36 | BA | 2100 | G | 2.6 |
| 25 | AZ | 339 | ARG | 2.6 |
| 40 | BE | 76 | ARG | 2.6 |
| 27 | B1 | 56 | GLN | 2.6 |
| 51 | BS | 84 | GLN | 2.6 |
| 25 | AZ | 340 | PRO | 2.6 |
| 36 | BA | 614(A) | U | 2.6 |
| 2 | AB | 132 | LYS | 2.6 |
| 57 | BY | 86 | ARG | 2.6 |
| 57 | BY | 5 | MET | 2.6 |
| 36 | BA | 1052 | C | 2.6 |
| 38 | BC | 158 | ALA | 2.6 |
| 2 | AB | 137 | ARG | 2.6 |
| 22 | AV | 60 | U | 2.6 |
| 36 | BA | 1509(A) | A | 2.6 |
| 36 | BA | 2111 | C | 2.6 |
| 12 | AL | 127 | GLU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | AV | 16 | U | 2.6 |
| 38 | BC | 205 | LYS | 2.6 |
| 58 | BZ | 153 | SER | 2.6 |
| 22 | AV | 18 | G | 2.6 |
| 25 | AZ | 38 | GLU | 2.6 |
| 41 | BF | 194 | MET | 2.6 |
| 28 | B2 | 66 | GLU | 2.6 |
| 36 | BA | 932 | G | 2.6 |
| 41 | BF | 207 | GLY | 2.6 |
| 43 | BH | 82 | GLY | 2.6 |
| 36 | BA | 1106 | G | 2.5 |
| 25 | AZ | 35 | THR | 2.5 |
| 46 | BN | 121 | LYS | 2.5 |
| 12 | AL | 28 | LYS | 2.5 |
| 58 | BZ | 7 | ALA | 2.5 |
| 38 | BC | 145 | VAL | 2.5 |
| 29 | B3 | 18 | ASP | 2.5 |
| 54 | BV | 27 | ALA | 2.5 |
| 56 | BX | 88 | LYS | 2.5 |
| 43 | BH | 167 | GLU | 2.5 |
| 2 | AB | 240 | GLN | 2.5 |
| 20 | AT | 90 | GLN | 2.5 |
| 41 | BF | 128 | ALA | 2.5 |
| 57 | BY | 84 | ARG | 2.5 |
| 2 | AB | 127 | ILE | 2.5 |
| 22 | AW | 8 | U | 2.5 |
| 36 | BA | 2177 | C | 2.5 |
| 43 | BH | 160 | LYS | 2.5 |
| 36 | BA | 2127 | G | 2.5 |
| 36 | BA | 2168 | G | 2.5 |
| 56 | BX | 64 | LYS | 2.5 |
| 48 | BP | 149 | GLU | 2.5 |
| 51 | BS | 107 | GLU | 2.5 |
| 36 | BA | 2833 | G | 2.5 |
| 36 | BA | 172 | C | 2.4 |
| 41 | BF | 135 | LYS | 2.4 |
| 54 | BV | 19 | LYS | 2.4 |
| 1 | AA | 78 | G | 2.4 |
| 25 | AZ | 333 | GLY | 2.4 |
| 36 | BA | 2172 | U | 2.4 |
| 2 | AB | 227 | GLY | 2.4 |
| 25 | AZ | 184 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | BA | 888 | C | 2.4 |
| 22 | AW | 26 | A | 2.4 |
| 20 | AT | 104 | LEU | 2.4 |
| 1 | AA | 1026 | G | 2.4 |
| 38 | BC | 203 | GLY | 2.4 |
| 42 | BG | 3 | LEU | 2.4 |
| 42 | BG | 127 | GLY | 2.4 |
| 57 | BY | 51 | VAL | 2.4 |
| 38 | BC | 179 | SER | 2.4 |
| 25 | AZ | 405 | GLU | 2.4 |
| 22 | AV | 66 | U | 2.4 |
| 1 | AA | 1268 | A | 2.4 |
| 57 | BY | 65 | ALA | 2.4 |
| 22 | AW | 53 | G | 2.4 |
| 29 | B3 | 59 | VAL | 2.4 |
| 38 | BC | 55 | ASP | 2.4 |
| 36 | BA | 229 | A | 2.4 |
| 22 | AW | 16 | U | 2.4 |
| 27 | B1 | 51 | VAL | 2.4 |
| 38 | BC | 226 | PRO | 2.4 |
| 52 | BT | 130 | ALA | 2.4 |
| 36 | BA | 1171 | G | 2.4 |
| 41 | BF | 199 | TRP | 2.4 |
| 48 | BP | 5 | ASP | 2.4 |
| 1 | AA | 1038 | C | 2.4 |
| 32 | B6 | 44 | ARG | 2.4 |
| 36 | BA | 885 | C | 2.4 |
| 9 | AI | 126 | SER | 2.4 |
| 34 | B8 | 64 | TYR | 2.4 |
| 52 | BT | 132 | LYS | 2.4 |
| 36 | BA | 2135 | A | 2.3 |
| 22 | AW | 59 | U | 2.3 |
| 38 | BC | 72 | VAL | 2.3 |
| 38 | BC | 114 | VAL | 2.3 |
| 40 | BE | 58 | ARG | 2.3 |
| 19 | AS | 12 | ASP | 2.3 |
| 40 | BE | 54 | GLN | 2.3 |
| 1 | AA | 97 | G | 2.3 |
| 36 | BA | 2101 | G | 2.3 |
| 36 | BA | 2115 | G | 2.3 |
| 35 | B9 | 34 | GLN | 2.3 |
| 36 | BA | 357 | A | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | AW | 51 | U | 2.3 |
| 42 | BG | 26 | GLN | 2.3 |
| 20 | AT | 10 | LEU | 2.3 |
| 36 | BA | 2792 | G | 2.3 |
| 36 | BA | 2891 | G | 2.3 |
| 38 | BC | 75 | LEU | 2.3 |
| 57 | BY | 95 | LYS | 2.3 |
| 36 | BA | 272(A) | U | 2.3 |
| 57 | BY | 98 | VAL | 2.3 |
| 54 | BV | 66 | ARG | 2.3 |
| 11 | AK | 12 | ARG | 2.3 |
| 49 | BQ | 1 | MET | 2.3 |
| 37 | BB | 87 | G | 2.3 |
| 52 | BT | 2 | ASN | 2.3 |
| 43 | BH | 66 | GLY | 2.3 |
| 38 | BC | 63 | SER | 2.3 |
| 36 | BA | 2189 | U | 2.3 |
| 43 | BH | 161 | GLY | 2.3 |
| 36 | BA | 363(F) | A | 2.3 |
| 36 | BA | 1077 | A | 2.3 |
| 36 | BA | 2126 | A | 2.3 |
| 41 | BF | 196 | LEU | 2.3 |
| 20 | AT | 84 | LEU | 2.3 |
| 25 | AZ | 403 | ILE | 2.3 |
| 9 | AI | 128 | ARG | 2.3 |
| 57 | BY | 58 | GLY | 2.2 |
| 39 | BD | 244 | ARG | 2.2 |
| 58 | BZ | 139 | VAL | 2.2 |
| 36 | BA | 2110 | G | 2.2 |
| 28 | B2 | 68 | ARG | 2.2 |
| 38 | BC | 82 | LYS | 2.2 |
| 43 | BH | 114 | VAL | 2.2 |
| 10 | AJ | 83 | GLU | 2.2 |
| 1 | AA | 92 | C | 2.2 |
| 48 | BP | 110 | TYR | 2.2 |
| 36 | BA | 1591 | G | 2.2 |
| 25 | AZ | 189 | ARG | 2.2 |
| 19 | AS | 28 | LYS | 2.2 |
| 51 | BS | 103 | GLU | 2.2 |
| 18 | AR | 31 | LEU | 2.2 |
| 49 | BQ | 89 | ASN | 2.2 |
| 22 | AV | 54 | U | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | BA | 2134 | A | 2.2 |
| 54 | BV | 70 | ILE | 2.2 |
| 29 | B3 | 8 | LEU | 2.2 |
| 41 | BF | 20 | LEU | 2.2 |
| 2 | AB | 130 | ARG | 2.2 |
| 36 | BA | 1043 | C | 2.2 |
| 29 | B3 | 17 | LYS | 2.2 |
| 22 | AW | 36 | A | 2.2 |
| 58 | BZ | 157 | LEU | 2.2 |
| 38 | BC | 117 | PRO | 2.2 |
| 43 | BH | 123 | PHE | 2.2 |
| 19 | AS | 43 | GLU | 2.2 |
| 38 | BC | 74 | VAL | 2.2 |
| 22 | AV | 53 | G | 2.2 |
| 37 | BB | 89 | G | 2.2 |
| 25 | AZ | 37 | ALA | 2.2 |
| 42 | BG | 86 | MET | 2.2 |
| 20 | AT | 37 | SER | 2.2 |
| 24 | AY | 57 | G | 2.2 |
| 36 | BA | 9 | U | 2.1 |
| 36 | BA | 1033 | U | 2.1 |
| 38 | BC | 56 | GLN | 2.1 |
| 4 | AD | 190 | ASP | 2.1 |
| 24 | AY | 44 | G | 2.1 |
| 36 | BA | 1044 | G | 2.1 |
| 42 | BG | 27 | ASN | 2.1 |
| 36 | BA | 2173 | A | 2.1 |
| 41 | BF | 167 | ALA | 2.1 |
| 3 | AC | 79 | ARG | 2.1 |
| 8 | AH | 98 | LYS | 2.1 |
| 48 | BP | 144 | GLU | 2.1 |
| 36 | BA | 362 | U | 2.1 |
| 57 | BY | 66 | PRO | 2.1 |
| 38 | BC | 15 | ASP | 2.1 |
| 43 | BH | 103 | LEU | 2.1 |
| 10 | AJ | 29 | ARG | 2.1 |
| 43 | BH | 115 | VAL | 2.1 |
| 12 | AL | 19 | ARG | 2.1 |
| 38 | BC | 30 | LYS | 2.1 |
| 53 | BU | 85 | LYS | 2.1 |
| 38 | BC | 58 | VAL | 2.1 |
| 22 | AW | 27 | G | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | AZ | 152 | MET | 2.1 |
| 26 | B0 | 84 | LEU | 2.1 |
| 32 | B6 | 31 | PRO | 2.1 |
| 40 | BE | 53 | PRO | 2.1 |
| 1 | AA | 90 | U | 2.1 |
| 36 | BA | 271(J) | C | 2.1 |
| 41 | BF | 146 | ALA | 2.1 |
| 53 | BU | 116 | ALA | 2.1 |
| 26 | B0 | 43 | THR | 2.1 |
| 38 | BC | 162 | GLU | 2.1 |
| 43 | BH | 45 | VAL | 2.1 |
| 2 | AB | 121 | LEU | 2.1 |
| 19 | AS | 30 | LEU | 2.1 |
| 43 | BH | 90 | LYS | 2.1 |
| 38 | BC | 142 | ALA | 2.1 |
| 1 | AA | 1137 | C | 2.1 |
| 27 | B1 | 57 | GLU | 2.1 |
| 43 | BH | 116 | GLU | 2.1 |
| 35 | B9 | 10 | ILE | 2.1 |
| 20 | AT | 85 | MET | 2.1 |
| 43 | BH | 59 | ARG | 2.1 |
| 38 | BC | 51 | PRO | 2.1 |
| 46 | BN | 10 | GLU | 2.1 |
| 58 | BZ | 138 | GLU | 2.1 |
| 22 | AW | 23 | A | 2.1 |
| 36 | BA | 1026 | U | 2.1 |
| 36 | BA | 1070 | A | 2.1 |
| 22 | AV | 65 | G | 2.1 |
| 29 | B3 | 5 | LYS | 2.1 |
| 36 | BA | 1543 | C | 2.1 |
| 54 | BV | 100 | ARG | 2.1 |
| 57 | BY | 92 | ASN | 2.1 |
| 12 | AL | 16 | GLU | 2.1 |
| 39 | BD | 275 | LYS | 2.1 |
| 36 | BA | 1046 | A | 2.1 |
| 1 | AA | 76 | C | 2.1 |
| 38 | BC | 197 | GLU | 2.1 |
| 41 | BF | 163 | VAL | 2.1 |
| 40 | BE | 88 | GLY | 2.1 |
| 4 | AD | 189 | PRO | 2.1 |
| 57 | BY | 74 | PRO | 2.1 |
| 1 | AA | 1036 | G | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | AJ | 88 | LEU | 2.1 |
| 36 | BA | 1051 | G | 2.1 |
| 36 | BA | 1538 | G | 2.1 |
| 2 | AB | 134 | GLU | 2.1 |
| 41 | BF | 27 | GLU | 2.1 |
| 48 | BP | 65 | ARG | 2.1 |
| 36 | BA | 1214 | A | 2.1 |
| 36 | BA | 1541 | G | 2.0 |
| 38 | BC | 81 | GLU | 2.0 |
| 39 | BD | 273 | ARG | 2.0 |
| 32 | B6 | 11 | LEU | 2.0 |
| 57 | BY | 82 | PRO | 2.0 |
| 50 | BR | 93 | GLY | 2.0 |
| 33 | B7 | 1 | MET | 2.0 |
| 53 | BU | 91 | ASP | 2.0 |
| 57 | BY | 35 | TYR | 2.0 |
| 42 | BG | 128 | ARG | 2.0 |
| 52 | BT | 39 | ARG | 2.0 |
| 36 | BA | 282 | A | 2.0 |
| 56 | BX | 70 | LEU | 2.0 |
| 25 | AZ | 347 | THR | 2.0 |
| 38 | BC | 159 | GLY | 2.0 |
| 19 | AS | 17 | GLU | 2.0 |
| 56 | BX | 82 | GLN | 2.0 |
| 38 | BC | 160 | ARG | 2.0 |
| 49 | BQ | 60 | ARG | 2.0 |
| 51 | BS | 26 | LEU | 2.0 |
| 58 | BZ | 163 | LEU | 2.0 |
| 1 | AA | 72 | C | 2.0 |
| 36 | BA | 2150 | U | 2.0 |
| 2 | AB | 19 | HIS | 2.0 |
| 19 | AS | 24 | ALA | 2.0 |
| 25 | AZ | 143 | ASP | 2.0 |
| 25 | AZ | 173 | GLY | 2.0 |
| 28 | B2 | 50 | ILE | 2.0 |
| 36 | BA | 276 | A | 2.0 |
| 13 | AM | 27 | LYS | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 24 | H2U | AY | 16 | 20/21 | 0.55 | 0.42 | 171,185,187,190 | 0 |
| 24 | H2U | AY | 17 | 20/21 | 0.61 | 0.80 | 191,199,200,200 | 0 |
| 24 | 5MU | AY | 54 | 21/22 | 0.65 | 0.36 | 145,152,154,155 | 0 |
| 24 | PSU | AY | 55 | 20/21 | 0.71 | 0.31 | 154,158,159,160 | 0 |
| 24 | H2U | AY | 20 | 20/21 | 0.75 | 0.31 | 185,187,191,191 | 0 |
| 24 | 4SU | AY | 8 | 20/21 | 0.79 | 0.24 | 104,105,107,108 | 0 |
| 24 | 7MG | AY | 46 | 24/25 | 0.88 | 0.24 | 112,114,120,121 | 0 |
| 24 | OMC | AY | 32 | 21/22 | 0.91 | 0.24 | 76,80,87,88 | 0 |
| 24 | MIA | AY | 37 | 29/30 | 0.94 | 0.27 | 48,63,74,86 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

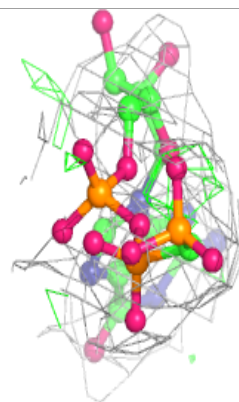
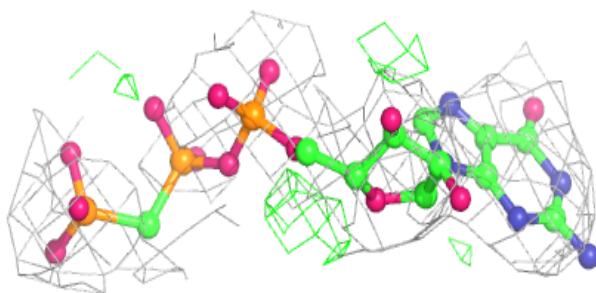
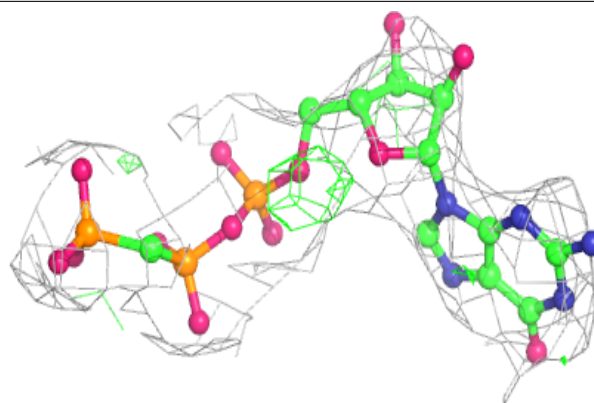
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60 | ZN | B4 | 101 | 1/1 | 0.92 | 0.08 | 132,132,132,132 | 0 |
| 62 | MG | AZ | 502 | 1/1 | 0.93 | 0.24 | 55,55,55,55 | 0 |
| 61 | GCP | AZ | 501 | 32/32 | 0.93 | 0.23 | 89,110,116,117 | 0 |
| 59 | PAR | AA | 1601 | 42/42 | 0.95 | 0.21 | 33,42,58,62 | 0 |
| 60 | ZN | AD | 301 | 1/1 | 0.98 | 0.33 | 58,58,58,58 | 0 |
| 60 | ZN | B9 | 101 | 1/1 | 0.99 | 0.12 | 92,92,92,92 | 0 |
| 60 | ZN | AN | 101 | 1/1 | 1.00 | 0.19 | 45,45,45,45 | 0 |

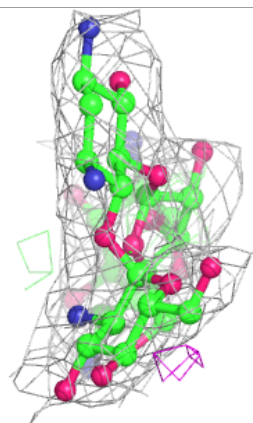
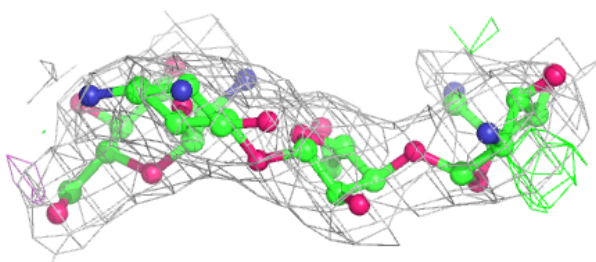
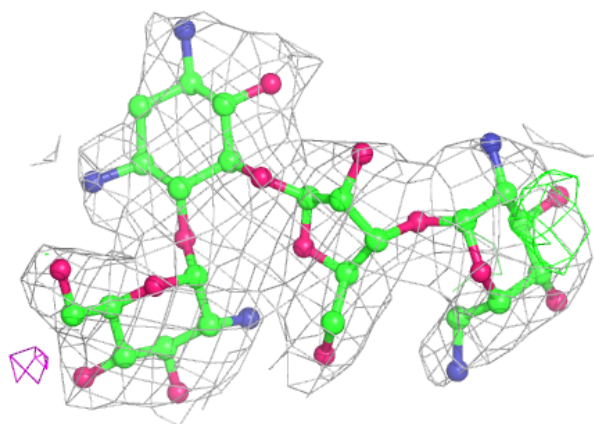
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GCP AZ 501:

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

**Electron density around PAR AA 1601:**

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



6.5 Other polymers

There are no such residues in this entry.