



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2024 – 04:55 PM EDT

PDB ID : 4U26
Title : Crystal structure of the E. coli ribosome bound to dalfopristin and quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 | : | 2.37.1 |
| 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) | : | 2.37.1 |

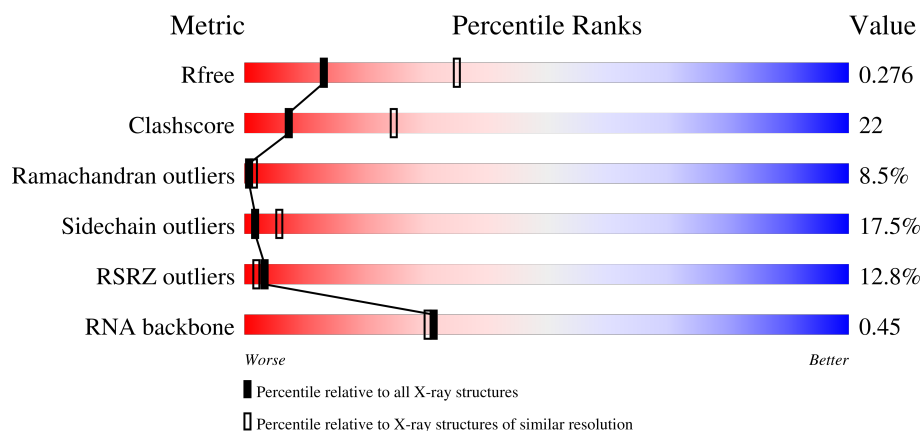
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 | 3140 (2.80-2.80) |
| Clashscore | 141614 | 3569 (2.80-2.80) |
| Ramachandran outliers | 138981 | 3498 (2.80-2.80) |
| Sidechain outliers | 138945 | 3500 (2.80-2.80) |
| RSRZ outliers | 127900 | 3078 (2.80-2.80) |
| RNA backbone | 3102 | 1227 (3.10-2.50) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 | 1539 | <div> <div>13%</div> <div>25%</div> <div>50%</div> <div>18%</div> <div>7%</div> </div> |
| 1 | CA | 1539 | <div> <div>4%</div> <div>31%</div> <div>54%</div> <div>16%</div> </div> |
| 2 | AB | 218 | <div> <div>13%</div> <div>25%</div> <div>50%</div> <div>18%</div> <div>7%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | CB | 218 | |
| 3 | AC | 206 | |
| 3 | CC | 206 | |
| 4 | AD | 205 | |
| 4 | CD | 205 | |
| 5 | AE | 150 | |
| 5 | CE | 150 | |
| 6 | AF | 100 | |
| 6 | CF | 100 | |
| 7 | AG | 151 | |
| 7 | CG | 151 | |
| 8 | AH | 129 | |
| 8 | CH | 129 | |
| 9 | AI | 127 | |
| 9 | CI | 127 | |
| 10 | AJ | 98 | |
| 10 | CJ | 98 | |
| 11 | AK | 117 | |
| 11 | CK | 117 | |
| 12 | AL | 123 | |
| 12 | CL | 123 | |
| 13 | AM | 114 | |
| 13 | CM | 114 | |
| 14 | AN | 100 | |
| 14 | CN | 100 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | AO | 88 | |
| 15 | CO | 88 | |
| 16 | AP | 82 | |
| 16 | CP | 82 | |
| 17 | AQ | 80 | |
| 17 | CQ | 80 | |
| 18 | AR | 55 | |
| 18 | CR | 55 | |
| 19 | AS | 79 | |
| 19 | CS | 79 | |
| 20 | AT | 85 | |
| 20 | CT | 85 | |
| 21 | AU | 51 | |
| 21 | CU | 51 | |
| 22 | BA | 2903 | |
| 22 | DA | 2903 | |
| 23 | BB | 119 | |
| 23 | DB | 119 | |
| 24 | BC | 271 | |
| 24 | DC | 271 | |
| 25 | BD | 209 | |
| 25 | DD | 209 | |
| 26 | BE | 201 | |
| 26 | DE | 201 | |
| 27 | BF | 177 | |












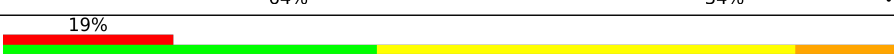
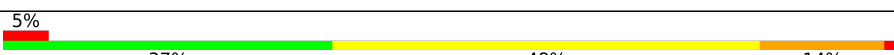
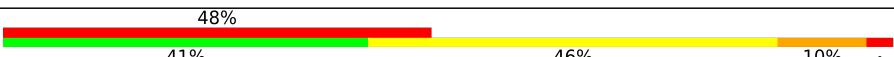

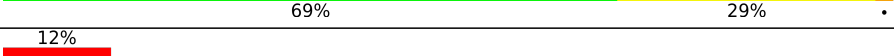


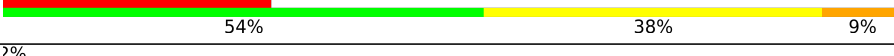

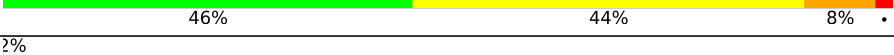




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27 | DF | 177 | |
| 28 | BG | 176 | |
| 28 | DG | 176 | |
| 29 | BH | 149 | |
| 29 | DH | 149 | |
| 30 | BI | 141 | |
| 30 | DI | 141 | |
| 31 | BJ | 142 | |
| 31 | DJ | 142 | |
| 32 | BK | 122 | |
| 32 | DK | 122 | |
| 33 | BL | 143 | |
| 33 | DL | 143 | |
| 34 | BM | 136 | |
| 34 | DM | 136 | |
| 35 | BN | 120 | |
| 35 | DN | 120 | |
| 36 | BO | 116 | |
| 36 | DO | 116 | |
| 37 | BP | 114 | |
| 37 | DP | 114 | |
| 38 | BQ | 117 | |
| 38 | DQ | 117 | |
| 39 | BR | 103 | |
| 39 | DR | 103 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 40 | BS | 110 |  |
| 40 | DS | 110 |  |
| 41 | BT | 93 |  |
| 41 | DT | 93 |  |
| 42 | BU | 102 |  |
| 42 | DU | 102 |  |
| 43 | BV | 94 |  |
| 43 | DV | 94 |  |
| 44 | BW | 76 |  |
| 44 | DW | 76 |  |
| 45 | BX | 77 |  |
| 45 | DX | 77 |  |
| 46 | BY | 63 |  |
| 46 | DY | 63 |  |
| 47 | BZ | 58 |  |
| 47 | DZ | 58 |  |
| 48 | B0 | 56 |  |
| 48 | D0 | 56 |  |
| 49 | B1 | 50 |  |
| 49 | D1 | 50 |  |
| 50 | B2 | 46 |  |
| 50 | D2 | 46 |  |
| 51 | B3 | 64 |  |
| 51 | D3 | 64 |  |
| 52 | B4 | 38 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52 | D4 | 38 | |
| 53 | B5 | 228 | |
| 54 | B6 | 8 | |
| 54 | D6 | 8 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55 | MG | AA | 1659 | - | - | - | X |
| 55 | MG | AM | 201 | - | - | - | X |
| 55 | MG | BA | 3134 | - | - | - | X |
| 55 | MG | DA | 3003 | - | - | - | X |
| 55 | MG | DA | 3005 | - | - | - | X |
| 55 | MG | DA | 3026 | - | - | - | X |
| 55 | MG | DA | 3028 | - | - | - | X |
| 55 | MG | DA | 3041 | - | - | - | X |
| 55 | MG | DA | 3048 | - | - | - | X |
| 55 | MG | DA | 3056 | - | - | - | X |
| 55 | MG | DA | 3062 | - | - | - | X |
| 55 | MG | DA | 3071 | - | - | - | X |
| 55 | MG | DA | 3072 | - | - | - | X |
| 55 | MG | DA | 3077 | - | - | - | X |
| 55 | MG | DA | 3131 | - | - | - | X |
| 55 | MG | DA | 3133 | - | - | - | X |
| 55 | MG | DA | 3155 | - | - | - | X |
| 56 | DOL | DA | 3001 | - | - | X | - |

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288423 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 | 1538 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32995 | 14716 | 6050 | 10691 | 1538 | | | |
| 1 | CA | 1539 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 33015 | 14725 | 6052 | 10699 | 1539 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1705 | 1081 | 305 | 312 | 7 | | | |
| 2 | CB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1705 | 1081 | 305 | 312 | 7 | | | |

- 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 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | | |
| 3 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- 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 |
| | | | 1106 | 687 | 211 | 202 | 6 | | | |
| 5 | CE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1106 | 687 | 211 | 202 | 6 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 515 | 148 | 149 | 6 | | | |
| 6 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 515 | 148 | 149 | 6 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | | |
| 7 | CG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 8 | CH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |

- 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 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 9 | CI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |

- 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 |
| | | | 787 | 493 | 150 | 143 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | CJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 787 | 493 | 150 | 143 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |
| 11 | CK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |
| 12 | CL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | | |
| 13 | CM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |
| 14 | CN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |

- 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 |
| | | | 710 | 437 | 143 | 129 | 1 | | | |
| 15 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 710 | 437 | 143 | 129 | 1 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 16 | CP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | | |
| 17 | CQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | AR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 288 | 86 | 82 | | | |
| 18 | CR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 288 | 86 | 82 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | | |
| 19 | CS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |
| 20 | CT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | AU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 426 | 265 | 86 | 74 | 1 | | | |
| 21 | CU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 426 | 265 | 86 | 74 | 1 | | | |

- Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22 | BA | 2897 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62195 | 27745 | 11446 | 20107 | 2897 | | | |
| 22 | DA | 2897 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62195 | 27745 | 11446 | 20107 | 2897 | | | |

- Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23 | BB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2549 | 1135 | 466 | 829 | 119 | | | |
| 23 | DB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24 | BC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2083 | 1288 | 423 | 365 | 7 | | | |
| 24 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2083 | 1288 | 423 | 365 | 7 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | BD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |
| 25 | DD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | BE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | BF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1411 | 899 | 249 | 257 | 6 | | | |
| 27 | DF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1411 | 899 | 249 | 257 | 6 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 28 | DG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | | |
| 29 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 30 | DI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 939 | 587 | 180 | 166 | 6 | | | |
| 32 | DK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 939 | 587 | 180 | 166 | 6 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 961 | 593 | 196 | 167 | 5 | | | |
| 35 | DN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 961 | 593 | 196 | 167 | 5 | | | |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 739 | 466 | 139 | 132 | 2 | | | |
| 41 | DT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 739 | 466 | 139 | 132 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BU | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 780 | 492 | 146 | 142 | | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42 | DU | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 780 | 492 | 146 | 142 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 43 | DV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BW | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 580 | 359 | 117 | 103 | 1 | | | |
| 44 | DW | 75 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 569 | 353 | 113 | 102 | 1 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 45 | DX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|---------|-------|
| 46 | BY | 63 | Total 509 | C 313 | N 99 | O 95 | S 2 | 0 | 0 | 0 |
| 46 | DY | 63 | Total 509 | C 313 | N 99 | O 95 | S 2 | 0 | 0 | 0 |

- Molecule 47 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|---------|-------|
| 47 | BZ | 58 | Total 449 | C 281 | N 87 | O 79 | S 2 | 0 | 0 | 0 |
| 47 | DZ | 58 | Total 449 | C 281 | N 87 | O 79 | S 2 | 0 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48 | B0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 48 | D0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49 | B1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 410 | 263 | 75 | 72 | | | |
| 49 | D1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 410 | 263 | 75 | 72 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 50 | D2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51 | B3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 51 | D3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 52 | D4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 53 | B5 | 191 | Total | C | N | O | 0 | 0 | 1 |
| | | | 1142 | 691 | 221 | 230 | | | |

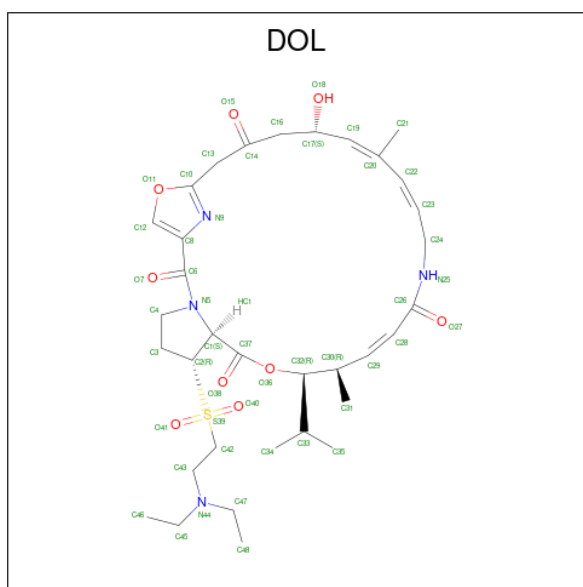
- Molecule 54 is a protein called Quinupristin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 54 | B6 | 8 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 73 | 53 | 9 | 10 | 1 | | | |
| 54 | D6 | 8 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 73 | 53 | 9 | 10 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 55 | AA | 71 | Total | Mg | 0 | 0 |
| | | | 71 | 71 | | |
| 55 | AM | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | BA | 194 | Total | Mg | 0 | 0 |
| | | | 194 | 194 | | |
| 55 | BB | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 55 | BQ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | CA | 56 | Total | Mg | 0 | 0 |
| | | | 56 | 56 | | |
| 55 | DA | 166 | Total | Mg | 0 | 0 |
| | | | 166 | 166 | | |
| 55 | DB | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 55 | DQ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | D2 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 56 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C₃₄H₅₀N₄O₉S).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 56 | BA | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 48 | 34 | 4 | 9 | 1 | | |
| 56 | DA | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 48 | 34 | 4 | 9 | 1 | | |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 58 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 58 | AA | 194 | Total | O | 0 | 0 |
| | | | 194 | 194 | | |
| 58 | AE | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 58 | AL | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | AN | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 58 | AT | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 58 | AU | 1 | Total O 1 1 | 0 | 0 |
| 58 | BA | 617 | Total O 617 617 | 0 | 0 |
| 58 | BB | 14 | Total O 14 14 | 0 | 0 |
| 58 | BC | 6 | Total O 6 6 | 0 | 0 |
| 58 | BD | 4 | Total O 4 4 | 0 | 0 |
| 58 | BE | 1 | Total O 1 1 | 0 | 0 |
| 58 | BF | 1 | Total O 1 1 | 0 | 0 |
| 58 | BG | 1 | Total O 1 1 | 0 | 0 |
| 58 | BJ | 1 | Total O 1 1 | 0 | 0 |
| 58 | BL | 7 | Total O 7 7 | 0 | 0 |
| 58 | BN | 5 | Total O 5 5 | 0 | 0 |
| 58 | BQ | 1 | Total O 1 1 | 0 | 0 |
| 58 | BS | 1 | Total O 1 1 | 0 | 0 |
| 58 | BT | 2 | Total O 2 2 | 0 | 0 |
| 58 | B3 | 3 | Total O 3 3 | 0 | 0 |
| 58 | B4 | 1 | Total O 1 1 | 0 | 0 |
| 58 | CA | 192 | Total O 192 192 | 0 | 0 |
| 58 | CL | 1 | Total O 1 1 | 0 | 0 |
| 58 | CN | 2 | Total O 2 2 | 0 | 0 |
| 58 | CT | 2 | Total O 2 2 | 0 | 0 |
| 58 | CU | 1 | Total O 1 1 | 0 | 0 |

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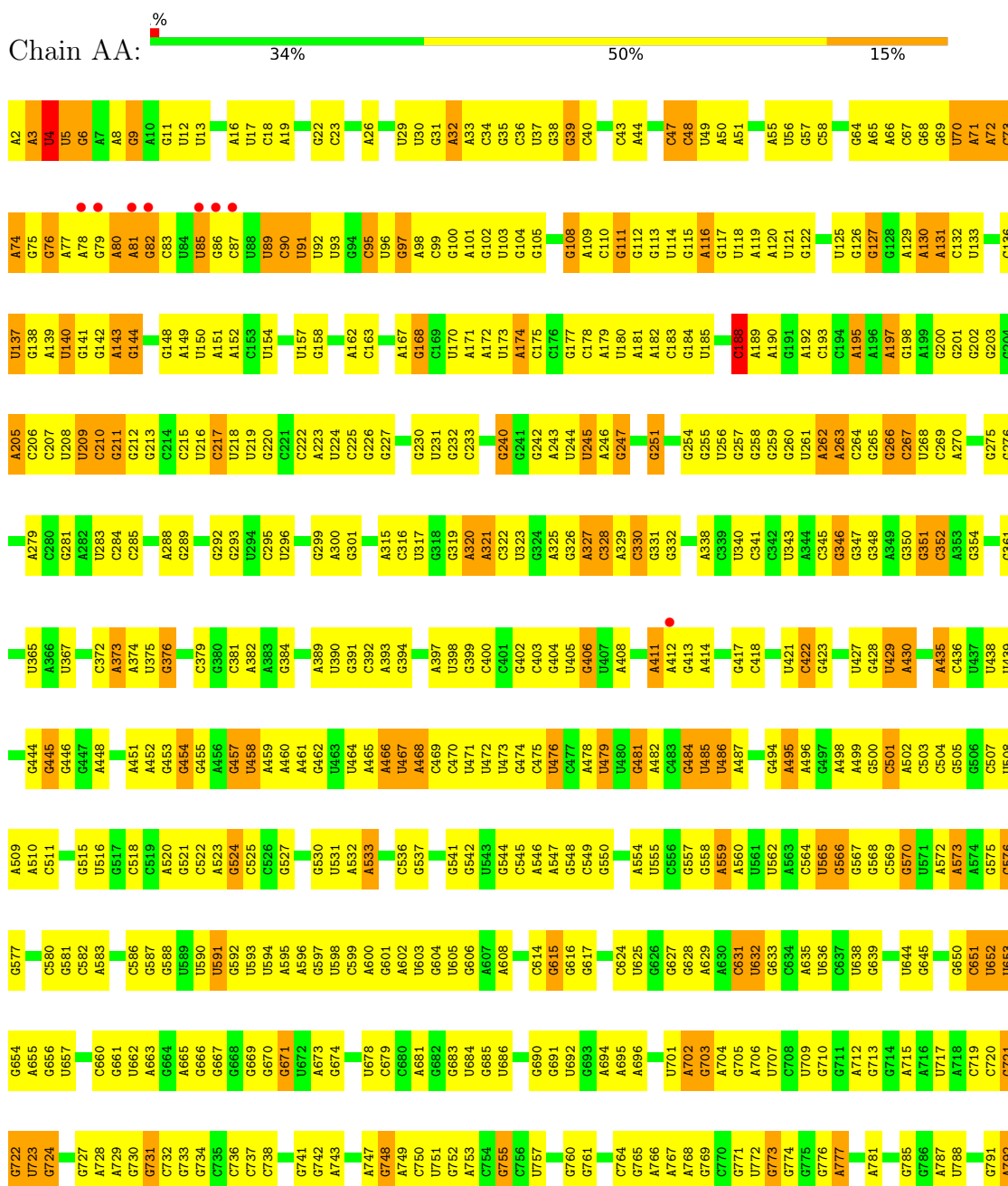
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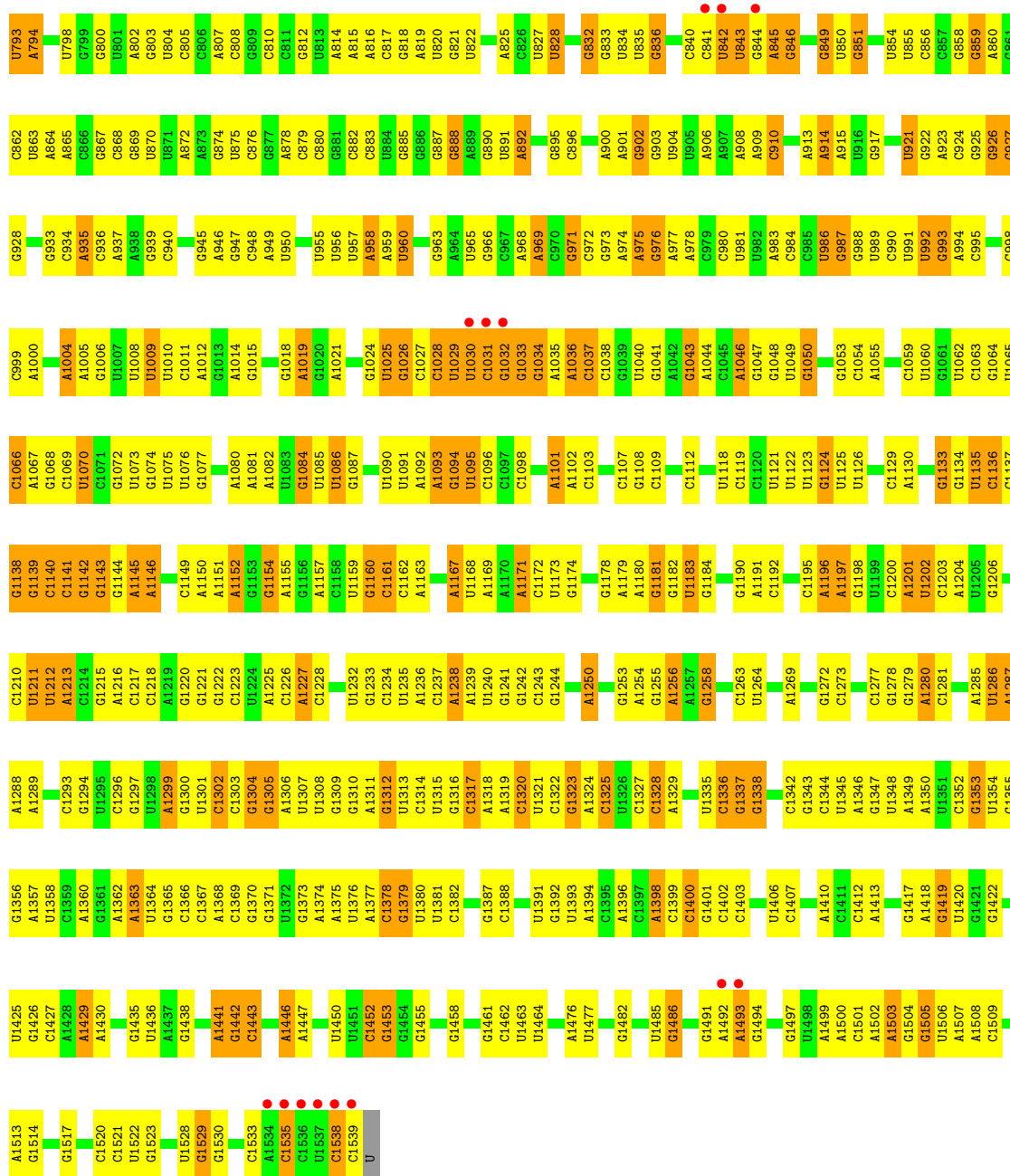
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 58 | DA | 610 | Total 610 | O 610 | 0 | 0 |
| 58 | DB | 13 | Total 13 | O 13 | 0 | 0 |
| 58 | DC | 8 | Total 8 | O 8 | 0 | 0 |
| 58 | DD | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | DE | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | DJ | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | DL | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | DN | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | DS | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | DT | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | DU | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | D2 | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | D3 | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | D4 | 1 | Total 1 | O 1 | 0 | 0 |

3 Residue-property plots

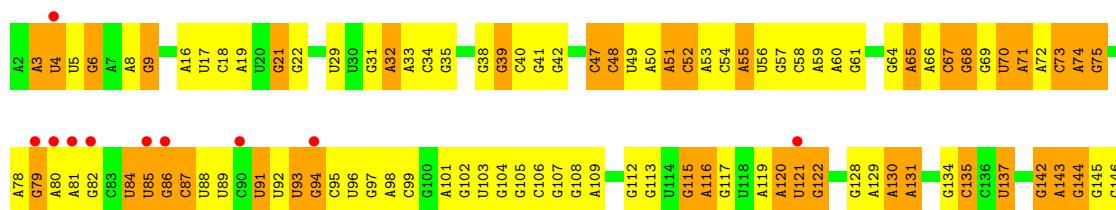
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

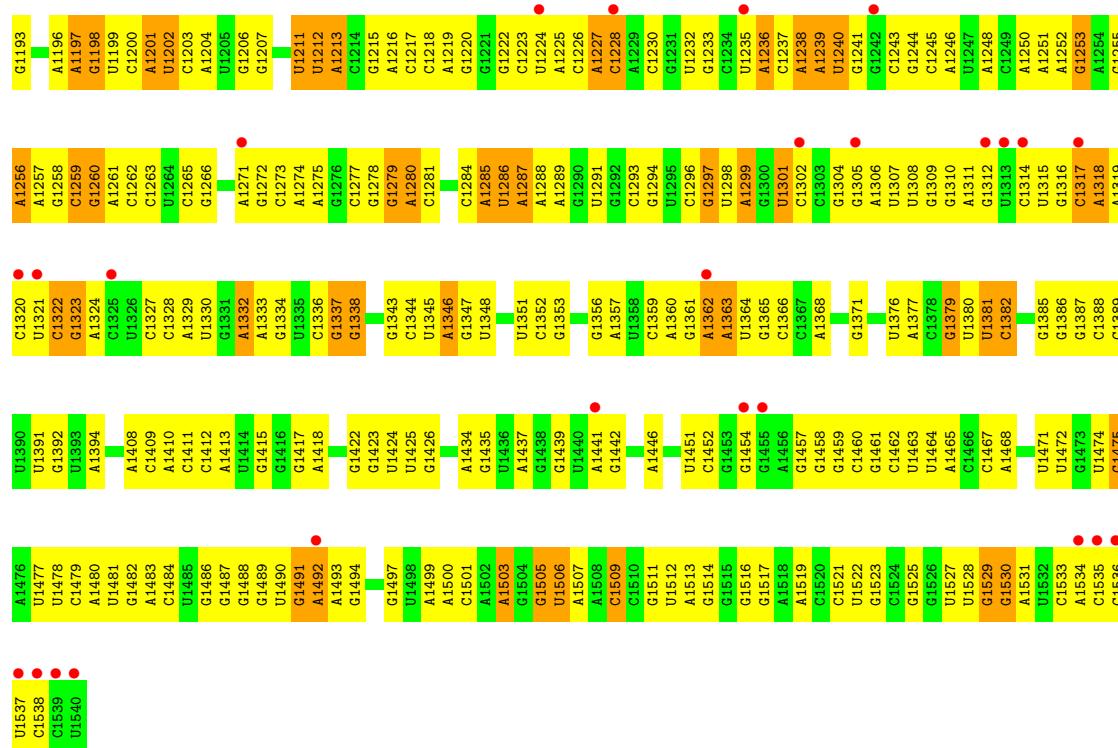




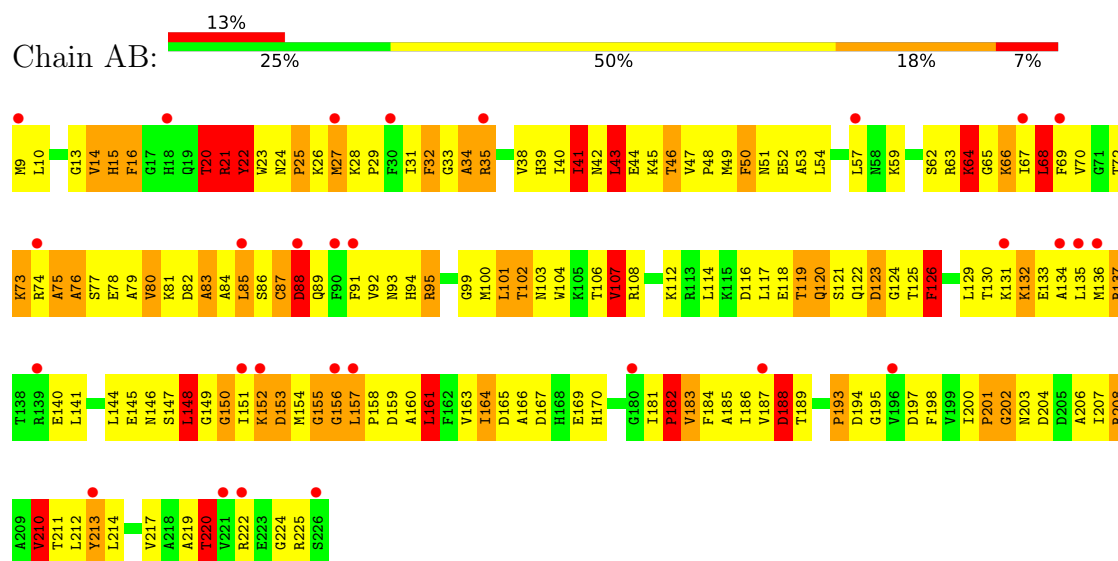
• Molecule 1: 16S rRNA



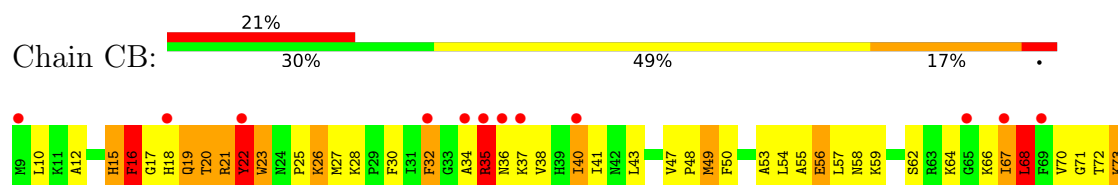
| | | | | | | | | | | | | | | |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| U1125 | U1052 | U991 | C912 | C839 | G774 | G711 | A642 | G567 | A499 | U426 | G353 | C271 | U209 | G147 |
| U1126 | G1053 | U992 | A913 | C840 | G775 | A712 | G643 | G568 | | U427 | G354 | G276 | C210 | G148 |
| C1054 | G993 | U993 | A914 | C841 | G776 | G713 | U644 | C569 | A502 | G428 | C355 | G277 | G211 | C149 |
| C1055 | A994 | G994 | U842 | U843 | A777 | G714 | U645 | G570 | C503 | U429 | A356 | G278 | G212 | U150 |
| C1129 | U1056 | A995 | A919 | G843 | G778 | A715 | G645 | U571 | C504 | A430 | G357 | G279 | G213 | A151 |
| A1130 | | C995 | U920 | U844 | C779 | A716 | A649 | A572 | G505 | A431 | G358 | C280 | C214 | A152 |
| | U1060 | C999 | U921 | A845 | A780 | U717 | G650 | A573 | G506 | A432 | G359 | G281 | C215 | G153 |
| G1133 | U1061 | A1000 | G922 | G846 | A781 | A718 | G651 | A574 | | A435 | G362 | G282 | U216 | U154 |
| G1134 | A1001 | C1001 | A923 | A782 | G719 | C719 | G652 | G575 | A509 | A436 | | A282 | C217 | U155 |
| U1135 | C924 | G1002 | C924 | A783 | G720 | C720 | U653 | C576 | A510 | U437 | U367 | U283 | U218 | C156 |
| G1064 | G1064 | G1002 | G925 | A784 | G721 | C721 | U654 | G577 | C511 | U438 | U368 | G284 | U219 | U157 |
| C1137 | U1065 | G1003 | G926 | G785 | G722 | C722 | G654 | C578 | U512 | U439 | G369 | C285 | G220 | G158 |
| G1066 | G927 | A1004 | G927 | G786 | U723 | C723 | G661 | C579 | C513 | U440 | C370 | C286 | G221 | G159 |
| G1138 | | A1005 | | A787 | G724 | C724 | U662 | C580 | C514 | | A371 | G289 | G222 | A160 |
| G1139 | A1067 | A1006 | C932 | | G725 | C725 | U663 | G581 | | U445 | G372 | C290 | A223 | A161 |
| C1140 | G1068 | U1007 | G933 | U854 | | | U664 | C582 | C517 | G446 | C373 | U291 | U224 | A162 |
| C1141 | C1069 | U1007 | G934 | G791 | A728 | C728 | G665 | A583 | C518 | | A374 | | G227 | C163 |
| G1142 | U1070 | U1008 | A935 | A792 | A729 | C729 | U666 | G584 | C519 | A451 | U375 | U294 | U228 | G164 |
| G1143 | C1071 | U1009 | | A793 | G730 | C730 | G667 | G585 | A520 | A452 | G376 | C295 | U229 | G165 |
| G1144 | U1072 | U1010 | A938 | U794 | G731 | C731 | U668 | G586 | | G453 | G377 | U296 | U230 | U167 |
| A1145 | U1073 | G1011 | G939 | A795 | | | G669 | U590 | G527 | G454 | G378 | C297 | U231 | G168 |
| A1146 | G1074 | A1012 | C940 | C795 | G734 | C734 | U670 | U591 | C528 | G455 | C379 | A298 | U232 | C169 |
| C1147 | | G1013 | G945 | U798 | G735 | C735 | G671 | | G529 | A456 | G384 | G299 | C233 | U170 |
| C1148 | | A1014 | G946 | G799 | G736 | C736 | U672 | G597 | C528 | G457 | C385 | A300 | C234 | A171 |
| C1149 | G1077 | G1015 | A946 | G800 | G737 | C737 | A673 | U598 | G530 | U458 | C386 | G301 | | A172 |
| A1150 | | A1016 | C947 | U801 | G738 | C738 | G674 | | U531 | A459 | U387 | G302 | G237 | U173 |
| A1151 | U1080 | U1017 | G948 | A802 | C739 | C739 | A675 | U603 | A532 | A460 | C388 | A303 | A238 | A174 |
| A1152 | A1081 | G1018 | C949 | G803 | U740 | C740 | A676 | G604 | A533 | A461 | C389 | | U239 | C175 |
| G1153 | U1082 | A1019 | G950 | U804 | G741 | C741 | A677 | G605 | U534 | A462 | A389 | A306 | G240 | C176 |
| G1154 | G1084 | G1020 | U950 | C905 | G742 | C742 | U678 | U606 | A535 | U463 | U390 | C307 | G241 | G177 |
| | U1085 | A1021 | G951 | C906 | G743 | C743 | C679 | A607 | G536 | U464 | C391 | C308 | G242 | C178 |
| A1157 | U1086 | A1022 | U952 | | G744 | C744 | C680 | A608 | G537 | A465 | C392 | A309 | U244 | A179 |
| C1158 | G1087 | U1023 | A872 | G809 | G745 | C745 | U681 | A609 | C538 | A466 | A393 | | U245 | U180 |
| C1159 | U1088 | G1024 | G874 | C910 | A746 | C746 | G682 | U610 | A539 | U467 | | C312 | G246 | A181 |
| G1160 | G1089 | U1025 | U875 | G811 | A747 | C747 | U683 | G612 | G540 | A468 | A397 | A313 | G247 | C182 |
| C1161 | U1090 | G1026 | C876 | G812 | G748 | C748 | U684 | C613 | G541 | C469 | U398 | C316 | G248 | C183 |
| C1162 | U1091 | C1027 | G877 | G813 | A749 | C749 | U685 | C614 | G542 | G470 | C399 | | U249 | G184 |
| A1167 | A1092 | C1028 | A878 | A815 | G750 | C750 | U686 | C615 | G543 | U471 | C400 | G319 | A250 | U185 |
| U1168 | U1093 | U1029 | C879 | A816 | U751 | C751 | A687 | G616 | C544 | U472 | G402 | A320 | G251 | C186 |
| U1169 | G1094 | C1031 | C880 | C817 | G752 | C752 | G688 | | C545 | U473 | C403 | A321 | U252 | G187 |
| A1170 | U1095 | G1032 | C881 | G818 | A753 | C753 | U689 | C618 | A546 | U474 | G404 | | G253 | C188 |
| A1171 | C1096 | G1033 | C882 | G819 | G754 | C754 | C690 | U619 | A547 | U475 | U405 | A327 | G254 | A189 |
| A1172 | C1097 | G1034 | C883 | A819 | C755 | C755 | G691 | C620 | | U476 | G406 | C328 | G255 | A190 |
| | C1098 | U1035 | U884 | U820 | G756 | C756 | G692 | A621 | G550 | C477 | U407 | A329 | U256 | G198 |
| | G1099 | A1036 | G885 | G821 | U757 | C757 | U693 | A622 | U551 | U478 | U408 | C330 | G257 | A199 |
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| G1178 | G1103 | G1039 | U891 | C826 | | | | | G555 | | A412 | G337 | U261 | A199 |
| A1179 | C1104 | U1040 | A892 | U827 | G763 | C763 | G700 | G628 | | G484 | A413 | A338 | A262 | G200 |
| A1180 | G1105 | G1041 | C893 | U828 | C764 | C764 | U701 | A629 | C556 | U485 | A414 | C339 | A263 | G201 |
| G1181 | C1107 | A1043 | | G829 | A765 | C765 | A702 | A630 | A559 | U486 | A415 | | G264 | G202 |
| U1182 | U1183 | A1044 | G976 | G832 | A767 | C767 | G703 | C631 | A560 | | | G345 | G265 | G203 |
| G1184 | G1184 | C1045 | A977 | G833 | A768 | C768 | U704 | U632 | U561 | C490 | U421 | C346 | G266 | G204 |
| | | A1046 | U978 | U834 | G769 | C769 | A705 | G633 | U562 | | C422 | G347 | C267 | A205 |
| G1187 | | A907 | C979 | U835 | G770 | C770 | A706 | G634 | A563 | A495 | U423 | | U268 | C206 |
| | A1117 | C980 | G979 | G836 | G771 | C771 | U707 | U635 | C564 | A496 | G424 | G351 | G269 | C207 |
| G1190 | U1049 | | A983 | U837 | U772 | C772 | | U636 | U565 | G497 | | | G270 | U208 |
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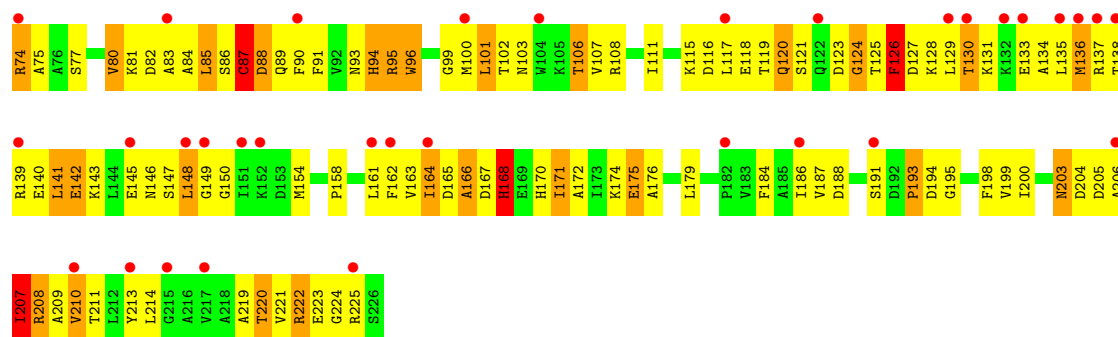


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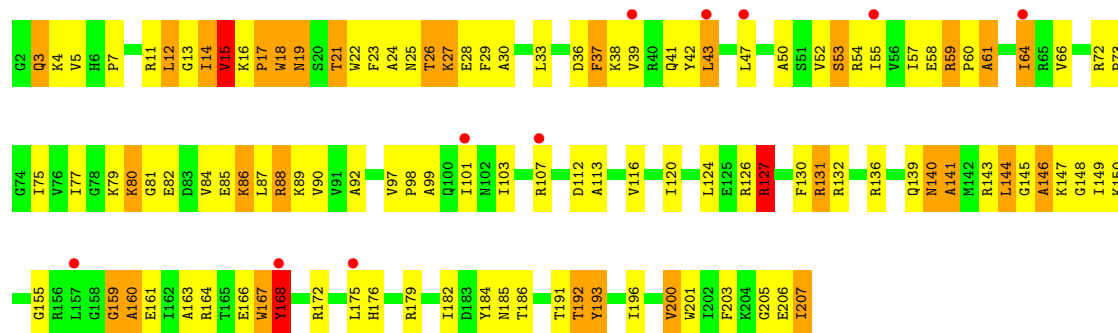


• Molecule 2: 30S ribosomal protein S2

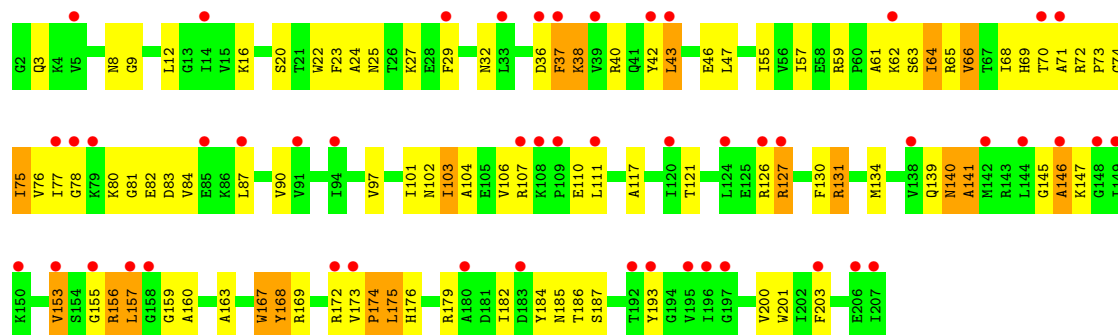




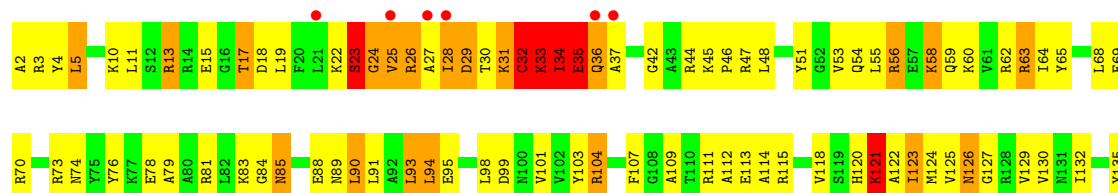
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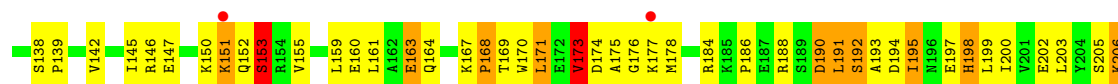


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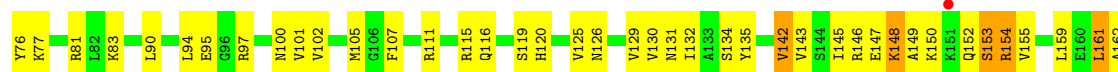
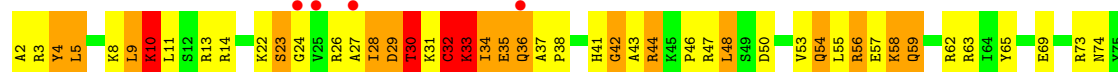


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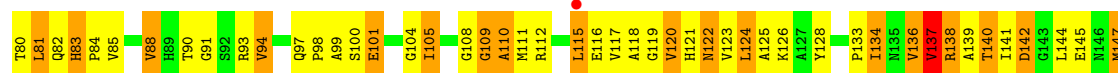




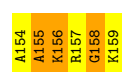
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

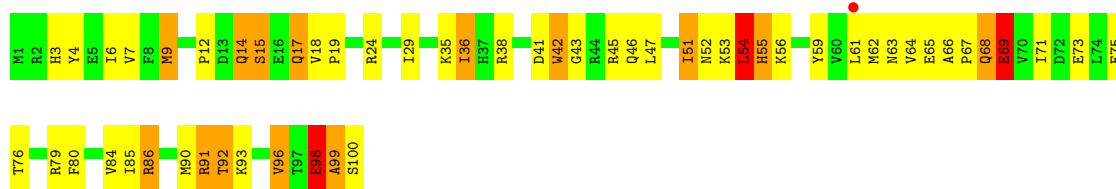


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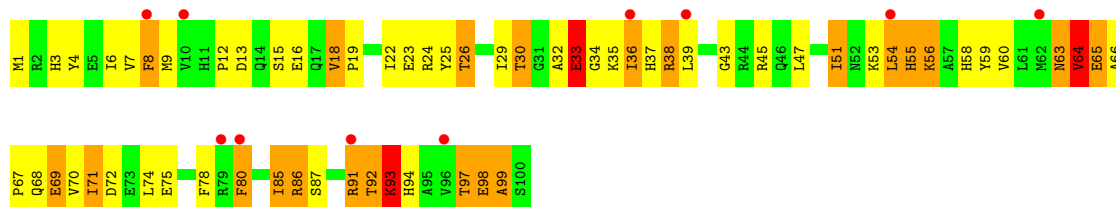


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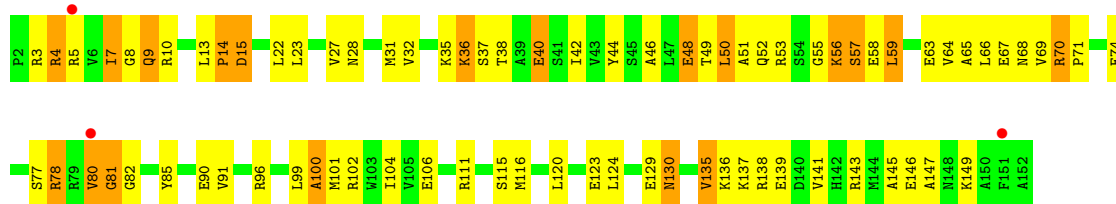




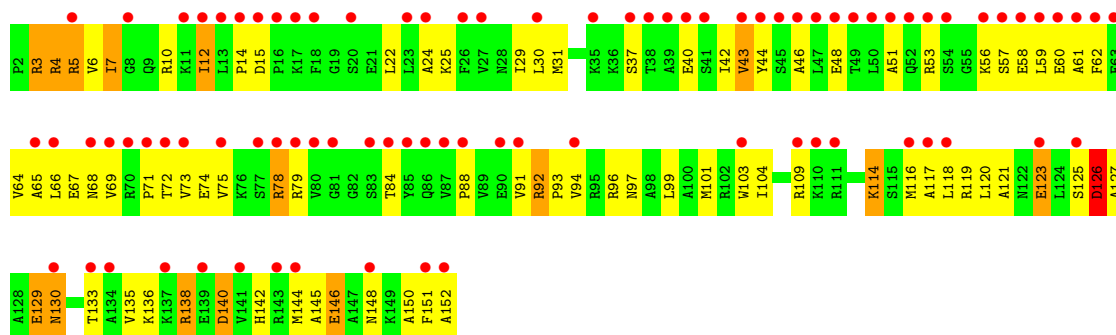
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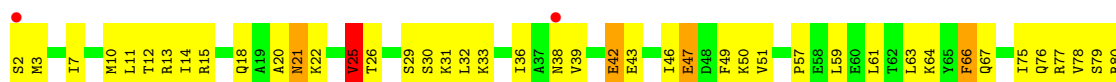
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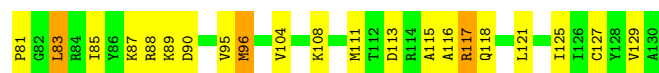


• Molecule 7: 30S ribosomal protein S7

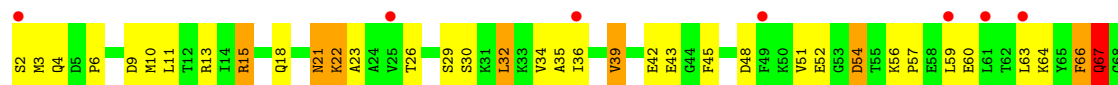


• Molecule 8: 30S ribosomal protein S8

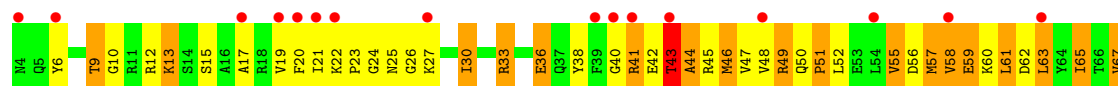
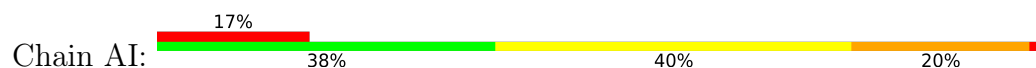




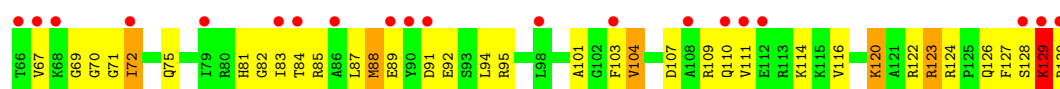
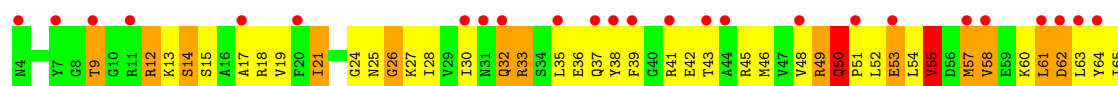
- Molecule 8: 30S ribosomal protein S8



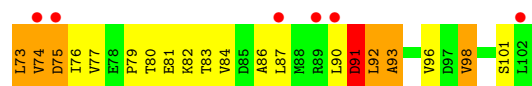
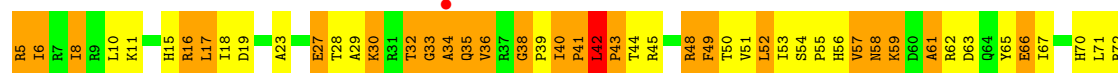
- Molecule 9: 30S ribosomal protein S9



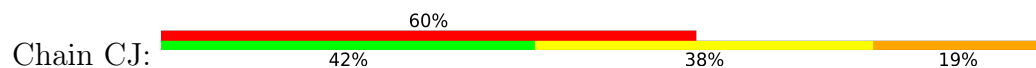
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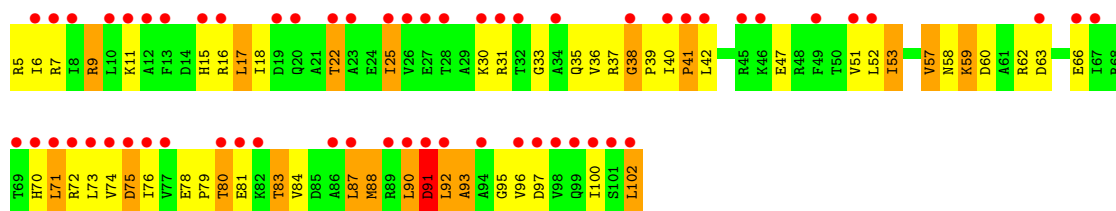


- Molecule 10: 30S ribosomal protein S10

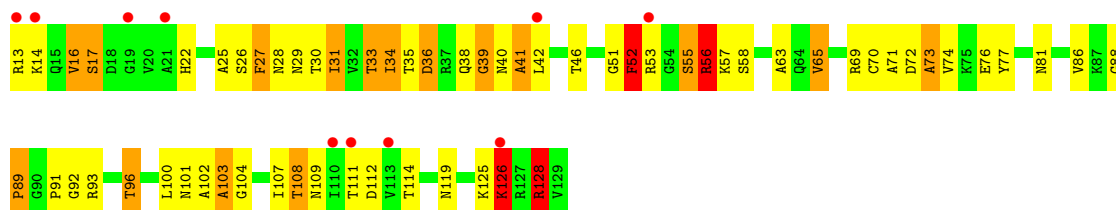


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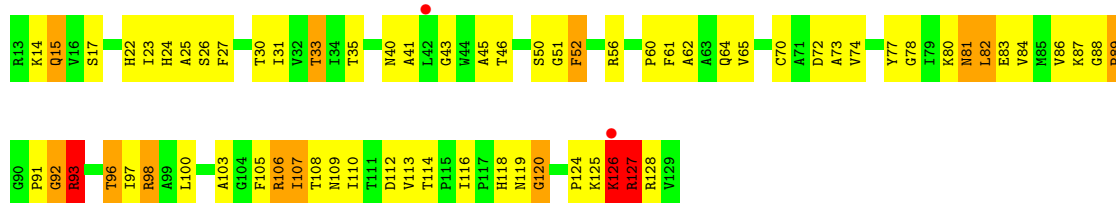
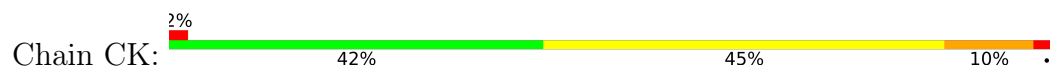




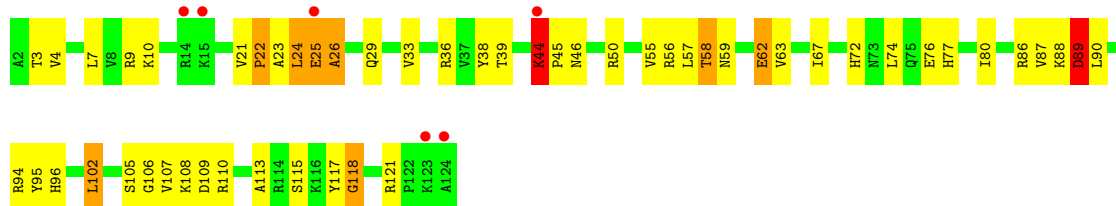
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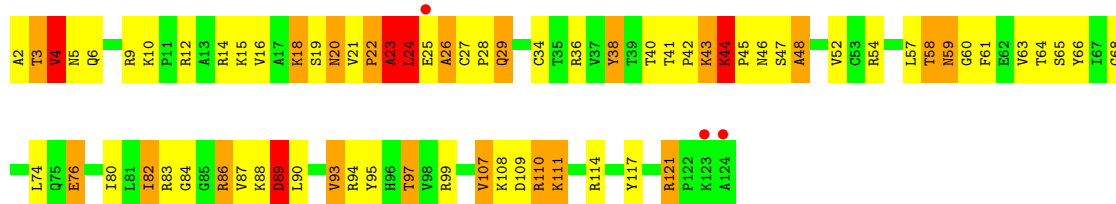
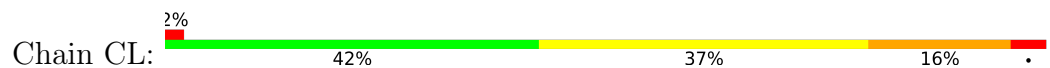
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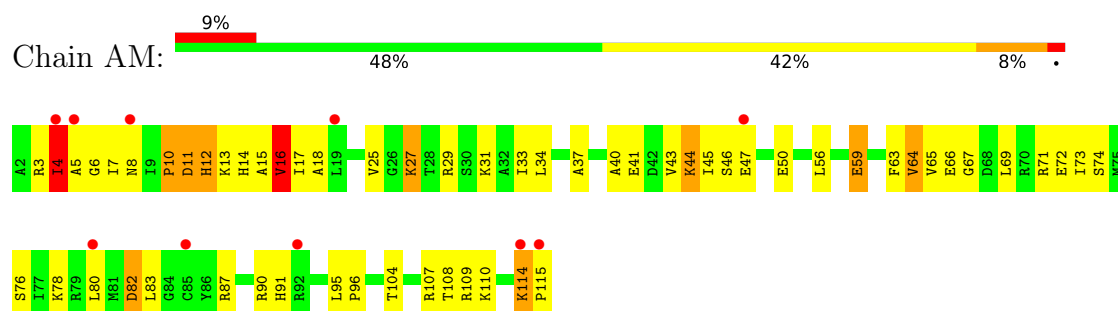
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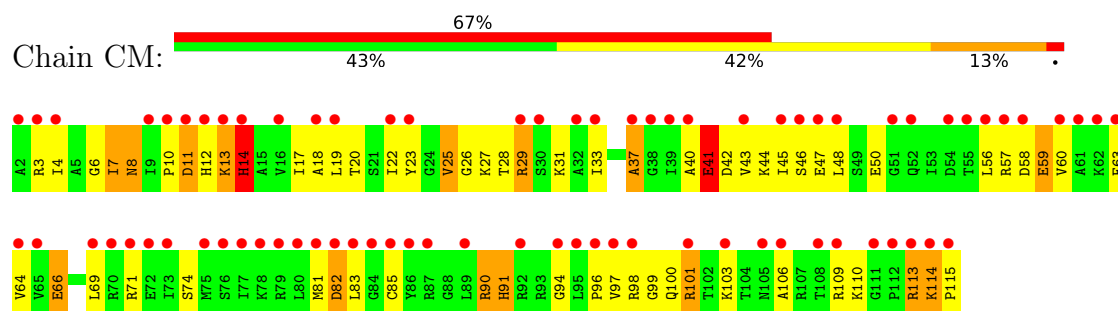
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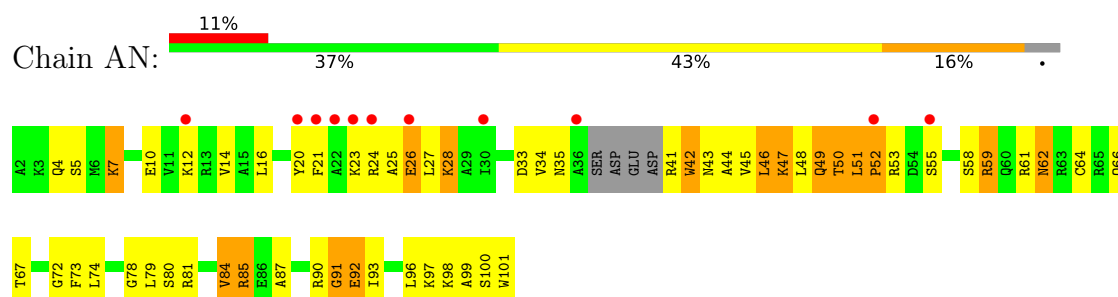
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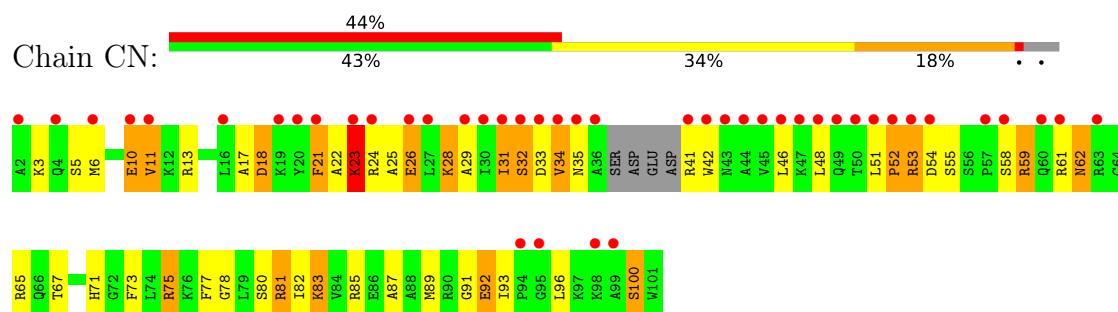
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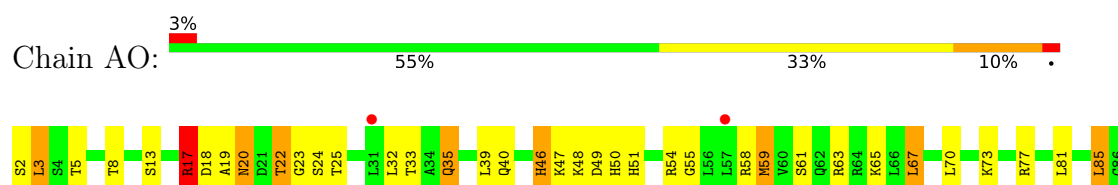
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

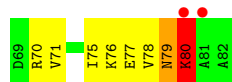
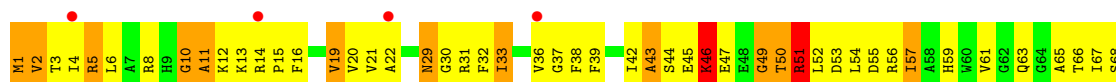




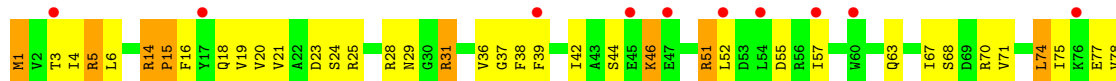
- Molecule 15: 30S ribosomal protein S15



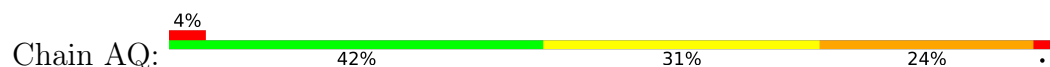
- Molecule 16: 30S ribosomal protein S16



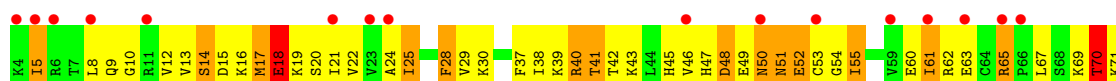
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17





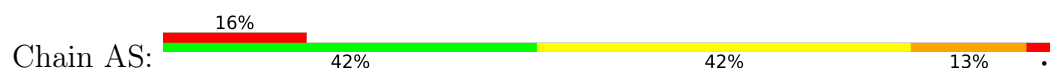
- Molecule 18: 30S ribosomal protein S18



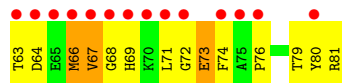
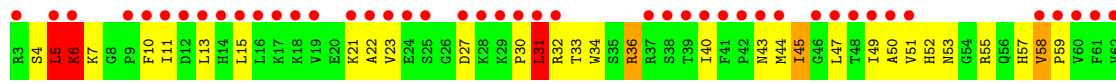
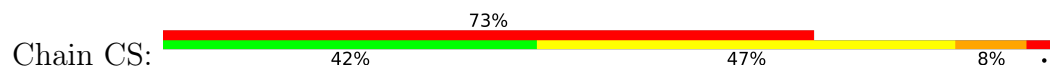
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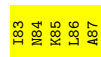
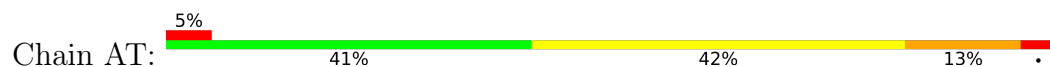
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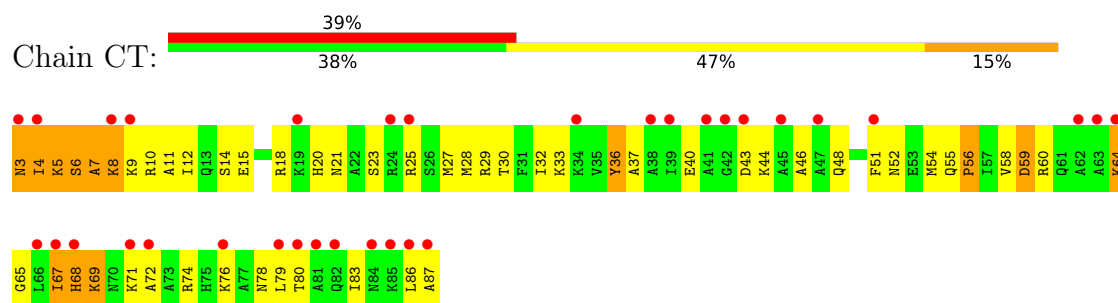
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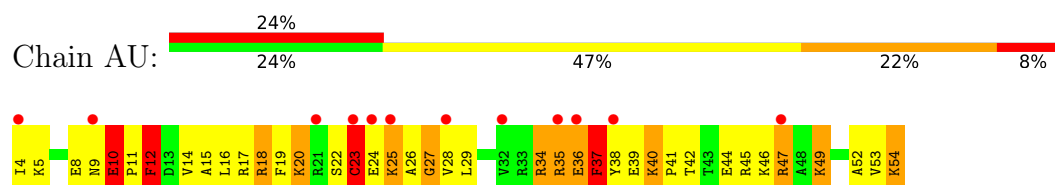
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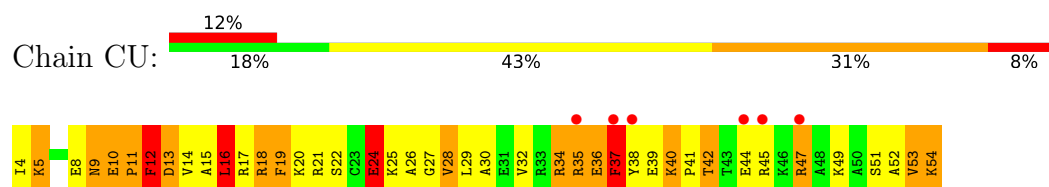
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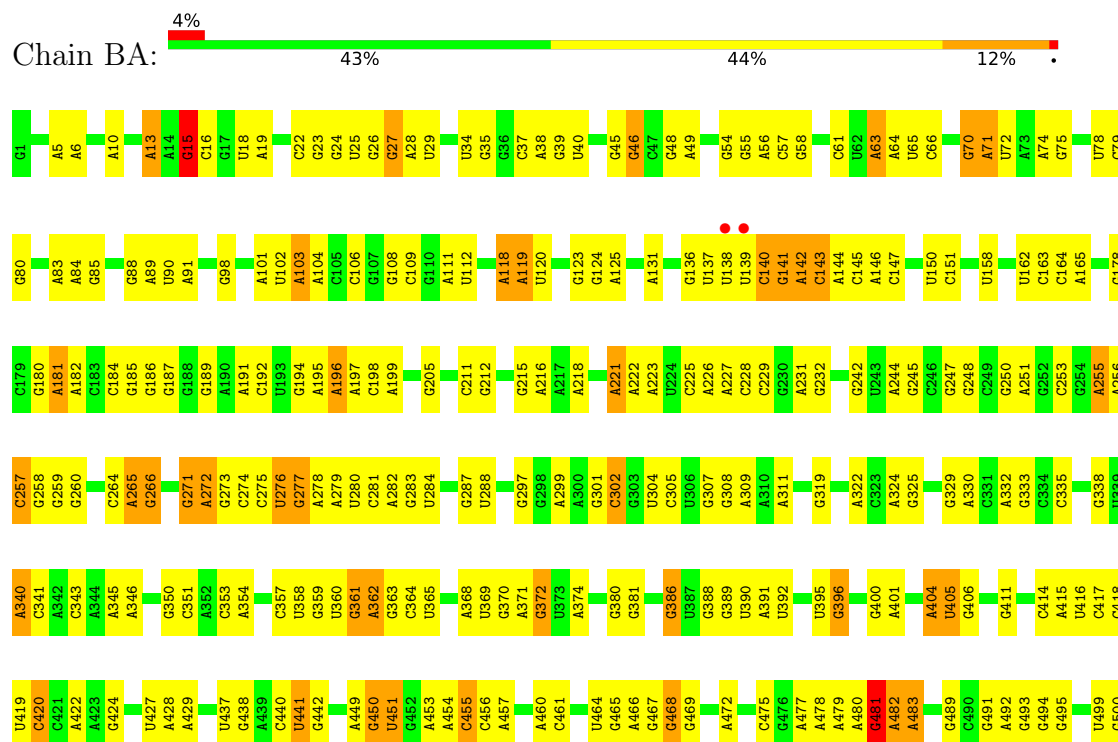
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

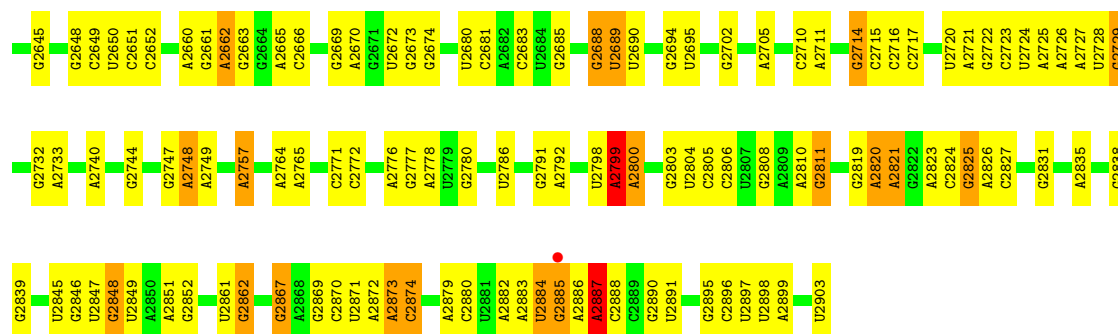


- Molecule 22: 23S rRNA

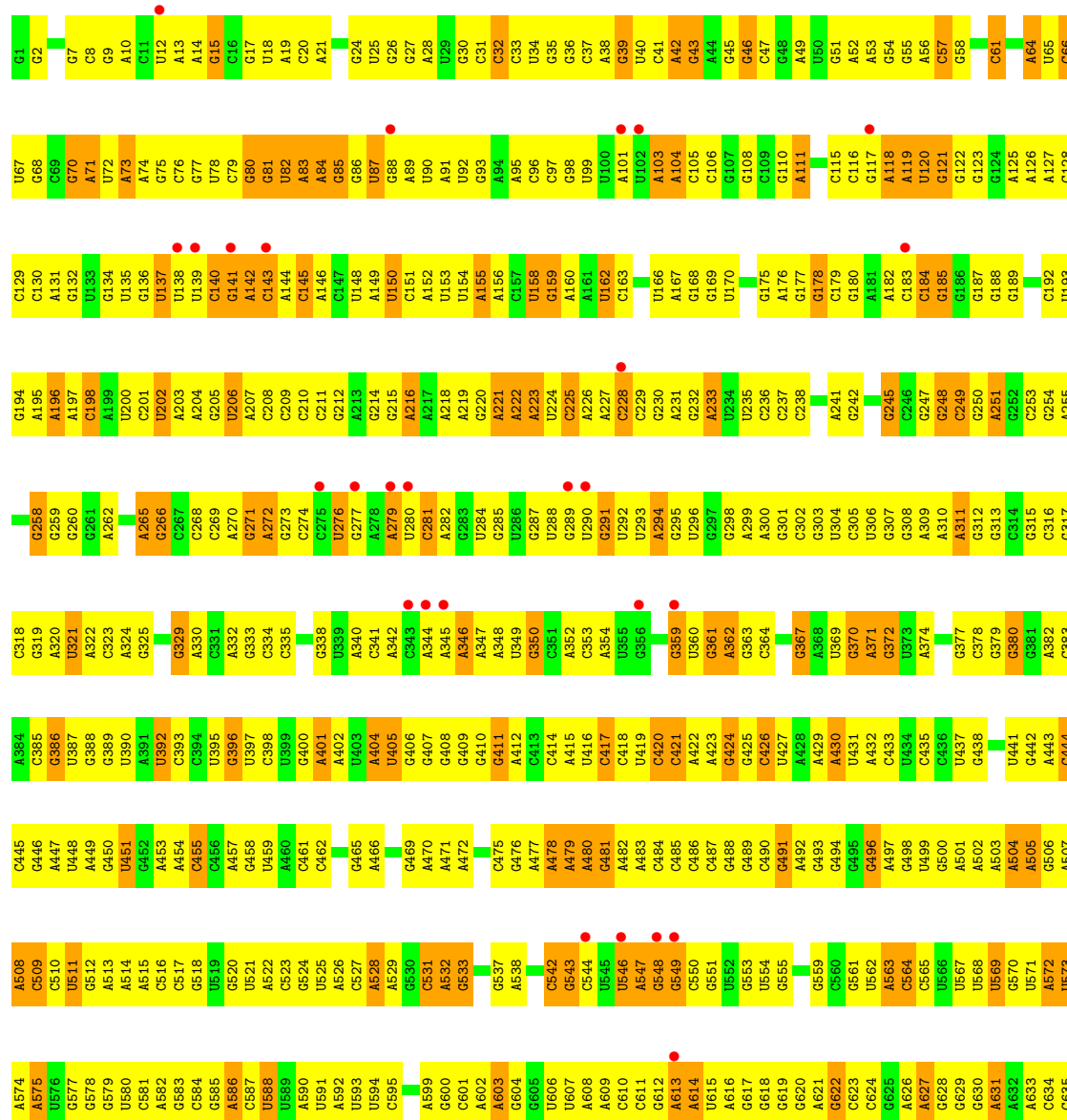


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| C2573 | C2498 | G2422 | U2334 | A2268 | U2189 | G2129 | G2057 | G1973 | | G1764 | | G1683 |
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| | G2501 | A2425 | C2339 | G2271 | A2192 | U2132 | A2059 | G1976 | G1839 | C1768 | | A1597 |
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| C2579 | U2504 | G2428 | C2343 | A2275 | C2197 | G2136 | C2063 | C1985 | G1843 | G1695 | | C1605 |
| G2580 | G2505 | G2429 | U2343 | C2275 | U2197 | U2137 | C2064 | C1986 | G1844 | U1775 | | C1606 |
| U2581 | U2506 | U2430 | U2344 | | A2198 | G2138 | C2065 | U1991 | G1845 | G1776 | | C1607 |
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| A2587 | | | C2353 | C2283 | | G2144 | | C1997 | U1852 | A1783 | | |
| G2588 | | | C2354 | | U2210 | G2145 | | C1998 | U1853 | A1784 | | A1618 |
| | U2514 | C2442 | G2355 | G2286 | A2211 | U2205 | | A1999 | | | | G1622 |
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| A2530 | | | G2366 | C2295 | U2220 | C2153 | | C2006 | G1869 | G1792 | | G1627 |
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| | | | | G2315 | U2240 | A2170 | | G2029 | U1886 | G1738 | | G1653 |
| | | | | G2316 | U2241 | G2170 | | A2030 | C1887 | G1739 | | |
| | | | | A2317 | U2242 | G2171 | | A2031 | G1888 | A1739 | | C1658 |
| | | | | G2318 | U2243 | U2172 | | G2032 | A1889 | G1817 | | |
| | | | | G2319 | U2244 | U2173 | | A2033 | A1890 | U1818 | | A1665 |
| | | | | U2320 | G2246 | C2174 | | U2034 | A1891 | U1820 | | G1666 |
| | | | | G2321 | A2247 | G2175 | | G2035 | C1893 | A1745 | | G1667 |
| | | | | U2322 | C2248 | A2176 | | A1894 | C1894 | U1746 | | A1668 |
| | | | | A2323 | U2249 | G2177 | | G2038 | C1895 | C1748 | | A1669 |

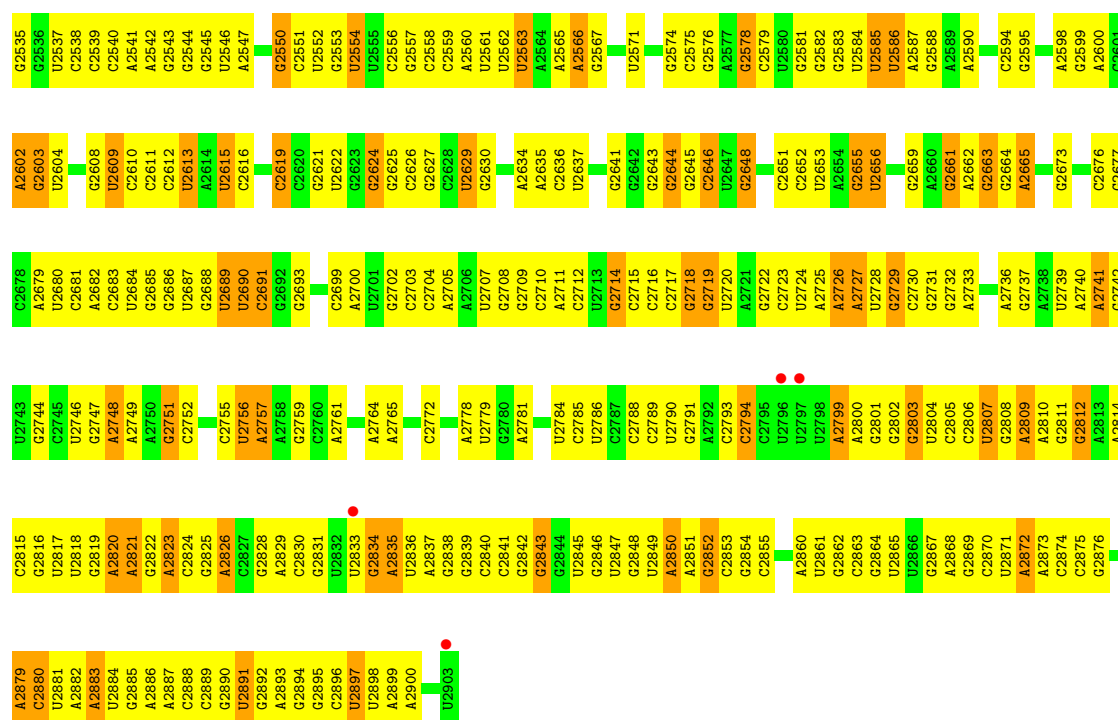


Molecule 22: 23S rRNA

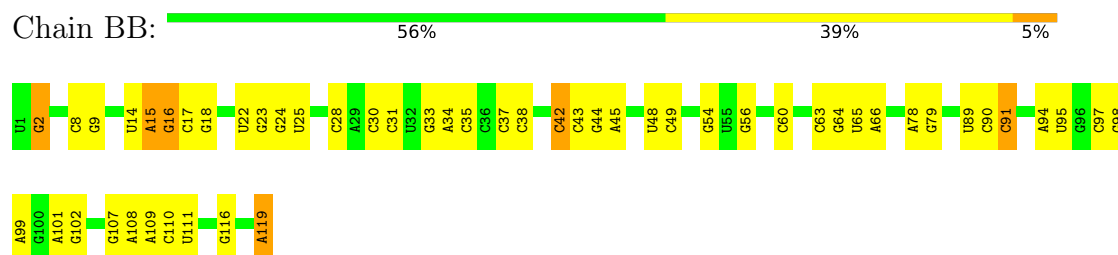


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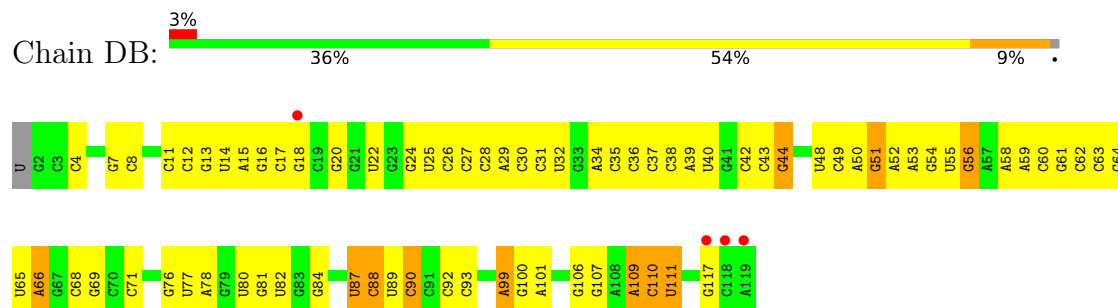
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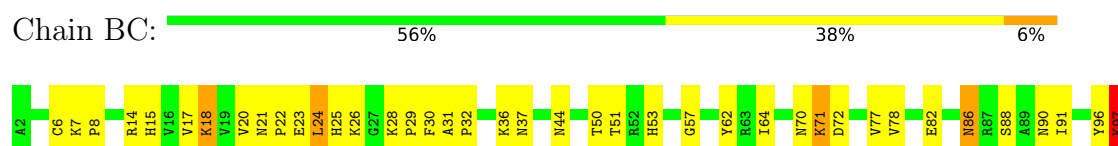
- Molecule 23: 5S rRNA

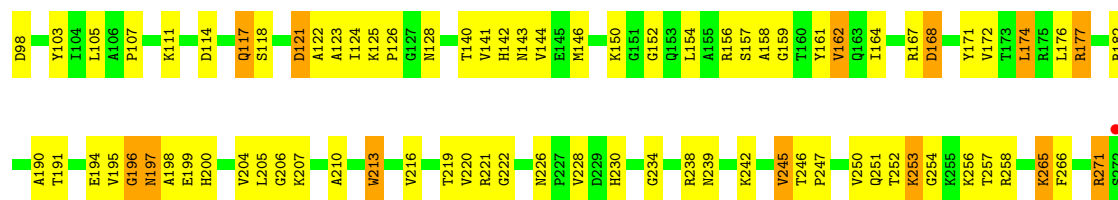


- Molecule 23: 5S rRNA

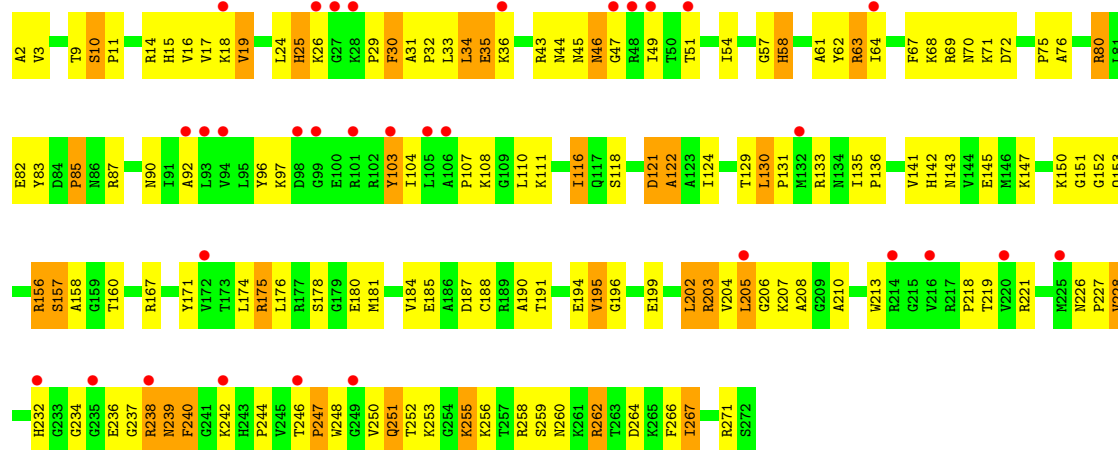


- Molecule 24: 50S ribosomal protein L2

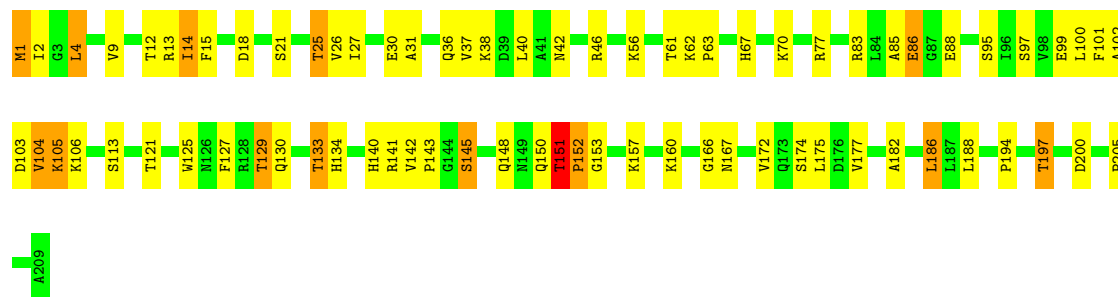




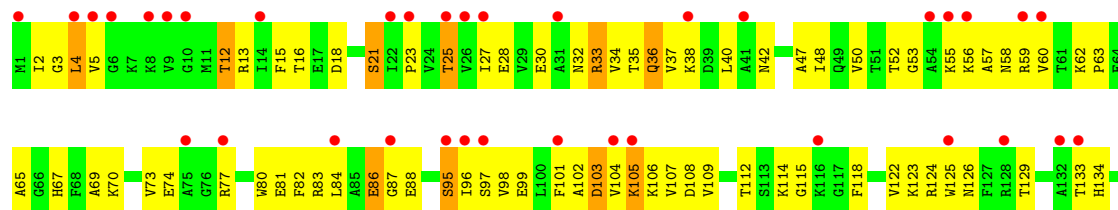
• Molecule 24: 50S ribosomal protein L2

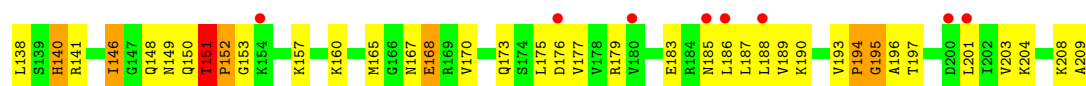


• Molecule 25: 50S ribosomal protein L3



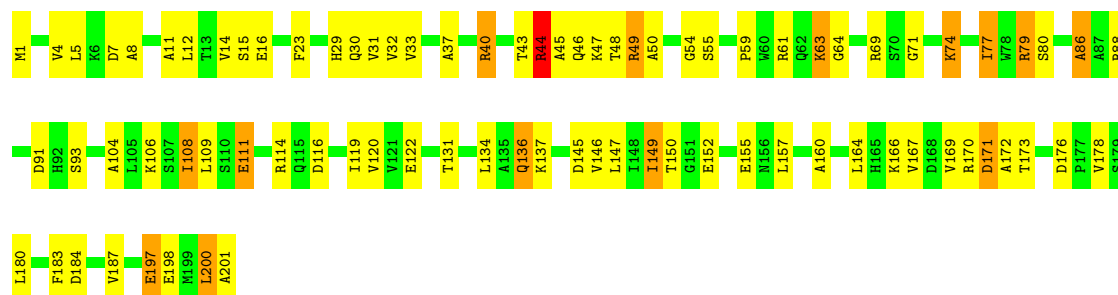
• Molecule 25: 50S ribosomal protein L3





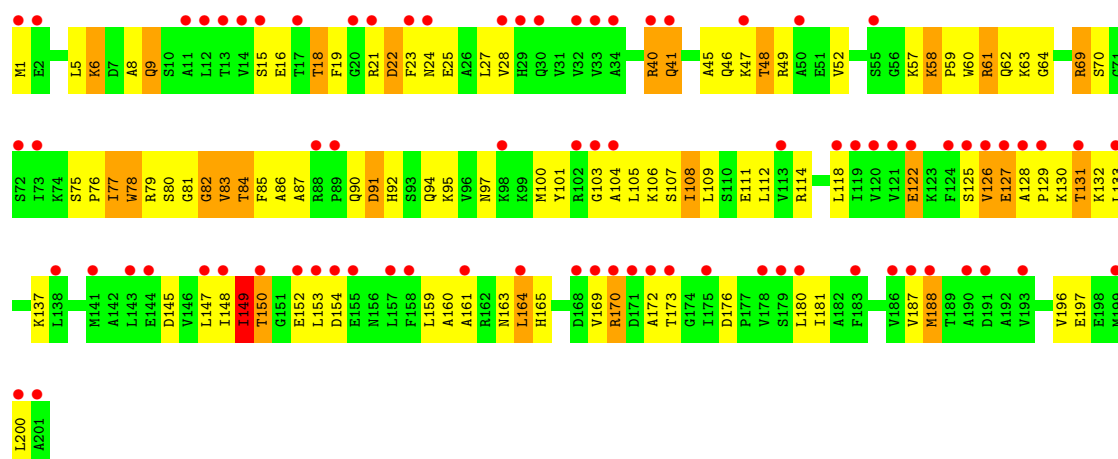
- Molecule 26: 50S ribosomal protein L4

Chain BE: 59% 34% 7%



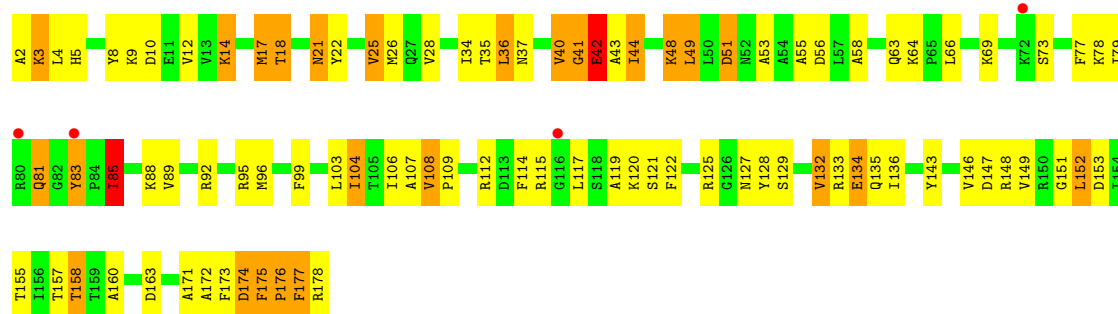
- Molecule 26: 50S ribosomal protein L4

Chain DE: 40% 49% 38% 12%

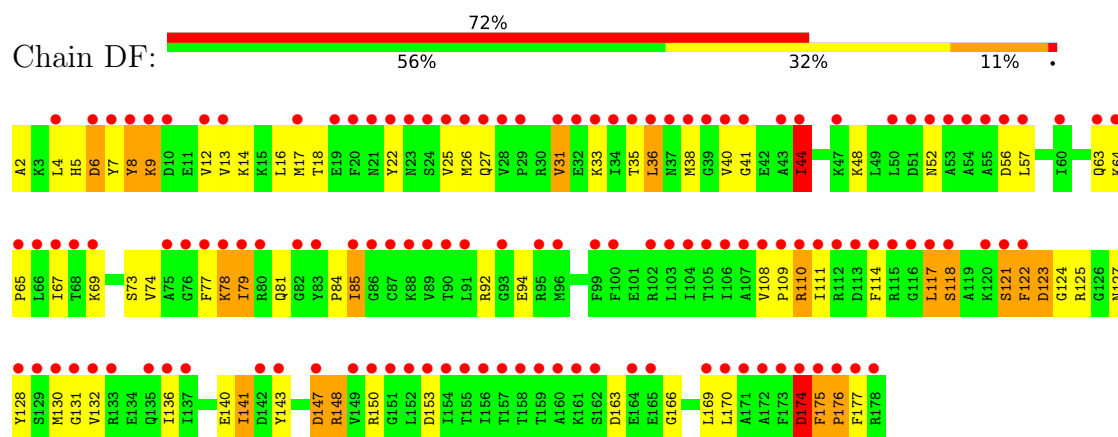


- Molecule 27: 50S ribosomal protein L5

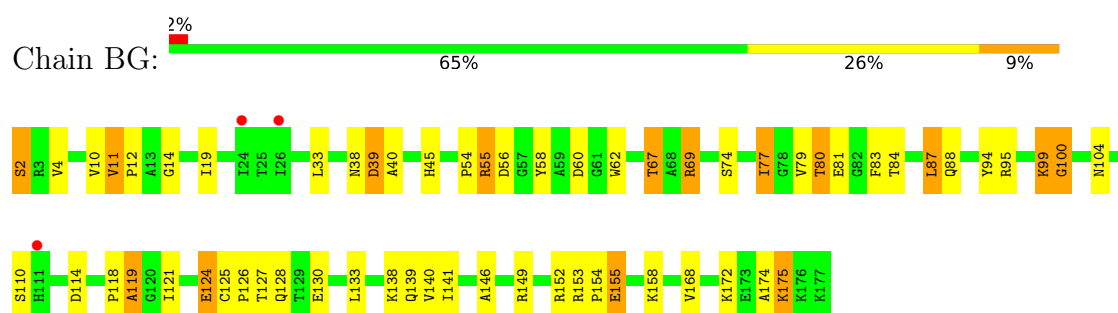
Chain BF: 2% 47% 37% 14%



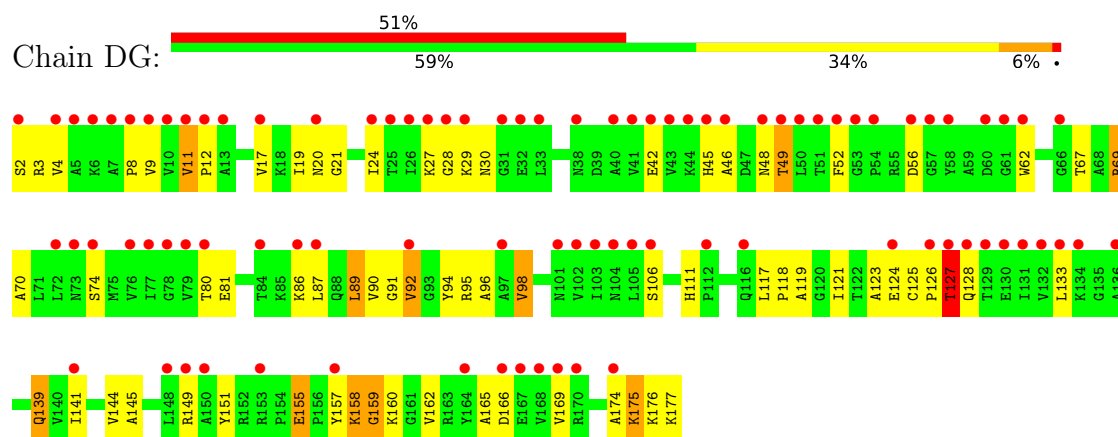
- Molecule 27: 50S ribosomal protein L5



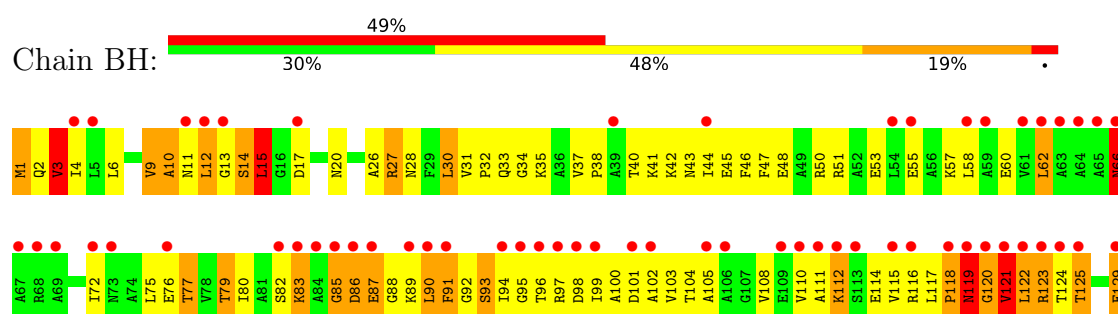
• Molecule 28: 50S ribosomal protein L6

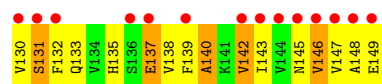


• Molecule 28: 50S ribosomal protein L6

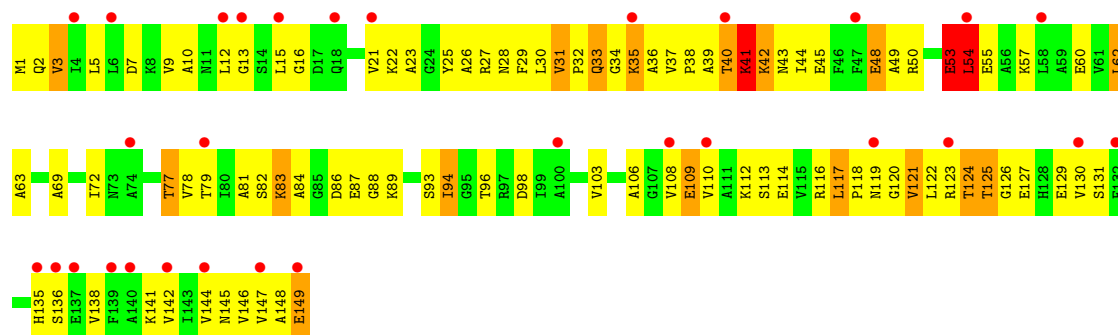


• Molecule 29: 50S ribosomal protein L9

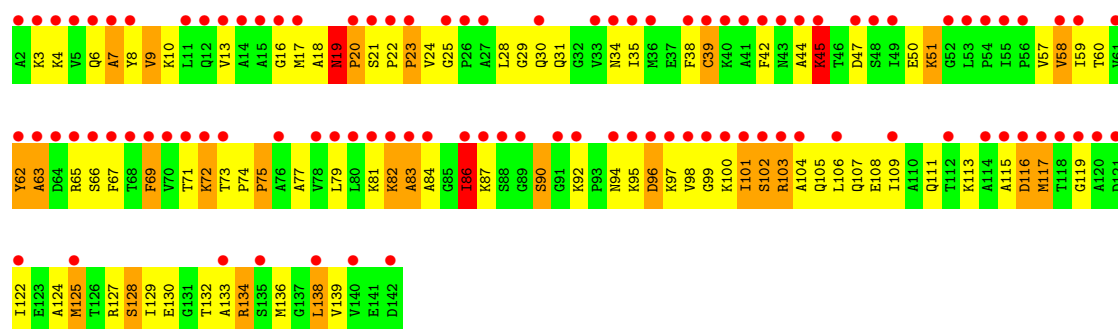
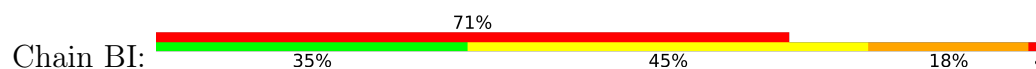




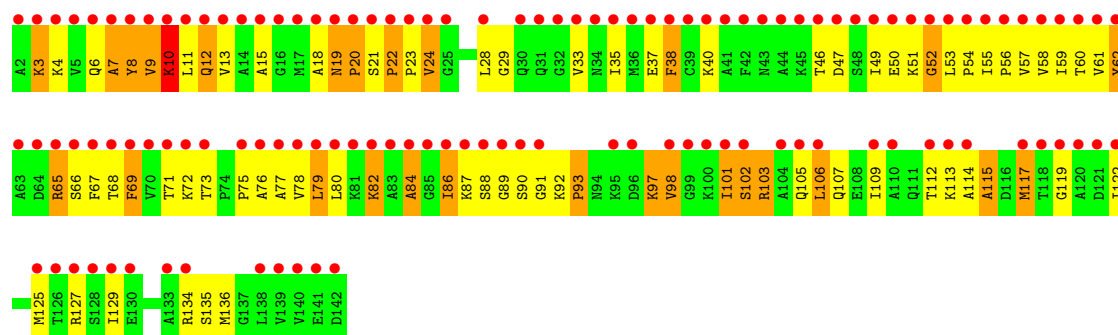
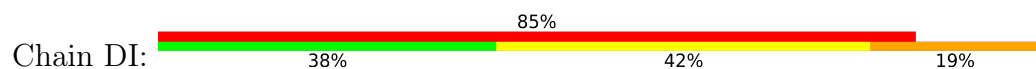
• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L11

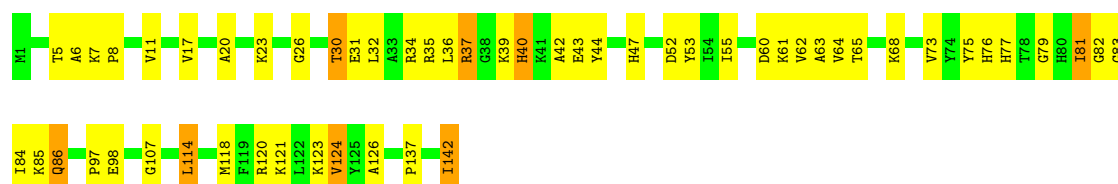


• Molecule 30: 50S ribosomal protein L11

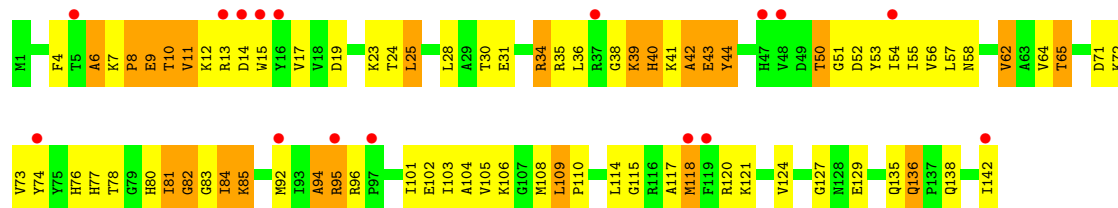
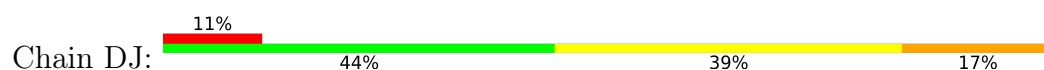


• Molecule 31: 50S ribosomal protein L13

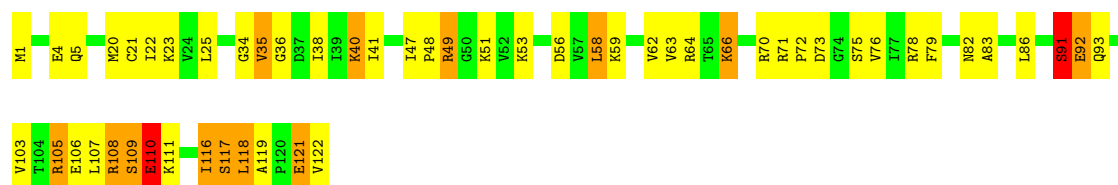




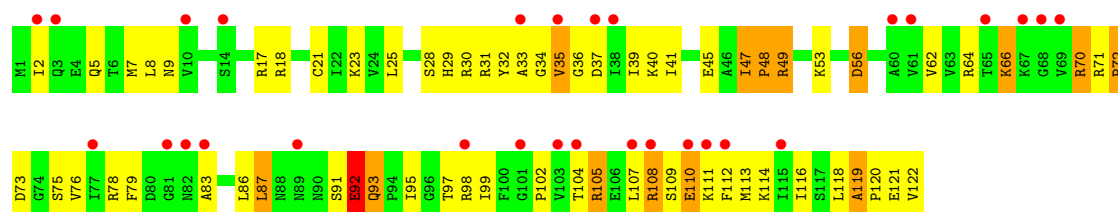
• Molecule 31: 50S ribosomal protein L13



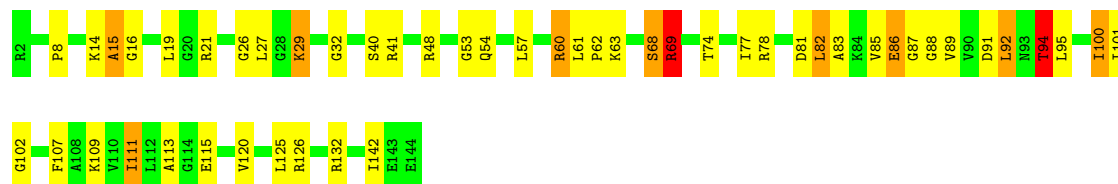
• Molecule 32: 50S ribosomal protein L14



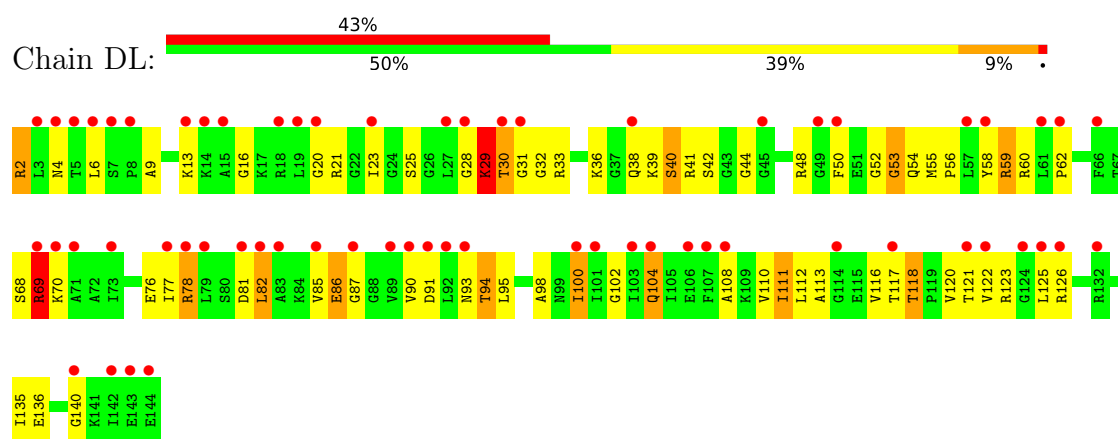
• Molecule 32: 50S ribosomal protein L14



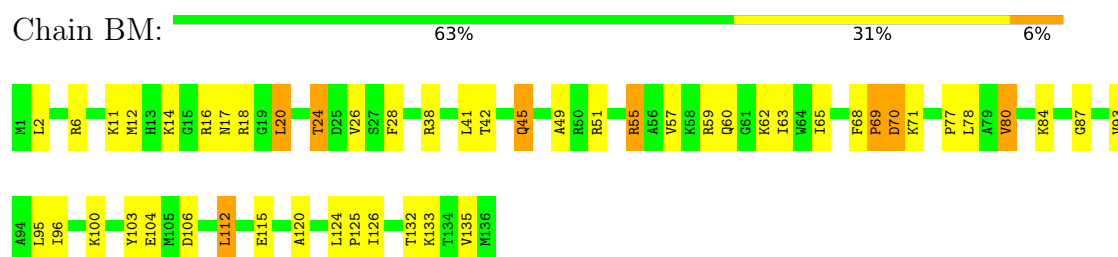
• Molecule 33: 50S ribosomal protein L15



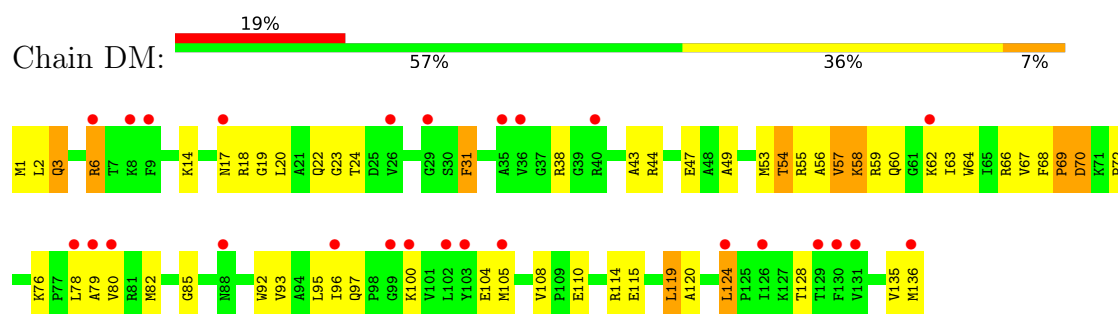
• Molecule 33: 50S ribosomal protein L15



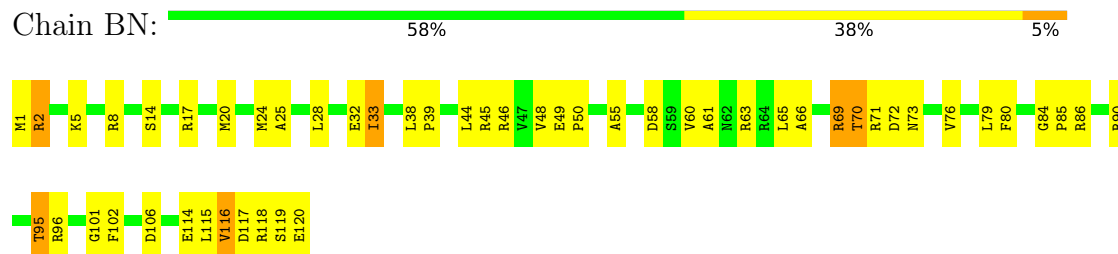
- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16

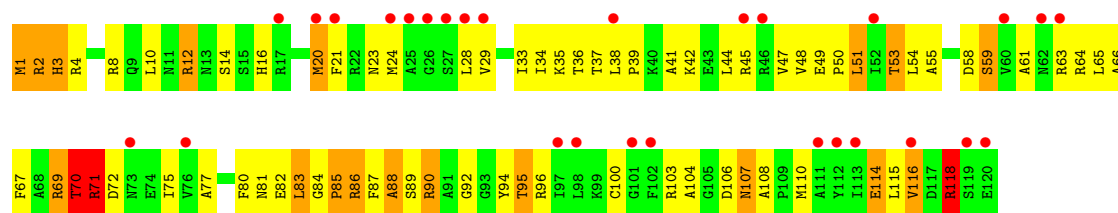


- Molecule 35: 50S ribosomal protein L17



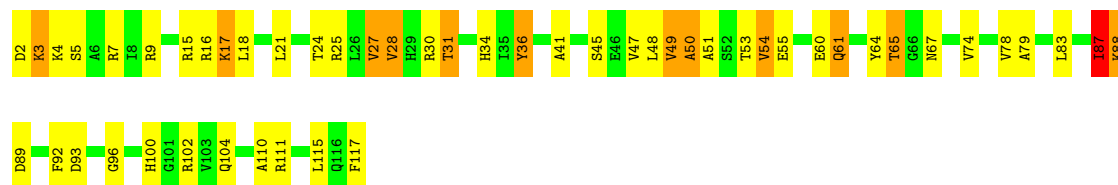
- Molecule 35: 50S ribosomal protein L17





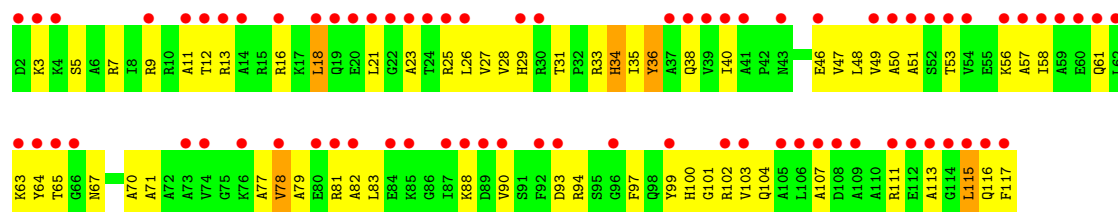
• Molecule 36: 50S ribosomal protein L18

Chain BO: 56% 33% 10% .



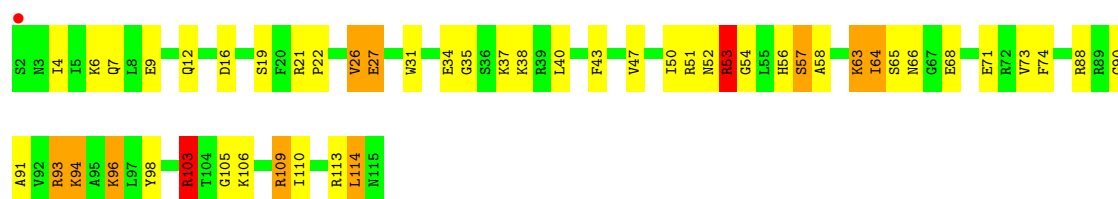
• Molecule 36: 50S ribosomal protein L18

Chain DO: 65% 46% 50% .



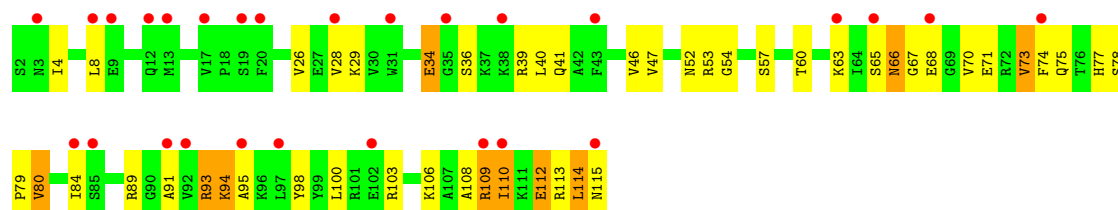
• Molecule 37: 50S ribosomal protein L19

Chain BP: 57% 32% 9% .



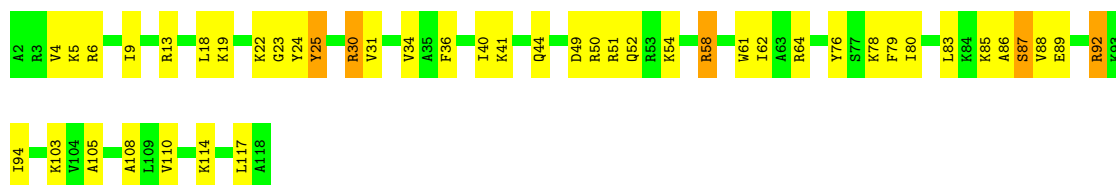
• Molecule 37: 50S ribosomal protein L19

Chain DP: 24% 58% 33% 9% .



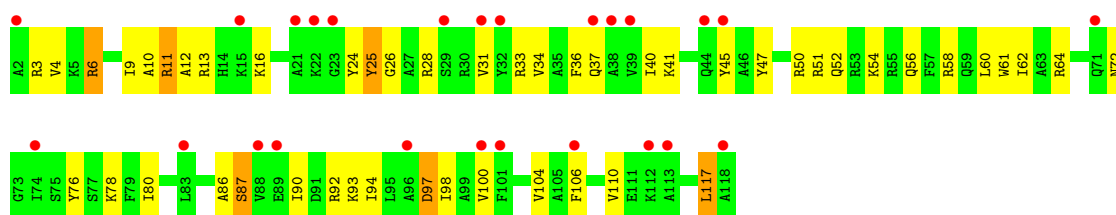
- Molecule 38: 50S ribosomal protein L20

Chain BQ: 



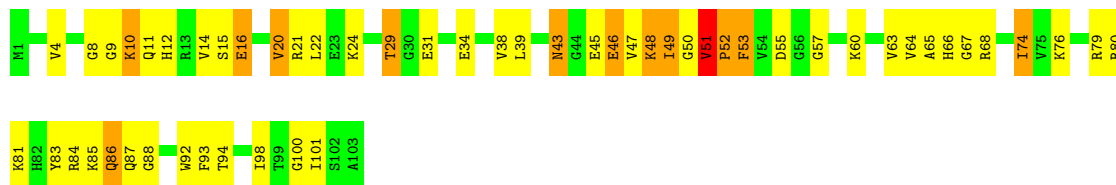
- Molecule 38: 50S ribosomal protein L20

Chain DQ: 



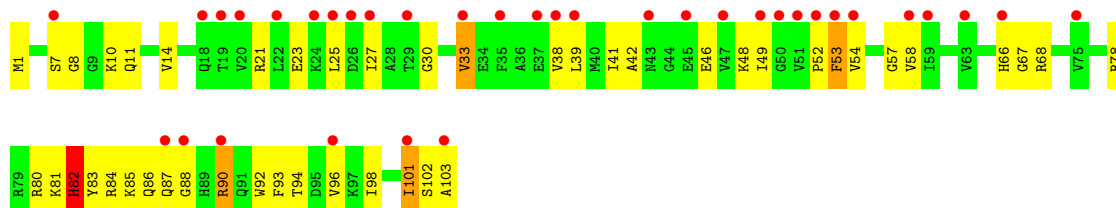
- Molecule 39: 50S ribosomal protein L21

Chain BR: 



- Molecule 39: 50S ribosomal protein L21

Chain DR: 



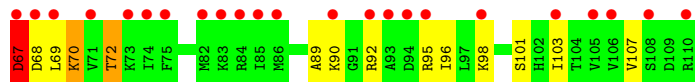
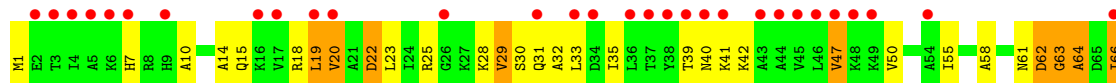
- Molecule 40: 50S ribosomal protein L22

Chain BS: 

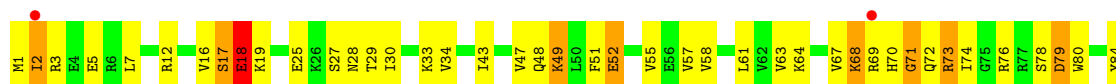




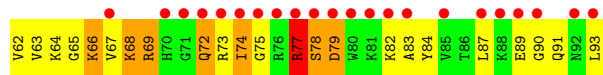
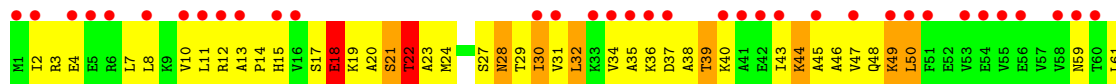
- Molecule 40: 50S ribosomal protein L22



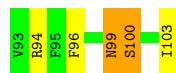
- Molecule 41: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L23

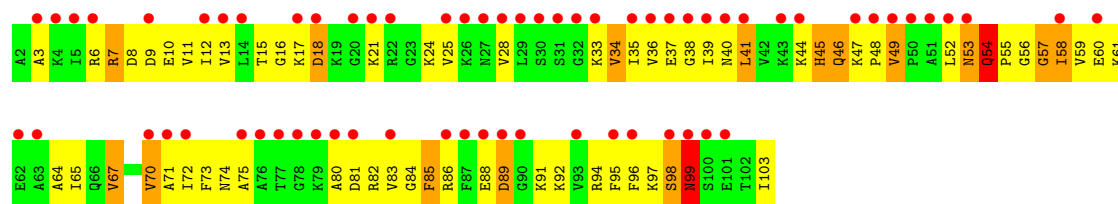


- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24





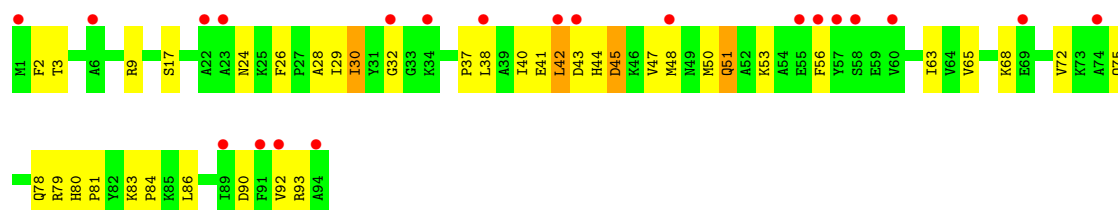
• Molecule 43: 50S ribosomal protein L25

Chain BV: 63% 27% 10% .



• Molecule 43: 50S ribosomal protein L25

Chain DV: 22% 59% 37% .



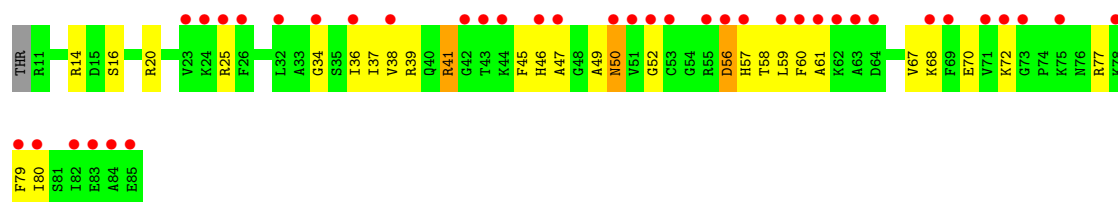
• Molecule 44: 50S ribosomal protein L27

Chain BW: 3% 63% 28% 8% .



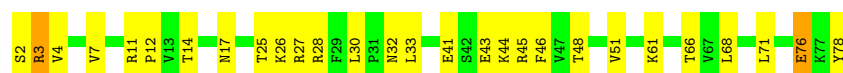
• Molecule 44: 50S ribosomal protein L27

Chain DW: 51% 61% 34% .

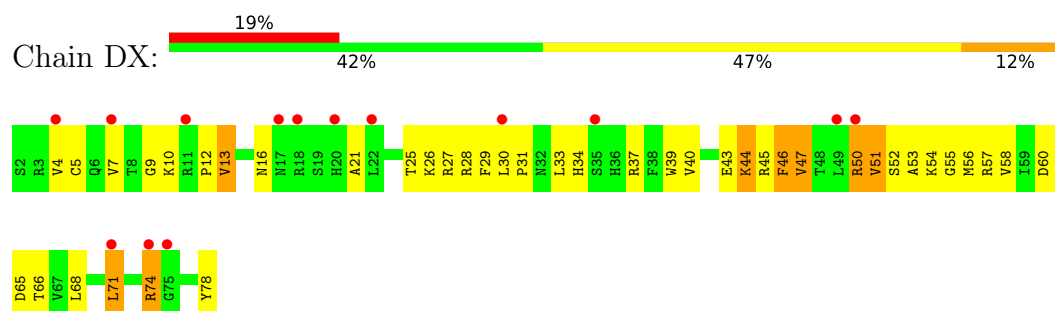


• Molecule 45: 50S ribosomal protein L28

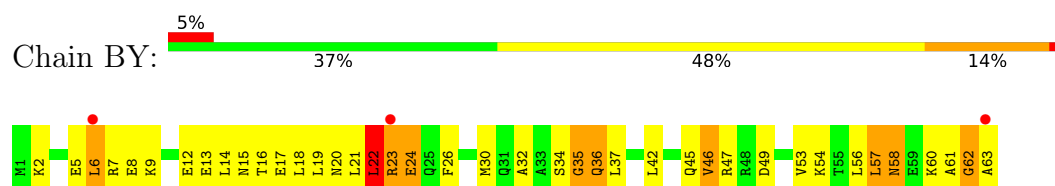
Chain BX: 64% 34% .



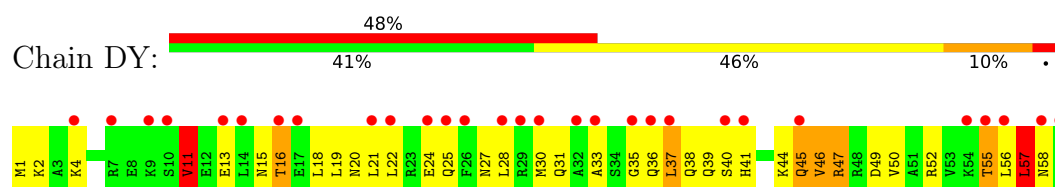
- Molecule 45: 50S ribosomal protein L28



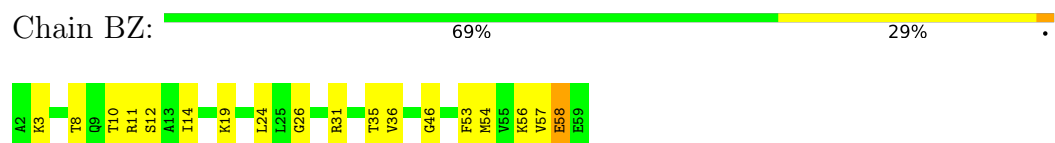
- Molecule 46: 50S ribosomal protein L29



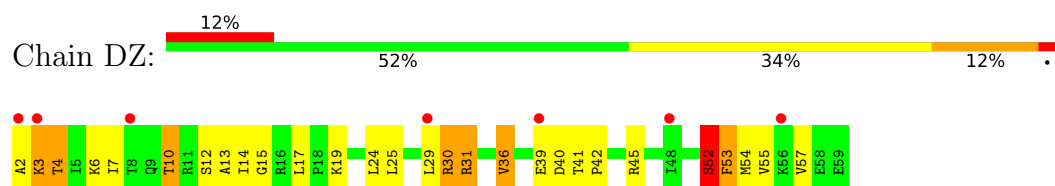
- Molecule 46: 50S ribosomal protein L29



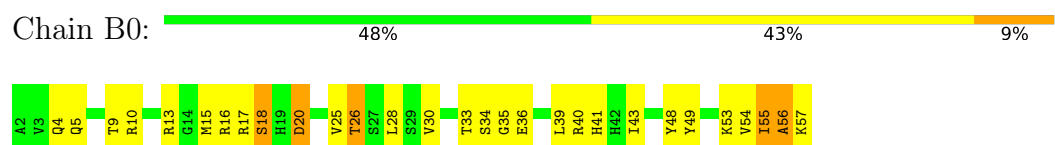
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

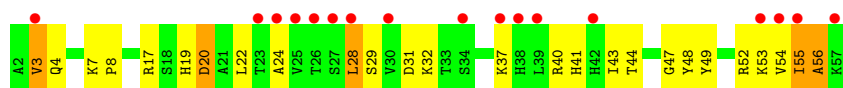


- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

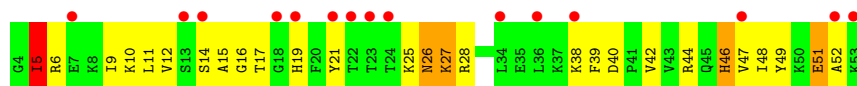




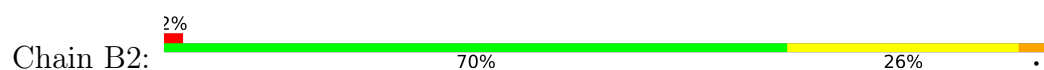
- Molecule 49: 50S ribosomal protein L33



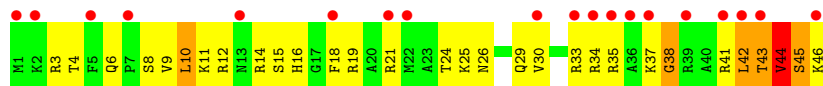
- Molecule 49: 50S ribosomal protein L33



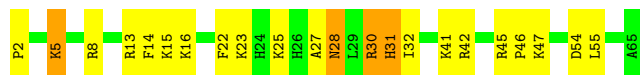
- Molecule 50: 50S ribosomal protein L34



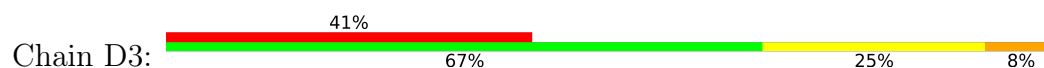
- Molecule 50: 50S ribosomal protein L34




- Molecule 51: 50S ribosomal protein L35

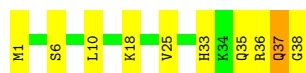


- Molecule 51: 50S ribosomal protein L35



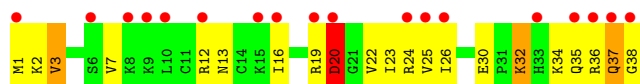
- Molecule 52: 50S ribosomal protein L36

Chain B4:  74% 24% .

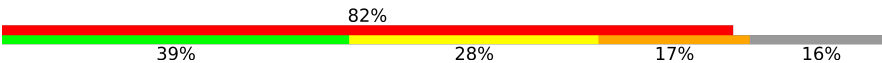


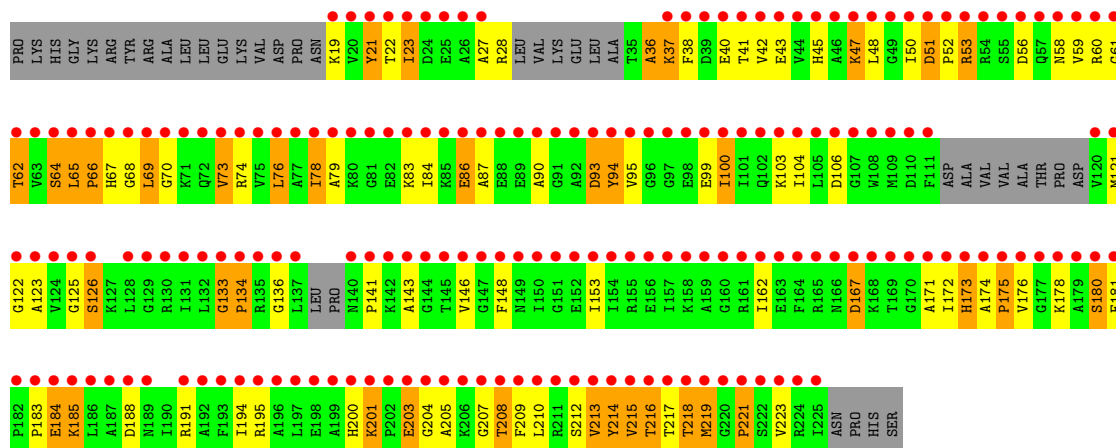
- Molecule 52: 50S ribosomal protein L36

Chain D4:  47% 45% 8% .



- Molecule 53: 50S ribosomal protein L1

Chain B5:  39% 82% 28% 17% 16%



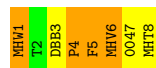
- Molecule 54: Quinupristin

Chain B6:  12% 75% 12%



- Molecule 54: Quinupristin

Chain D6:  12% 38% 50%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.26Å 432.34Å 621.39Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 69.08 – 2.80 69.08 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 94.1 (69.08-2.80) 94.1 (69.08-2.80) | Depositor EDS |
| R_{merge} | 0.14 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.40 (at 2.81Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.1_1160) | Depositor |
| R, R_{free} | 0.225 , 0.271 0.230 , 0.276 | Depositor DCC |
| R_{free} test set | 5217 reflections (0.40%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 48.8 | Xtriage |
| Anisotropy | 0.379 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 54.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 288423 | wwPDB-VP |
| Average B, all atoms (Å ²) | 61.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MHW, 004, MHV, MG, DOL, ZN, DBB, MHU, MHT

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 | 0.34 | 0/36944 | 0.80 | 3/57632 (0.0%) |
| 1 | CA | 0.28 | 0/36966 | 0.78 | 1/57666 (0.0%) |
| 2 | AB | 0.28 | 0/1736 | 0.56 | 0/2338 |
| 2 | CB | 0.26 | 0/1736 | 0.50 | 0/2338 |
| 3 | AC | 0.28 | 0/1652 | 0.53 | 0/2225 |
| 3 | CC | 0.25 | 0/1652 | 0.48 | 0/2225 |
| 4 | AD | 0.29 | 0/1665 | 0.55 | 0/2227 |
| 4 | CD | 0.31 | 0/1665 | 0.55 | 0/2227 |
| 5 | AE | 0.31 | 0/1119 | 0.61 | 0/1504 |
| 5 | CE | 0.29 | 0/1119 | 0.59 | 0/1504 |
| 6 | AF | 0.30 | 0/836 | 0.55 | 0/1128 |
| 6 | CF | 0.27 | 0/836 | 0.57 | 1/1128 (0.1%) |
| 7 | AG | 0.26 | 0/1196 | 0.48 | 0/1602 |
| 7 | CG | 0.25 | 0/1196 | 0.49 | 0/1602 |
| 8 | AH | 0.31 | 0/989 | 0.50 | 0/1326 |
| 8 | CH | 0.25 | 0/989 | 0.48 | 0/1326 |
| 9 | AI | 0.26 | 0/1034 | 0.54 | 0/1375 |
| 9 | CI | 0.26 | 0/1034 | 0.52 | 0/1375 |
| 10 | AJ | 0.29 | 0/797 | 0.55 | 0/1077 |
| 10 | CJ | 0.25 | 0/797 | 0.50 | 0/1077 |
| 11 | AK | 0.29 | 0/893 | 0.63 | 1/1205 (0.1%) |
| 11 | CK | 0.26 | 0/893 | 0.52 | 0/1205 |
| 12 | AL | 0.31 | 0/969 | 0.58 | 0/1300 |
| 12 | CL | 0.29 | 0/969 | 0.60 | 0/1300 |
| 13 | AM | 0.27 | 0/893 | 0.55 | 0/1193 |
| 13 | CM | 0.26 | 0/893 | 0.50 | 0/1193 |
| 14 | AN | 0.28 | 0/785 | 0.55 | 0/1043 |
| 14 | CN | 0.25 | 0/785 | 0.46 | 0/1043 |
| 15 | AO | 0.28 | 0/718 | 0.53 | 0/959 |
| 15 | CO | 0.26 | 0/718 | 0.46 | 0/959 |
| 16 | AP | 0.30 | 0/659 | 0.66 | 1/884 (0.1%) |
| 16 | CP | 0.27 | 0/659 | 0.49 | 0/884 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.30 | 0/658 | 0.58 | 0/881 |
| 17 | CQ | 0.28 | 0/658 | 0.51 | 0/881 |
| 18 | AR | 0.26 | 0/463 | 0.53 | 0/621 |
| 18 | CR | 0.26 | 0/463 | 0.49 | 0/621 |
| 19 | AS | 0.27 | 0/653 | 0.50 | 0/877 |
| 19 | CS | 0.27 | 0/653 | 0.54 | 0/877 |
| 20 | AT | 0.31 | 0/671 | 0.55 | 0/888 |
| 20 | CT | 0.25 | 0/671 | 0.50 | 0/888 |
| 21 | AU | 0.36 | 0/431 | 0.62 | 0/570 |
| 21 | CU | 0.33 | 0/431 | 0.56 | 0/570 |
| 22 | BA | 0.59 | 5/69659 (0.0%) | 0.99 | 92/108672 (0.1%) |
| 22 | DA | 0.27 | 0/69659 | 0.79 | 4/108672 (0.0%) |
| 23 | BB | 0.52 | 0/2850 | 0.93 | 0/4444 |
| 23 | DB | 0.23 | 0/2828 | 0.76 | 0/4410 |
| 24 | BC | 0.38 | 0/2122 | 0.60 | 0/2852 |
| 24 | DC | 0.27 | 0/2122 | 0.52 | 0/2852 |
| 25 | BD | 0.42 | 0/1586 | 0.63 | 1/2134 (0.0%) |
| 25 | DD | 0.26 | 0/1586 | 0.51 | 0/2134 |
| 26 | BE | 0.37 | 0/1571 | 0.60 | 0/2113 |
| 26 | DE | 0.26 | 0/1571 | 0.51 | 0/2113 |
| 27 | BF | 0.30 | 0/1435 | 0.52 | 0/1926 |
| 27 | DF | 0.24 | 0/1435 | 0.46 | 0/1926 |
| 28 | BG | 0.30 | 0/1343 | 0.53 | 0/1816 |
| 28 | DG | 0.25 | 0/1343 | 0.46 | 0/1816 |
| 29 | BH | 0.36 | 0/1121 | 0.66 | 1/1515 (0.1%) |
| 29 | DH | 0.35 | 0/1121 | 0.56 | 0/1515 |
| 30 | BI | 0.29 | 0/1046 | 0.54 | 0/1410 |
| 30 | DI | 0.28 | 0/1046 | 0.52 | 0/1410 |
| 31 | BJ | 0.42 | 0/1152 | 0.58 | 0/1551 |
| 31 | DJ | 0.25 | 0/1152 | 0.51 | 0/1551 |
| 32 | BK | 0.41 | 0/948 | 0.64 | 0/1268 |
| 32 | DK | 0.27 | 0/948 | 0.51 | 0/1268 |
| 33 | BL | 0.39 | 0/1054 | 0.64 | 0/1403 |
| 33 | DL | 0.26 | 0/1054 | 0.51 | 0/1403 |
| 34 | BM | 0.42 | 0/1093 | 0.63 | 0/1460 |
| 34 | DM | 0.25 | 0/1093 | 0.46 | 0/1460 |
| 35 | BN | 0.43 | 0/974 | 0.68 | 0/1301 |
| 35 | DN | 0.27 | 0/974 | 0.56 | 1/1301 (0.1%) |
| 36 | BO | 0.34 | 0/902 | 0.55 | 0/1209 |
| 36 | DO | 0.24 | 0/902 | 0.45 | 0/1209 |
| 37 | BP | 0.42 | 0/929 | 0.69 | 2/1242 (0.2%) |
| 37 | DP | 0.26 | 0/929 | 0.47 | 0/1242 |
| 38 | BQ | 0.50 | 0/960 | 0.66 | 0/1278 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DQ | 0.26 | 0/960 | 0.47 | 0/1278 |
| 39 | BR | 0.47 | 0/829 | 0.73 | 1/1107 (0.1%) |
| 39 | DR | 0.25 | 0/829 | 0.50 | 0/1107 |
| 40 | BS | 0.51 | 0/864 | 0.64 | 0/1156 |
| 40 | DS | 0.26 | 0/864 | 0.50 | 0/1156 |
| 41 | BT | 0.36 | 0/745 | 0.60 | 0/994 |
| 41 | DT | 0.25 | 0/745 | 0.49 | 0/994 |
| 42 | BU | 0.36 | 0/788 | 0.57 | 0/1051 |
| 42 | DU | 0.28 | 0/788 | 0.52 | 0/1051 |
| 43 | BV | 0.37 | 0/766 | 0.58 | 0/1025 |
| 43 | DV | 0.24 | 0/766 | 0.44 | 0/1025 |
| 44 | BW | 0.44 | 0/587 | 0.71 | 2/776 (0.3%) |
| 44 | DW | 0.25 | 0/576 | 0.47 | 0/762 |
| 45 | BX | 0.34 | 0/635 | 0.57 | 0/848 |
| 45 | DX | 0.28 | 0/635 | 0.53 | 0/848 |
| 46 | BY | 0.32 | 0/510 | 0.63 | 0/677 |
| 46 | DY | 0.25 | 0/510 | 0.50 | 0/677 |
| 47 | BZ | 0.43 | 0/453 | 0.61 | 0/605 |
| 47 | DZ | 0.26 | 0/453 | 0.48 | 0/605 |
| 48 | B0 | 0.44 | 0/450 | 0.64 | 0/599 |
| 48 | D0 | 0.27 | 0/450 | 0.50 | 0/599 |
| 49 | B1 | 0.37 | 0/417 | 0.53 | 0/554 |
| 49 | D1 | 0.28 | 0/417 | 0.49 | 0/554 |
| 50 | B2 | 0.44 | 0/380 | 0.69 | 0/498 |
| 50 | D2 | 0.28 | 0/380 | 0.51 | 0/498 |
| 51 | B3 | 0.38 | 0/513 | 0.57 | 0/676 |
| 51 | D3 | 0.25 | 0/513 | 0.44 | 0/676 |
| 52 | B4 | 0.43 | 0/303 | 0.63 | 0/397 |
| 52 | D4 | 0.25 | 0/303 | 0.49 | 0/397 |
| 53 | B5 | 0.25 | 0/1145 | 0.49 | 0/1556 |
| 54 | B6 | 1.77 | 0/13 | 2.40 | 1/15 (6.7%) |
| 54 | D6 | 1.44 | 0/13 | 2.02 | 1/15 (6.7%) |
| All | All | 0.39 | 5/310652 (0.0%) | 0.79 | 113/464396 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6 | CF | 0 | 1 |
| 11 | AK | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 12 | CL | 0 | 2 |
| 25 | BD | 0 | 1 |
| 25 | DD | 0 | 1 |
| All | All | 0 | 6 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | BA | 984 | A | N9-C4 | -8.33 | 1.32 | 1.37 |
| 22 | BA | 1142 | A | N9-C4 | -7.64 | 1.33 | 1.37 |
| 22 | BA | 1936 | A | N9-C4 | -7.63 | 1.33 | 1.37 |
| 22 | BA | 528 | A | N9-C4 | -7.62 | 1.33 | 1.37 |
| 22 | BA | 528 | A | N3-C4 | -5.47 | 1.31 | 1.34 |

All (113) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | BA | 974 | G | C4-C5-N7 | 10.83 | 115.13 | 110.80 |
| 22 | BA | 974 | G | C6-C5-N7 | -10.21 | 124.27 | 130.40 |
| 25 | BD | 151 | THR | C-N-CD | -9.98 | 98.64 | 120.60 |
| 22 | BA | 984 | A | C2-N3-C4 | -9.95 | 105.62 | 110.60 |
| 22 | BA | 974 | G | C5-N7-C8 | -9.65 | 99.48 | 104.30 |
| 22 | BA | 974 | G | C5-C6-O6 | -9.39 | 122.96 | 128.60 |
| 22 | BA | 974 | G | N1-C6-O6 | 9.23 | 125.44 | 119.90 |
| 22 | BA | 528 | A | C2-N3-C4 | -8.94 | 106.13 | 110.60 |
| 22 | BA | 984 | A | N3-C4-C5 | 8.82 | 132.97 | 126.80 |
| 22 | BA | 752 | A | C5-N7-C8 | -8.81 | 99.50 | 103.90 |
| 22 | BA | 752 | A | N1-C6-N6 | 8.79 | 123.87 | 118.60 |
| 22 | BA | 984 | A | N3-C4-N9 | -8.56 | 120.55 | 127.40 |
| 16 | AP | 51 | ARG | NE-CZ-NH1 | 8.43 | 124.51 | 120.30 |
| 22 | BA | 528 | A | N1-C6-N6 | 8.42 | 123.65 | 118.60 |
| 22 | BA | 974 | G | N7-C8-N9 | 8.29 | 117.25 | 113.10 |
| 22 | BA | 752 | A | C4-C5-N7 | 8.03 | 114.71 | 110.70 |
| 22 | BA | 1142 | A | C2-N3-C4 | -7.99 | 106.60 | 110.60 |
| 37 | BP | 103 | ARG | NE-CZ-NH1 | 7.92 | 124.26 | 120.30 |
| 37 | BP | 53 | ARG | NE-CZ-NH1 | 7.84 | 124.22 | 120.30 |
| 22 | BA | 1936 | A | C2-N3-C4 | -7.70 | 106.75 | 110.60 |
| 22 | BA | 704 | G | O4'-C1'-N9 | 7.38 | 114.11 | 108.20 |
| 22 | BA | 1936 | A | N3-C4-C5 | 7.36 | 131.95 | 126.80 |
| 22 | BA | 784 | G | O4'-C1'-N9 | -7.22 | 102.42 | 108.20 |
| 11 | AK | 128 | ARG | NE-CZ-NH1 | 7.19 | 123.89 | 120.30 |
| 35 | DN | 71 | ARG | NE-CZ-NH2 | 7.19 | 123.89 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 974 | G | C4-N9-C1' | 7.04 | 135.65 | 126.50 |
| 22 | BA | 752 | A | C6-C5-N7 | -7.01 | 127.39 | 132.30 |
| 22 | BA | 586 | A | O5'-P-OP1 | -6.96 | 99.44 | 105.70 |
| 22 | BA | 528 | A | C5-N7-C8 | -6.81 | 100.49 | 103.90 |
| 22 | BA | 2588 | G | O5'-P-OP2 | -6.80 | 99.58 | 105.70 |
| 22 | BA | 783 | A | C5-N7-C8 | -6.70 | 100.55 | 103.90 |
| 22 | BA | 752 | A | N7-C8-N9 | 6.68 | 117.14 | 113.80 |
| 22 | BA | 1936 | A | N1-C6-N6 | 6.55 | 122.53 | 118.60 |
| 22 | BA | 2499 | C | N1-C2-O2 | -6.55 | 114.97 | 118.90 |
| 22 | BA | 2250 | G | C5-N7-C8 | -6.46 | 101.07 | 104.30 |
| 22 | BA | 2606 | C | C6-N1-C2 | 6.45 | 122.88 | 120.30 |
| 22 | BA | 1936 | A | N3-C4-N9 | -6.32 | 122.35 | 127.40 |
| 22 | BA | 1985 | C | N1-C2-O2 | -6.30 | 115.12 | 118.90 |
| 22 | BA | 752 | A | C5-C6-N6 | -6.28 | 118.68 | 123.70 |
| 22 | BA | 2645 | G | O4'-C1'-N9 | 6.24 | 113.19 | 108.20 |
| 22 | DA | 1313 | U | C2-N1-C1' | 6.18 | 125.12 | 117.70 |
| 22 | BA | 967 | U | N3-C4-O4 | -6.17 | 115.08 | 119.40 |
| 22 | BA | 481 | G | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 22 | BA | 2453 | A | N1-C6-N6 | 6.08 | 122.25 | 118.60 |
| 22 | BA | 752 | A | O4'-C1'-N9 | 6.07 | 113.06 | 108.20 |
| 22 | BA | 967 | U | C5-C4-O4 | 6.06 | 129.54 | 125.90 |
| 22 | BA | 784 | G | P-O3'-C3' | 6.03 | 126.94 | 119.70 |
| 22 | BA | 963 | U | O5'-P-OP2 | -5.99 | 100.31 | 105.70 |
| 22 | BA | 783 | A | C4-C5-N7 | 5.95 | 113.67 | 110.70 |
| 22 | BA | 1331 | G | N1-C6-O6 | -5.93 | 116.34 | 119.90 |
| 1 | AA | 4 | U | C2-N1-C1' | 5.93 | 124.82 | 117.70 |
| 6 | CF | 86 | ARG | NE-CZ-NH1 | 5.91 | 123.25 | 120.30 |
| 22 | BA | 783 | A | C2-N3-C4 | -5.90 | 107.65 | 110.60 |
| 22 | BA | 2250 | G | C4-C5-N7 | 5.87 | 113.15 | 110.80 |
| 22 | BA | 705 | A | N1-C6-N6 | 5.87 | 122.12 | 118.60 |
| 22 | BA | 1779 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 22 | BA | 2799 | A | N1-C6-N6 | 5.86 | 122.11 | 118.60 |
| 22 | BA | 528 | A | O4'-C1'-N9 | -5.83 | 103.54 | 108.20 |
| 22 | BA | 837 | C | N1-C2-O2 | -5.81 | 115.41 | 118.90 |
| 22 | BA | 1779 | U | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 22 | BA | 1142 | A | N3-C4-C5 | 5.80 | 130.86 | 126.80 |
| 22 | BA | 783 | A | N3-C4-C5 | 5.79 | 130.85 | 126.80 |
| 54 | D6 | 4 | PRO | N-CA-CB | 5.78 | 110.23 | 103.30 |
| 22 | BA | 1452 | G | C5-N7-C8 | -5.75 | 101.43 | 104.30 |
| 22 | BA | 2286 | G | N3-C4-C5 | 5.74 | 131.47 | 128.60 |
| 44 | BW | 41 | ARG | NE-CZ-NH2 | -5.71 | 117.44 | 120.30 |
| 1 | AA | 188 | C | C2-N1-C1' | 5.71 | 125.08 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 2542 | A | N1-C6-N6 | -5.69 | 115.19 | 118.60 |
| 22 | BA | 1452 | G | C4-C5-N7 | 5.67 | 113.07 | 110.80 |
| 22 | BA | 2890 | G | C4-C5-N7 | 5.62 | 113.05 | 110.80 |
| 1 | CA | 4 | U | C2-N1-C1' | 5.59 | 124.41 | 117.70 |
| 22 | BA | 1645 | G | C6-C5-N7 | -5.55 | 127.07 | 130.40 |
| 22 | BA | 698 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 22 | BA | 2887 | A | N1-C6-N6 | 5.53 | 121.92 | 118.60 |
| 54 | B6 | 4 | PRO | N-CA-CB | 5.52 | 109.93 | 103.30 |
| 22 | BA | 2580 | U | OP2-P-O3' | 5.48 | 117.26 | 105.20 |
| 39 | BR | 51 | VAL | C-N-CD | 5.48 | 139.91 | 128.40 |
| 22 | DA | 2447 | G | C4-N9-C1' | -5.43 | 119.43 | 126.50 |
| 22 | BA | 1658 | C | C6-N1-C2 | 5.42 | 122.47 | 120.30 |
| 22 | BA | 974 | G | C8-N9-C1' | -5.41 | 119.97 | 127.00 |
| 22 | BA | 528 | A | C6-C5-N7 | -5.38 | 128.53 | 132.30 |
| 22 | BA | 1645 | G | C4-C5-N7 | 5.37 | 112.95 | 110.80 |
| 22 | BA | 984 | A | C4-N9-C1' | -5.37 | 116.64 | 126.30 |
| 22 | BA | 2512 | C | N1-C2-O2 | -5.36 | 115.69 | 118.90 |
| 22 | BA | 1761 | C | O5'-P-OP1 | -5.35 | 100.88 | 105.70 |
| 22 | BA | 1783 | A | O5'-P-OP2 | -5.34 | 100.90 | 105.70 |
| 22 | BA | 528 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 22 | BA | 2705 | A | N1-C6-N6 | 5.29 | 121.77 | 118.60 |
| 44 | BW | 41 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 22 | BA | 2447 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 22 | BA | 1230 | A | O5'-P-OP2 | -5.27 | 100.96 | 105.70 |
| 22 | BA | 2501 | C | C2-N1-C1' | -5.24 | 113.04 | 118.80 |
| 22 | BA | 990 | A | C5-C6-N6 | -5.23 | 119.52 | 123.70 |
| 22 | BA | 2609 | U | C2-N1-C1' | -5.20 | 111.46 | 117.70 |
| 22 | BA | 1331 | G | C5-C6-O6 | 5.18 | 131.71 | 128.60 |
| 22 | BA | 2030 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 1 | AA | 279 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 22 | DA | 2501 | C | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 22 | BA | 974 | G | C8-N9-C4 | -5.16 | 104.33 | 106.40 |
| 29 | BH | 121 | VAL | C-N-CA | 5.15 | 134.57 | 121.70 |
| 22 | BA | 2030 | A | C5-C6-N6 | 5.14 | 127.81 | 123.70 |
| 22 | DA | 2447 | G | C8-N9-C1' | 5.14 | 133.69 | 127.00 |
| 22 | BA | 15 | G | C5-C6-O6 | 5.13 | 131.68 | 128.60 |
| 22 | BA | 1134 | A | O5'-P-OP1 | -5.13 | 101.08 | 105.70 |
| 22 | BA | 528 | A | C4-C5-N7 | 5.13 | 113.27 | 110.70 |
| 22 | BA | 2017 | U | O5'-P-OP1 | -5.09 | 101.12 | 105.70 |
| 22 | BA | 563 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 22 | BA | 528 | A | N3-C4-C5 | 5.07 | 130.35 | 126.80 |
| 22 | BA | 2581 | G | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 1900 | A | O5'-P-OP1 | -5.07 | 101.14 | 105.70 |
| 22 | BA | 2848 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 22 | BA | 2060 | A | N1-C6-N6 | -5.05 | 115.57 | 118.60 |
| 22 | BA | 984 | A | C8-N9-C1' | 5.03 | 136.75 | 127.70 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 11 | AK | 126 | LYS | Peptide |
| 25 | BD | 151 | THR | Peptide |
| 6 | CF | 54 | LEU | Peptide |
| 12 | CL | 23 | ALA | Peptide |
| 12 | CL | 24 | LEU | Peptide |
| 25 | DD | 151 | THR | Peptide |

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 | 32995 | 0 | 16607 | 962 | 0 |
| 1 | CA | 33015 | 0 | 16617 | 1107 | 1 |
| 2 | AB | 1705 | 0 | 1732 | 164 | 0 |
| 2 | CB | 1705 | 0 | 1732 | 135 | 0 |
| 3 | AC | 1625 | 0 | 1696 | 78 | 0 |
| 3 | CC | 1625 | 0 | 1696 | 69 | 0 |
| 4 | AD | 1643 | 0 | 1707 | 116 | 0 |
| 4 | CD | 1643 | 0 | 1707 | 116 | 0 |
| 5 | AE | 1106 | 0 | 1148 | 88 | 0 |
| 5 | CE | 1106 | 0 | 1148 | 99 | 0 |
| 6 | AF | 818 | 0 | 808 | 47 | 0 |
| 6 | CF | 818 | 0 | 808 | 60 | 0 |
| 7 | AG | 1182 | 0 | 1238 | 58 | 0 |
| 7 | CG | 1182 | 0 | 1238 | 66 | 0 |
| 8 | AH | 979 | 0 | 1031 | 49 | 0 |
| 8 | CH | 979 | 0 | 1031 | 52 | 0 |
| 9 | AI | 1022 | 0 | 1070 | 87 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | CI | 1022 | 0 | 1070 | 66 | 0 |
| 10 | AJ | 787 | 0 | 828 | 81 | 0 |
| 10 | CJ | 787 | 0 | 828 | 56 | 0 |
| 11 | AK | 877 | 0 | 887 | 68 | 0 |
| 11 | CK | 877 | 0 | 887 | 55 | 0 |
| 12 | AL | 955 | 0 | 1016 | 44 | 0 |
| 12 | CL | 955 | 0 | 1016 | 74 | 0 |
| 13 | AM | 884 | 0 | 941 | 44 | 0 |
| 13 | CM | 884 | 0 | 941 | 51 | 0 |
| 14 | AN | 774 | 0 | 824 | 58 | 0 |
| 14 | CN | 774 | 0 | 824 | 51 | 0 |
| 15 | AO | 710 | 0 | 728 | 31 | 0 |
| 15 | CO | 710 | 0 | 728 | 29 | 0 |
| 16 | AP | 649 | 0 | 666 | 53 | 0 |
| 16 | CP | 649 | 0 | 666 | 36 | 0 |
| 17 | AQ | 649 | 0 | 691 | 63 | 0 |
| 17 | CQ | 649 | 0 | 691 | 53 | 0 |
| 18 | AR | 456 | 0 | 478 | 17 | 0 |
| 18 | CR | 456 | 0 | 478 | 25 | 0 |
| 19 | AS | 638 | 0 | 665 | 39 | 0 |
| 19 | CS | 638 | 0 | 665 | 42 | 0 |
| 20 | AT | 665 | 0 | 714 | 65 | 0 |
| 20 | CT | 665 | 0 | 714 | 46 | 0 |
| 21 | AU | 426 | 0 | 449 | 52 | 0 |
| 21 | CU | 426 | 0 | 449 | 53 | 0 |
| 22 | BA | 62195 | 0 | 31280 | 1486 | 0 |
| 22 | DA | 62195 | 0 | 31280 | 2451 | 1 |
| 23 | BB | 2549 | 0 | 1291 | 37 | 0 |
| 23 | DB | 2529 | 0 | 1281 | 66 | 0 |
| 24 | BC | 2083 | 0 | 2154 | 102 | 0 |
| 24 | DC | 2083 | 0 | 2154 | 128 | 0 |
| 25 | BD | 1565 | 0 | 1616 | 66 | 0 |
| 25 | DD | 1565 | 0 | 1616 | 97 | 0 |
| 26 | BE | 1552 | 0 | 1619 | 67 | 0 |
| 26 | DE | 1552 | 0 | 1619 | 91 | 0 |
| 27 | BF | 1411 | 0 | 1444 | 84 | 0 |
| 27 | DF | 1411 | 0 | 1444 | 54 | 0 |
| 28 | BG | 1323 | 0 | 1371 | 41 | 0 |
| 28 | DG | 1323 | 0 | 1371 | 42 | 0 |
| 29 | BH | 1110 | 0 | 1147 | 139 | 0 |
| 29 | DH | 1110 | 0 | 1148 | 87 | 0 |
| 30 | BI | 1032 | 0 | 1085 | 76 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30 | DI | 1032 | 0 | 1085 | 85 | 0 |
| 31 | BJ | 1129 | 0 | 1162 | 48 | 0 |
| 31 | DJ | 1129 | 0 | 1162 | 62 | 0 |
| 32 | BK | 939 | 0 | 1012 | 45 | 0 |
| 32 | DK | 939 | 0 | 1012 | 53 | 0 |
| 33 | BL | 1045 | 0 | 1117 | 54 | 0 |
| 33 | DL | 1045 | 0 | 1117 | 75 | 0 |
| 34 | BM | 1074 | 0 | 1157 | 43 | 0 |
| 34 | DM | 1074 | 0 | 1157 | 41 | 0 |
| 35 | BN | 961 | 0 | 1000 | 39 | 0 |
| 35 | DN | 961 | 0 | 1000 | 71 | 0 |
| 36 | BO | 892 | 0 | 923 | 38 | 0 |
| 36 | DO | 892 | 0 | 923 | 41 | 0 |
| 37 | BP | 917 | 0 | 962 | 45 | 0 |
| 37 | DP | 917 | 0 | 962 | 42 | 0 |
| 38 | BQ | 947 | 0 | 1019 | 39 | 0 |
| 38 | DQ | 947 | 0 | 1019 | 47 | 0 |
| 39 | BR | 816 | 0 | 839 | 66 | 0 |
| 39 | DR | 816 | 0 | 839 | 36 | 0 |
| 40 | BS | 857 | 0 | 922 | 33 | 0 |
| 40 | DS | 857 | 0 | 922 | 37 | 0 |
| 41 | BT | 739 | 0 | 807 | 41 | 0 |
| 41 | DT | 739 | 0 | 807 | 60 | 0 |
| 42 | BU | 780 | 0 | 831 | 37 | 0 |
| 42 | DU | 780 | 0 | 831 | 68 | 0 |
| 43 | BV | 753 | 0 | 780 | 28 | 0 |
| 43 | DV | 753 | 0 | 780 | 21 | 0 |
| 44 | BW | 580 | 0 | 594 | 20 | 0 |
| 44 | DW | 569 | 0 | 581 | 23 | 0 |
| 45 | BX | 625 | 0 | 652 | 15 | 0 |
| 45 | DX | 625 | 0 | 652 | 46 | 0 |
| 46 | BY | 509 | 0 | 543 | 34 | 0 |
| 46 | DY | 509 | 0 | 543 | 26 | 0 |
| 47 | BZ | 449 | 0 | 488 | 9 | 0 |
| 47 | DZ | 449 | 0 | 488 | 24 | 0 |
| 48 | B0 | 444 | 0 | 458 | 27 | 0 |
| 48 | D0 | 444 | 0 | 458 | 23 | 0 |
| 49 | B1 | 410 | 0 | 440 | 19 | 0 |
| 49 | D1 | 410 | 0 | 440 | 22 | 0 |
| 50 | B2 | 377 | 0 | 418 | 10 | 0 |
| 50 | D2 | 377 | 0 | 418 | 31 | 0 |
| 51 | B3 | 504 | 0 | 572 | 28 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 51 | D3 | 504 | 0 | 572 | 22 | 0 |
| 52 | B4 | 302 | 0 | 340 | 7 | 0 |
| 52 | D4 | 302 | 0 | 340 | 15 | 0 |
| 53 | B5 | 1142 | 0 | 865 | 69 | 0 |
| 54 | B6 | 73 | 0 | 64 | 3 | 0 |
| 54 | D6 | 73 | 0 | 65 | 12 | 0 |
| 55 | AA | 71 | 0 | 0 | 0 | 0 |
| 55 | AM | 1 | 0 | 0 | 0 | 0 |
| 55 | BA | 194 | 0 | 0 | 0 | 0 |
| 55 | BB | 4 | 0 | 0 | 0 | 0 |
| 55 | BQ | 1 | 0 | 0 | 0 | 0 |
| 55 | CA | 56 | 0 | 0 | 0 | 0 |
| 55 | D2 | 1 | 0 | 0 | 0 | 0 |
| 55 | DA | 166 | 0 | 0 | 0 | 0 |
| 55 | DB | 3 | 0 | 0 | 0 | 0 |
| 55 | DQ | 1 | 0 | 0 | 0 | 0 |
| 56 | BA | 48 | 0 | 50 | 15 | 0 |
| 56 | DA | 48 | 0 | 50 | 25 | 0 |
| 57 | B4 | 1 | 0 | 0 | 0 | 0 |
| 57 | D4 | 1 | 0 | 0 | 0 | 0 |
| 58 | AA | 194 | 0 | 0 | 18 | 0 |
| 58 | AE | 2 | 0 | 0 | 0 | 0 |
| 58 | AL | 1 | 0 | 0 | 0 | 0 |
| 58 | AN | 3 | 0 | 0 | 0 | 0 |
| 58 | AT | 2 | 0 | 0 | 0 | 0 |
| 58 | AU | 1 | 0 | 0 | 0 | 0 |
| 58 | B3 | 3 | 0 | 0 | 0 | 0 |
| 58 | B4 | 1 | 0 | 0 | 0 | 0 |
| 58 | BA | 617 | 0 | 0 | 66 | 0 |
| 58 | BB | 14 | 0 | 0 | 1 | 0 |
| 58 | BC | 6 | 0 | 0 | 1 | 0 |
| 58 | BD | 4 | 0 | 0 | 2 | 0 |
| 58 | BE | 1 | 0 | 0 | 0 | 0 |
| 58 | BF | 1 | 0 | 0 | 1 | 0 |
| 58 | BG | 1 | 0 | 0 | 1 | 0 |
| 58 | BJ | 1 | 0 | 0 | 0 | 0 |
| 58 | BL | 7 | 0 | 0 | 0 | 0 |
| 58 | BN | 5 | 0 | 0 | 0 | 0 |
| 58 | BQ | 1 | 0 | 0 | 0 | 0 |
| 58 | BS | 1 | 0 | 0 | 0 | 0 |
| 58 | BT | 2 | 0 | 0 | 0 | 0 |
| 58 | CA | 192 | 0 | 0 | 12 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58 | CL | 1 | 0 | 0 | 0 | 0 |
| 58 | CN | 2 | 0 | 0 | 0 | 0 |
| 58 | CT | 2 | 0 | 0 | 0 | 0 |
| 58 | CU | 1 | 0 | 0 | 1 | 0 |
| 58 | D2 | 1 | 0 | 0 | 1 | 0 |
| 58 | D3 | 1 | 0 | 0 | 0 | 0 |
| 58 | D4 | 1 | 0 | 0 | 0 | 0 |
| 58 | DA | 610 | 0 | 0 | 84 | 0 |
| 58 | DB | 13 | 0 | 0 | 1 | 0 |
| 58 | DC | 8 | 0 | 0 | 1 | 0 |
| 58 | DD | 4 | 0 | 0 | 2 | 0 |
| 58 | DE | 4 | 0 | 0 | 0 | 0 |
| 58 | DJ | 1 | 0 | 0 | 0 | 0 |
| 58 | DL | 4 | 0 | 0 | 1 | 0 |
| 58 | DN | 2 | 0 | 0 | 0 | 0 |
| 58 | DS | 2 | 0 | 0 | 0 | 0 |
| 58 | DT | 3 | 0 | 0 | 1 | 0 |
| 58 | DU | 1 | 0 | 0 | 0 | 0 |
| 58 | DV | 1 | 0 | 0 | 0 | 0 |
| All | All | 288423 | 0 | 193016 | 10587 | 1 |

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 22.

All (10587) 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) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:BH:117:LEU:O | 29:BH:121:VAL:HG23 | 1.34 | 1.22 |
| 22:BA:730:A:OP2 | 58:BA:3693:HOH:O | 1.58 | 1.21 |
| 1:AA:533:A:OP1 | 58:AA:1848:HOH:O | 1.65 | 1.15 |
| 29:BH:117:LEU:O | 29:BH:121:VAL:CG2 | 1.95 | 1.14 |
| 22:BA:2498:C:OP2 | 58:BA:3684:HOH:O | 1.64 | 1.13 |
| 22:BA:627:A:OP1 | 33:BL:78:ARG:NH1 | 1.83 | 1.11 |
| 22:BA:731:C:OP2 | 58:BA:3693:HOH:O | 1.66 | 1.11 |
| 25:DD:151:THR:O | 25:DD:153:GLY:N | 1.84 | 1.10 |
| 29:BH:123:ARG:O | 29:BH:124:THR:CG2 | 2.01 | 1.09 |
| 22:DA:1378:A:O2' | 22:DA:1380:G:N7 | 1.86 | 1.08 |
| 5:CE:101:GLU:O | 5:CE:103:THR:N | 1.89 | 1.05 |
| 22:BA:2720:U:OP1 | 37:BP:53:ARG:NH2 | 1.89 | 1.04 |
| 22:DA:2711:A:OP2 | 58:DA:3546:HOH:O | 1.73 | 1.03 |
| 56:DA:3001:DOL:H483 | 56:DA:3001:DOL:H463 | 1.41 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:BA:1395:A:OP1 | 58:BA:3411:HOH:O | 1.76 | 1.02 |
| 22:DA:1439:A:OP2 | 58:DA:3627:HOH:O | 1.76 | 1.02 |
| 22:DA:842:U:O4 | 58:DA:3577:HOH:O | 1.75 | 1.02 |
| 22:BA:842:U:O4 | 58:BA:3587:HOH:O | 1.75 | 1.02 |
| 22:DA:310:A:O2' | 22:DA:311:A:OP2 | 1.77 | 1.01 |
| 22:BA:1342:A:OP2 | 58:BA:3712:HOH:O | 1.76 | 1.01 |
| 22:DA:784:G:OP1 | 58:DA:3315:HOH:O | 1.79 | 1.01 |
| 22:DA:2349:G:OP1 | 51:D3:45:ARG:NH2 | 1.93 | 1.01 |
| 23:DB:28:C:OP1 | 36:DO:36:TYR:OH | 1.78 | 1.01 |
| 22:DA:789:A:N1 | 58:DA:3311:HOH:O | 1.91 | 1.00 |
| 13:AM:11:ASP:OD1 | 13:AM:12:HIS:N | 1.94 | 1.00 |
| 22:BA:1153:C:OP2 | 58:BA:3359:HOH:O | 1.78 | 1.00 |
| 25:BD:140:HIS:NE2 | 58:BD:303:HOH:O | 1.95 | 0.99 |
| 2:AB:193:PRO:O | 2:AB:195:GLY:N | 1.95 | 0.99 |
| 29:BH:117:LEU:HD21 | 29:BH:121:VAL:H | 1.23 | 0.99 |
| 22:BA:517:C:OP2 | 48:B0:10:ARG:NH2 | 1.94 | 0.99 |
| 29:BH:123:ARG:O | 29:BH:124:THR:HG23 | 1.61 | 0.99 |
| 28:DG:126:PRO:O | 28:DG:127:THR:OG1 | 1.81 | 0.99 |
| 22:BA:1001:A:OP2 | 58:BA:3735:HOH:O | 1.78 | 0.98 |
| 5:CE:157:ARG:O | 5:CE:159:LYS:N | 1.96 | 0.98 |
| 22:DA:2588:G:OP1 | 58:DA:3315:HOH:O | 1.81 | 0.98 |
| 4:CD:41:HIS:O | 4:CD:43:ALA:N | 1.97 | 0.98 |
| 1:CA:1500:A:OP2 | 58:CA:1883:HOH:O | 1.82 | 0.97 |
| 22:DA:2714:G:OP2 | 58:DA:3546:HOH:O | 1.82 | 0.97 |
| 22:BA:797:G:O6 | 58:BA:3322:HOH:O | 1.83 | 0.97 |
| 1:AA:516:U:O4 | 58:AA:1848:HOH:O | 1.82 | 0.97 |
| 29:DH:40:THR:O | 29:DH:42:LYS:N | 1.98 | 0.96 |
| 22:BA:1923:U:H2' | 22:BA:1924:C:H5' | 1.46 | 0.96 |
| 2:CB:73:LYS:O | 2:CB:75:ALA:N | 1.98 | 0.96 |
| 22:DA:2627:G:O2' | 22:DA:2781:A:N1 | 1.98 | 0.96 |
| 1:AA:980:C:OP2 | 58:AA:1835:HOH:O | 1.82 | 0.96 |
| 2:AB:21:ARG:O | 2:AB:23:TRP:N | 1.97 | 0.96 |
| 22:DA:602:A:O2' | 22:DA:604:G:O2' | 1.84 | 0.96 |
| 22:DA:182:A:O2' | 22:DA:433:C:O2' | 1.83 | 0.96 |
| 6:AF:91:ARG:O | 6:AF:92:THR:OG1 | 1.84 | 0.95 |
| 29:BH:120:GLY:C | 29:BH:122:LEU:HA | 1.85 | 0.95 |
| 22:DA:514:A:N3 | 22:DA:581:C:O2' | 1.98 | 0.95 |
| 5:AE:157:ARG:O | 5:AE:159:LYS:N | 2.00 | 0.94 |
| 22:DA:370:G:N7 | 58:DA:3555:HOH:O | 1.97 | 0.94 |
| 56:BA:3001:DOL:HC1 | 56:BA:3001:DOL:H463 | 1.49 | 0.94 |
| 9:CI:107:ASP:OD1 | 9:CI:109:ARG:NH1 | 1.99 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 22:BA:1916:A:C4 | 22:BA:1917:U:H1' | 2.02 | 0.93 |
| 22:DA:790:U:OP2 | 58:DA:3755:HOH:O | 1.84 | 0.93 |
| 22:BA:1062:G:N2 | 22:BA:1077:A:N1 | 2.16 | 0.93 |
| 22:BA:2428:G:OP1 | 58:BA:3699:HOH:O | 1.85 | 0.93 |
| 22:DA:621:A:OP2 | 58:DA:3293:HOH:O | 1.85 | 0.93 |
| 22:DA:2056:G:OP2 | 58:DA:3485:HOH:O | 1.86 | 0.92 |
| 4:CD:28:ILE:O | 4:CD:31:LYS:NZ | 2.04 | 0.91 |
| 22:BA:2269:G:OP1 | 58:BA:3512:HOH:O | 1.89 | 0.91 |
| 40:DS:28:LYS:O | 40:DS:30:SER:N | 2.02 | 0.91 |
| 22:DA:299:A:N3 | 22:DA:319:G:O2' | 2.02 | 0.91 |
| 35:DN:87:PHE:O | 35:DN:89:SER:N | 2.04 | 0.91 |
| 1:AA:1312:G:N7 | 19:AS:3:ARG:N | 2.17 | 0.91 |
| 22:BA:1602:U:O4 | 58:BA:3712:HOH:O | 1.87 | 0.91 |
| 39:DR:101:ILE:O | 39:DR:103:ALA:N | 2.03 | 0.91 |
| 23:DB:43:C:O2 | 27:DF:92:ARG:NH2 | 2.04 | 0.90 |
| 29:DH:83:LYS:HG3 | 29:DH:149:GLU:CG | 2.02 | 0.90 |
| 22:DA:450:G:O6 | 58:DA:3242:HOH:O | 1.90 | 0.90 |
| 22:DA:1817:G:OP1 | 24:DC:62:TYR:OH | 1.89 | 0.90 |
| 22:DA:1050:A:N6 | 22:DA:1109:C:O2 | 2.04 | 0.90 |
| 1:AA:880:C:OP1 | 12:AL:9:ARG:NH1 | 2.05 | 0.90 |
| 1:CA:858:G:N7 | 58:CA:1819:HOH:O | 2.04 | 0.90 |
| 2:CB:87:CYS:O | 2:CB:89:GLN:N | 2.05 | 0.90 |
| 22:DA:729:G:OP2 | 24:DC:207:LYS:NZ | 2.03 | 0.90 |
| 22:DA:488:G:N2 | 22:DA:493:G:O6 | 2.05 | 0.89 |
| 5:CE:102:GLY:O | 5:CE:104:GLY:N | 2.06 | 0.89 |
| 22:BA:1964:G:O2' | 22:BA:1967:C:OP2 | 1.89 | 0.89 |
| 22:DA:2615:U:OP1 | 58:DA:3745:HOH:O | 1.90 | 0.89 |
| 3:AC:85:GLU:OE1 | 3:AC:88:ARG:NH1 | 2.05 | 0.89 |
| 17:CQ:69:LYS:O | 17:CQ:70:THR:OG1 | 1.91 | 0.89 |
| 22:DA:58:G:OP1 | 41:DT:78:SER:OG | 1.88 | 0.89 |
| 22:BA:1924:C:H2' | 22:BA:1925:C:H5'' | 1.54 | 0.89 |
| 31:DJ:80:HIS:O | 31:DJ:82:GLY:N | 2.06 | 0.89 |
| 22:DA:1464:G:N7 | 58:DA:3633:HOH:O | 2.05 | 0.88 |
| 22:BA:1823:G:N7 | 58:BA:3657:HOH:O | 2.06 | 0.88 |
| 22:DA:1268:A:OP1 | 58:DA:3378:HOH:O | 1.89 | 0.88 |
| 13:AM:82:ASP:OD1 | 27:BF:112:ARG:NH2 | 2.06 | 0.88 |
| 22:BA:1073:A:H3' | 22:BA:1074:G:C5' | 2.04 | 0.88 |
| 50:D2:11:LYS:NZ | 58:D2:201:HOH:O | 2.06 | 0.88 |
| 22:BA:2271:G:O6 | 58:BA:3511:HOH:O | 1.91 | 0.88 |
| 29:BH:123:ARG:O | 29:BH:124:THR:HG22 | 1.74 | 0.88 |
| 14:CN:41:ARG:NH1 | 14:CN:42:TRP:O | 2.07 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:BH:117:LEU:C | 29:BH:121:VAL:HG23 | 1.93 | 0.87 |
| 22:BA:747:U:C5 | 22:BA:2613:U:C5 | 2.62 | 0.87 |
| 22:BA:1909:C:N4 | 22:BA:1921:G:O6 | 2.06 | 0.87 |
| 1:CA:1256:A:O2' | 1:CA:1278:G:O6 | 1.91 | 0.87 |
| 22:DA:528:A:OP1 | 58:DA:3246:HOH:O | 1.90 | 0.87 |
| 1:CA:1046:A:N6 | 1:CA:1211:U:O2 | 2.08 | 0.87 |
| 16:AP:42:ILE:O | 16:AP:44:SER:N | 2.08 | 0.87 |
| 29:DH:83:LYS:HG3 | 29:DH:149:GLU:HG2 | 1.56 | 0.87 |
| 22:DA:2834:G:O6 | 22:DA:2879:A:O2' | 1.93 | 0.86 |
| 4:AD:125:VAL:O | 4:AD:127:GLY:N | 2.07 | 0.86 |
| 22:BA:2448:A:OP2 | 58:BA:3684:HOH:O | 1.92 | 0.86 |
| 1:CA:912:C:OP1 | 12:CL:43:LYS:NZ | 2.07 | 0.86 |
| 4:CD:192:SER:OG | 4:CD:193:ALA:N | 2.04 | 0.86 |
| 20:CT:5:LYS:O | 20:CT:7:ALA:N | 2.09 | 0.86 |
| 7:AG:55:GLY:O | 7:AG:57:SER:N | 2.08 | 0.86 |
| 25:BD:103:ASP:O | 25:BD:105:LYS:N | 2.07 | 0.86 |
| 36:BO:31:THR:O | 36:BO:102:ARG:NH1 | 2.09 | 0.86 |
| 22:DA:18:U:O4 | 58:DA:3205:HOH:O | 1.94 | 0.86 |
| 22:BA:622:G:OP2 | 58:BA:3293:HOH:O | 1.94 | 0.86 |
| 1:AA:1108:G:O6 | 58:AA:1861:HOH:O | 1.92 | 0.86 |
| 29:BH:147:VAL:HG12 | 29:BH:149:GLU:HG3 | 1.57 | 0.86 |
| 22:DA:1010:A:OP2 | 58:DA:3778:HOH:O | 1.94 | 0.86 |
| 22:DA:1508:A:O2' | 22:DA:1509:A:O4' | 1.93 | 0.85 |
| 31:DJ:41:LYS:O | 31:DJ:43:GLU:N | 2.09 | 0.85 |
| 1:AA:537:G:OP1 | 12:AL:110:ARG:NH2 | 2.09 | 0.85 |
| 22:DA:858:G:O2' | 22:DA:2268:A:N3 | 2.08 | 0.85 |
| 22:DA:618:G:O6 | 58:DA:3292:HOH:O | 1.94 | 0.85 |
| 48:B0:20:ASP:OD2 | 48:B0:20:ASP:N | 2.09 | 0.85 |
| 22:DA:1371:G:N7 | 58:DA:3399:HOH:O | 2.08 | 0.85 |
| 4:AD:163:GLU:OE2 | 4:AD:164:GLN:N | 2.10 | 0.85 |
| 2:AB:118:GLU:O | 2:AB:121:SER:N | 2.09 | 0.85 |
| 14:AN:61:ARG:O | 14:AN:62:ASN:HB2 | 1.77 | 0.84 |
| 1:CA:1007:U:O4 | 1:CA:1022:A:N6 | 2.10 | 0.84 |
| 17:AQ:17:MET:SD | 17:AQ:17:MET:N | 2.50 | 0.84 |
| 1:CA:684:U:O2' | 11:CK:40:ASN:O | 1.94 | 0.84 |
| 56:DA:3001:DOL:C6 | 56:DA:3001:DOL:H432 | 2.07 | 0.84 |
| 1:CA:1198:G:N7 | 58:CA:1852:HOH:O | 2.09 | 0.84 |
| 39:DR:8:GLY:O | 39:DR:10:LYS:NZ | 2.09 | 0.84 |
| 29:BH:117:LEU:O | 29:BH:119:ASN:N | 2.08 | 0.84 |
| 5:CE:41:ASP:OD1 | 5:CE:42:GLY:N | 2.10 | 0.84 |
| 56:DA:3001:DOL:H432 | 56:DA:3001:DOL:O7 | 1.76 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BH:117:LEU:HD21 | 29:BH:121:VAL:N | 1.93 | 0.84 |
| 1:CA:319:G:O6 | 58:CA:1735:HOH:O | 1.95 | 0.84 |
| 29:DH:82:SER:O | 29:DH:84:ALA:N | 2.10 | 0.84 |
| 22:BA:2453:A:N7 | 58:BA:3524:HOH:O | 2.11 | 0.84 |
| 47:DZ:52:SER:O | 47:DZ:54:MET:N | 2.10 | 0.84 |
| 22:BA:1651:G:O6 | 58:BA:3800:HOH:O | 1.95 | 0.84 |
| 22:DA:2243:U:OP1 | 58:DA:3737:HOH:O | 1.95 | 0.84 |
| 22:BA:1093:G:N3 | 22:BA:1098:A:N6 | 2.25 | 0.84 |
| 1:CA:736:C:OP1 | 18:CR:61:ARG:NH1 | 2.10 | 0.84 |
| 22:DA:2684:U:O4' | 32:DK:70:ARG:NH1 | 2.11 | 0.84 |
| 50:D2:43:THR:OG1 | 50:D2:44:VAL:N | 2.09 | 0.83 |
| 1:AA:1222:G:O6 | 58:AA:1835:HOH:O | 1.96 | 0.83 |
| 22:DA:2004:G:OP1 | 58:DA:3800:HOH:O | 1.96 | 0.83 |
| 29:DH:94:ILE:HB | 29:DH:122:LEU:HD12 | 1.60 | 0.83 |
| 46:DY:11:VAL:O | 46:DY:15:ASN:ND2 | 2.10 | 0.83 |
| 14:AN:33:ASP:O | 14:AN:35:ASN:N | 2.11 | 0.83 |
| 21:AU:35:ARG:O | 21:AU:37:PHE:N | 2.11 | 0.83 |
| 1:CA:484:G:H4' | 1:CA:485:U:O5' | 1.79 | 0.83 |
| 21:CU:51:SER:O | 21:CU:53:VAL:N | 2.12 | 0.83 |
| 4:CD:29:ASP:O | 4:CD:31:LYS:N | 2.10 | 0.83 |
| 18:CR:20:GLU:O | 18:CR:22:ASP:N | 2.11 | 0.83 |
| 22:DA:1515:A:O2' | 22:DA:1556:C:O2' | 1.97 | 0.83 |
| 22:BA:2048:G:O6 | 58:BA:3678:HOH:O | 1.96 | 0.83 |
| 39:BR:49:ILE:HG22 | 39:BR:53:PHE:N | 1.94 | 0.83 |
| 22:DA:1266:G:O2' | 22:DA:2012:G:O6 | 1.96 | 0.83 |
| 4:AD:22:LYS:O | 4:AD:24:GLY:N | 2.12 | 0.82 |
| 22:BA:2445:G:OP1 | 26:BE:69:ARG:NH2 | 2.12 | 0.82 |
| 22:BA:2572:A:N7 | 25:BD:150:GLN:HG3 | 1.95 | 0.82 |
| 22:DA:1287:A:O4' | 35:DN:103:ARG:NH1 | 2.12 | 0.82 |
| 23:DB:40:U:N3 | 23:DB:44:G:OP2 | 2.13 | 0.82 |
| 29:BH:120:GLY:C | 29:BH:122:LEU:CA | 2.47 | 0.82 |
| 9:AI:57:MET:N | 9:AI:57:MET:SD | 2.52 | 0.82 |
| 1:CA:614:C:OP1 | 4:CD:83:LYS:NZ | 2.13 | 0.82 |
| 9:AI:42:GLU:O | 9:AI:45:ARG:NH1 | 2.12 | 0.82 |
| 1:CA:32:A:C2 | 1:CA:33:A:C5 | 2.67 | 0.82 |
| 1:CA:201:G:N2 | 1:CA:469:C:O2 | 2.13 | 0.82 |
| 22:DA:2134:A:OP2 | 22:DA:2157:G:N2 | 2.11 | 0.82 |
| 6:CF:12:PRO:O | 6:CF:15:SER:OG | 1.98 | 0.82 |
| 22:DA:1378:A:O2' | 58:DA:3751:HOH:O | 1.96 | 0.81 |
| 39:DR:82:HIS:ND1 | 39:DR:82:HIS:O | 2.13 | 0.81 |
| 22:BA:1064:C:N4 | 22:BA:1070:A:OP2 | 2.13 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CA:72:A:C6 | 1:CA:73:C:N4 | 2.48 | 0.81 |
| 8:AH:113:ASP:OD2 | 8:AH:117:ARG:NH2 | 2.13 | 0.81 |
| 26:BE:7:ASP:OD2 | 26:BE:8:ALA:N | 2.14 | 0.81 |
| 1:CA:209:U:H4' | 1:CA:210:C:OP2 | 1.81 | 0.81 |
| 26:DE:21:ARG:O | 26:DE:114:ARG:NH2 | 2.12 | 0.81 |
| 22:BA:2116:G:O6 | 22:BA:2171:A:N6 | 2.14 | 0.81 |
| 2:CB:193:PRO:O | 2:CB:195:GLY:N | 2.13 | 0.81 |
| 43:BV:80:HIS:CE1 | 43:BV:83:LYS:HG3 | 2.15 | 0.81 |
| 22:DA:258:G:O2' | 33:DL:104:GLN:OE1 | 1.97 | 0.81 |
| 22:DA:2307:G:OP1 | 22:DA:2308:G:N2 | 2.14 | 0.81 |
| 1:AA:825:A:O2' | 8:AH:13:ARG:NH1 | 2.14 | 0.81 |
| 5:CE:99:ALA:O | 5:CE:101:GLU:N | 2.14 | 0.80 |
| 22:DA:188:G:O2' | 22:DA:1365:A:N6 | 2.14 | 0.80 |
| 1:AA:207:C:O2 | 1:AA:213:G:N2 | 2.14 | 0.80 |
| 22:BA:2269:G:OP1 | 58:BA:3510:HOH:O | 1.97 | 0.80 |
| 31:BJ:114:LEU:HG | 31:BJ:118:MET:HE3 | 1.61 | 0.80 |
| 22:DA:225:C:N4 | 22:DA:419:U:O2' | 2.13 | 0.80 |
| 22:DA:2550:G:OP1 | 58:DA:3720:HOH:O | 1.99 | 0.80 |
| 7:AG:80:VAL:O | 7:AG:82:GLY:N | 2.14 | 0.80 |
| 7:CG:93:PRO:O | 7:CG:97:ASN:ND2 | 2.14 | 0.80 |
| 22:DA:613:A:O2' | 22:DA:614:A:OP1 | 1.98 | 0.80 |
| 22:BA:370:G:OP2 | 58:BA:3560:HOH:O | 2.00 | 0.80 |
| 1:AA:1232:U:OP1 | 9:AI:126:GLN:NE2 | 2.15 | 0.80 |
| 22:BA:2579:C:OP1 | 58:BA:3541:HOH:O | 1.99 | 0.80 |
| 21:AU:44:GLU:OE2 | 21:AU:45:ARG:NH1 | 2.15 | 0.80 |
| 13:CM:40:ALA:O | 13:CM:42:ASP:N | 2.14 | 0.80 |
| 46:BY:61:ALA:O | 46:BY:63:ALA:N | 2.14 | 0.80 |
| 1:CA:195:A:OP1 | 20:CT:60:ARG:NH1 | 2.15 | 0.80 |
| 22:DA:1606:C:O2' | 22:DA:1607:C:OP2 | 1.99 | 0.80 |
| 22:BA:2611:C:OP2 | 58:BA:3543:HOH:O | 2.00 | 0.79 |
| 22:DA:2575:C:OP2 | 58:DA:3707:HOH:O | 2.00 | 0.79 |
| 22:DA:83:A:OP2 | 42:DU:92:LYS:NZ | 2.15 | 0.79 |
| 22:DA:1269:A:OP2 | 58:DA:3385:HOH:O | 1.98 | 0.79 |
| 1:AA:650:G:H2' | 1:AA:651:C:H5' | 1.62 | 0.79 |
| 22:BA:194:G:N7 | 58:BA:3758:HOH:O | 2.14 | 0.79 |
| 22:BA:2305:U:C2 | 27:BF:151:GLY:HA3 | 2.17 | 0.79 |
| 7:AG:99:LEU:O | 7:AG:102:ARG:N | 2.16 | 0.79 |
| 22:DA:1427:A:N6 | 22:DA:1571:A:OP2 | 2.15 | 0.79 |
| 2:AB:73:LYS:O | 2:AB:75:ALA:N | 2.15 | 0.79 |
| 1:AA:319:G:N7 | 58:AA:1708:HOH:O | 2.15 | 0.79 |
| 22:DA:1667:G:O2' | 22:DA:1991:U:O4 | 1.99 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CA:890:G:O2' | 1:CA:906:A:N6 | 2.16 | 0.79 |
| 22:BA:1179:G:C5 | 22:BA:1180:U:H1' | 2.18 | 0.79 |
| 22:BA:1653:G:H3' | 35:BN:2:ARG:HG3 | 1.65 | 0.79 |
| 40:BS:53:SER:O | 40:BS:57:ASN:ND2 | 2.16 | 0.79 |
| 22:DA:279:A:N6 | 22:DA:361:G:O2' | 2.16 | 0.79 |
| 33:BL:87:GLY:O | 33:BL:89:VAL:N | 2.16 | 0.78 |
| 22:DA:732:C:OP2 | 58:DA:3298:HOH:O | 2.02 | 0.78 |
| 24:BC:70:ASN:O | 24:BC:72:ASP:N | 2.16 | 0.78 |
| 22:BA:1827:U:O4 | 58:BA:3787:HOH:O | 1.99 | 0.78 |
| 23:BB:8:C:O3' | 36:BO:25:ARG:NH1 | 2.16 | 0.78 |
| 20:CT:59:ASP:OD2 | 20:CT:76:LYS:NZ | 2.14 | 0.78 |
| 22:BA:1061:U:O2' | 22:BA:1062:G:O5' | 2.00 | 0.78 |
| 1:CA:1095:U:OP2 | 58:CA:1857:HOH:O | 2.01 | 0.78 |
| 35:DN:106:ASP:O | 35:DN:108:ALA:N | 2.16 | 0.78 |
| 22:DA:2576:G:O2' | 22:DA:2579:C:OP2 | 2.01 | 0.78 |
| 22:BA:1509:A:O2' | 22:BA:1510:G:OP2 | 2.00 | 0.78 |
| 22:DA:300:A:N6 | 58:DA:3551:HOH:O | 2.16 | 0.78 |
| 22:DA:1377:G:OP2 | 58:DA:3394:HOH:O | 2.00 | 0.78 |
| 22:BA:1746:A:H2' | 22:BA:1747:U:C6 | 2.20 | 0.77 |
| 22:DA:1469:A:H2' | 22:DA:1470:A:C8 | 2.19 | 0.77 |
| 16:AP:43:ALA:O | 16:AP:44:SER:OG | 2.01 | 0.77 |
| 20:AT:43:ASP:OD1 | 20:AT:46:ALA:N | 2.17 | 0.77 |
| 22:BA:1923:U:C2' | 22:BA:1924:C:H5' | 2.14 | 0.77 |
| 47:BZ:8:THR:OG1 | 47:BZ:35:THR:OG1 | 2.02 | 0.77 |
| 22:DA:1363:C:O2 | 22:DA:1369:G:C2 | 2.37 | 0.77 |
| 22:DA:2453:A:N7 | 58:DA:3525:HOH:O | 2.17 | 0.77 |
| 7:AG:111:ARG:NH1 | 7:AG:123:GLU:OE2 | 2.17 | 0.77 |
| 22:BA:2874:C:OP1 | 58:BA:3803:HOH:O | 2.02 | 0.77 |
| 22:DA:1091:G:O2' | 22:DA:1092:C:OP2 | 2.03 | 0.77 |
| 22:DA:1344:U:O2' | 22:DA:1345:C:OP2 | 2.03 | 0.77 |
| 1:CA:183:C:O2' | 1:CA:184:G:O5' | 2.01 | 0.77 |
| 15:CO:18:ASP:OD1 | 15:CO:20:ASN:N | 2.17 | 0.77 |
| 28:DG:158:LYS:O | 28:DG:160:LYS:N | 2.18 | 0.77 |
| 2:CB:103:ASN:ND2 | 2:CB:106:THR:OG1 | 2.18 | 0.77 |
| 22:DA:370:G:OP2 | 58:DA:3556:HOH:O | 2.03 | 0.77 |
| 1:CA:1061:G:O4' | 10:CJ:58:ASN:ND2 | 2.18 | 0.77 |
| 22:DA:2055:C:OP2 | 58:DA:3569:HOH:O | 2.01 | 0.77 |
| 22:DA:2286:G:H4' | 22:DA:2287:A:O5' | 1.83 | 0.77 |
| 29:DH:1:MET:SD | 29:DH:27:ARG:NH1 | 2.58 | 0.77 |
| 25:BD:77:ARG:NH2 | 25:BD:200:ASP:OD1 | 2.17 | 0.77 |
| 12:CL:66:TYR:O | 12:CL:97:THR:OG1 | 2.03 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:DP:65:SER:O | 37:DP:67:GLY:N | 2.18 | 0.77 |
| 1:AA:928:G:O2' | 1:AA:1533:C:OP1 | 2.03 | 0.76 |
| 1:CA:243:A:H4' | 1:CA:244:U:H5' | 1.67 | 0.76 |
| 1:CA:992:U:O4' | 1:CA:993:G:N2 | 2.19 | 0.76 |
| 22:BA:1998:A:OP2 | 25:BD:141:ARG:NH2 | 2.19 | 0.76 |
| 22:DA:1607:C:N4 | 22:DA:1622:G:N7 | 2.34 | 0.76 |
| 22:DA:1613:G:O6 | 58:DA:3638:HOH:O | 2.03 | 0.76 |
| 22:BA:560:C:OP2 | 58:BA:3250:HOH:O | 2.01 | 0.76 |
| 29:DH:45:GLU:O | 29:DH:49:ALA:N | 2.19 | 0.76 |
| 14:AN:91:GLY:O | 14:AN:93:ILE:N | 2.19 | 0.76 |
| 1:CA:243:A:H4' | 1:CA:244:U:C5' | 2.15 | 0.76 |
| 22:DA:622:G:OP2 | 58:DA:3293:HOH:O | 2.03 | 0.76 |
| 22:DA:1009:A:N3 | 22:DA:1153:C:O2' | 2.18 | 0.76 |
| 29:DH:53:GLU:O | 29:DH:55:GLU:N | 2.19 | 0.76 |
| 1:CA:205:A:N6 | 1:CA:213:G:O6 | 2.17 | 0.76 |
| 1:CA:949:A:O2' | 1:CA:971:G:O6 | 2.04 | 0.76 |
| 17:CQ:19:LYS:O | 17:CQ:71:LYS:NZ | 2.14 | 0.76 |
| 29:BH:97:ARG:NH1 | 1:CA:369:G:O2' | 2.18 | 0.76 |
| 22:DA:449:A:OP2 | 58:DA:3244:HOH:O | 2.04 | 0.76 |
| 1:CA:404:G:N7 | 4:CD:2:ALA:N | 2.33 | 0.76 |
| 22:DA:1359:A:OP1 | 58:DA:3610:HOH:O | 2.04 | 0.76 |
| 37:BP:54:GLY:O | 37:BP:57:SER:OG | 2.04 | 0.76 |
| 22:DA:761:A:OP2 | 58:DA:3295:HOH:O | 2.03 | 0.76 |
| 34:DM:66:ARG:NH1 | 34:DM:104:GLU:OE1 | 2.19 | 0.76 |
| 22:BA:1776:G:P | 58:BA:3449:HOH:O | 2.43 | 0.75 |
| 22:DA:910:A:N3 | 22:DA:2264:C:O2' | 2.18 | 0.75 |
| 27:DF:123:ASP:OD1 | 27:DF:124:GLY:N | 2.19 | 0.75 |
| 31:DJ:41:LYS:NZ | 31:DJ:52:ASP:OD2 | 2.16 | 0.75 |
| 22:DA:58:G:N3 | 22:DA:70:G:N2 | 2.34 | 0.75 |
| 29:DH:124:THR:OG1 | 29:DH:125:THR:N | 2.17 | 0.75 |
| 22:BA:370:G:N7 | 58:BA:3561:HOH:O | 2.19 | 0.75 |
| 22:BA:1253:A:N7 | 58:BA:3335:HOH:O | 2.18 | 0.75 |
| 22:BA:528:A:C2 | 22:BA:2043:C:H5' | 2.21 | 0.75 |
| 22:DA:1475:G:O2' | 22:DA:1476:U:OP1 | 2.05 | 0.75 |
| 22:BA:372:G:O2' | 22:BA:400:G:O6 | 2.01 | 0.75 |
| 22:BA:481:G:C4 | 22:BA:507:A:C2 | 2.75 | 0.75 |
| 1:CA:495:A:C2 | 1:CA:496:A:C6 | 2.75 | 0.75 |
| 22:DA:2563:U:O4' | 22:DA:2566:A:N6 | 2.18 | 0.75 |
| 1:AA:1403:C:O2 | 1:AA:1499:A:N6 | 2.19 | 0.75 |
| 11:AK:102:ALA:O | 11:AK:104:GLY:N | 2.20 | 0.75 |
| 1:AA:702:A:N6 | 22:BA:1846:G:O2' | 2.20 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:81:LEU:HB3 | 5:AE:147:MET:HE3 | 1.69 | 0.75 |
| 22:DA:1223:G:N2 | 22:DA:1226:A:OP2 | 2.19 | 0.75 |
| 22:BA:1378:A:O2' | 22:BA:1380:G:OP2 | 2.05 | 0.75 |
| 22:BA:1385:A:H1' | 22:BA:1386:C:C6 | 2.22 | 0.74 |
| 38:BQ:49:ASP:HA | 38:BQ:52:GLN:HB2 | 1.68 | 0.74 |
| 13:CM:13:LYS:O | 13:CM:14:HIS:ND1 | 2.20 | 0.74 |
| 22:DA:27:G:O2' | 22:DA:28:A:OP2 | 2.04 | 0.74 |
| 22:DA:374:A:N6 | 22:DA:400:G:O2' | 2.19 | 0.74 |
| 22:DA:878:A:N6 | 22:DA:899:A:O2' | 2.20 | 0.74 |
| 4:AD:95:GLU:OE2 | 4:AD:104:ARG:NH1 | 2.20 | 0.74 |
| 29:BH:88:GLY:O | 29:BH:125:THR:OG1 | 2.04 | 0.74 |
| 1:AA:208:U:C5 | 1:AA:210:C:C4 | 2.76 | 0.74 |
| 1:AA:251:G:C6 | 1:AA:266:G:C6 | 2.75 | 0.74 |
| 16:AP:50:THR:O | 16:AP:50:THR:HG22 | 1.87 | 0.74 |
| 29:BH:123:ARG:C | 29:BH:124:THR:HG23 | 2.06 | 0.74 |
| 19:CS:4:SER:O | 19:CS:5:LEU:HB2 | 1.87 | 0.74 |
| 22:DA:733:G:OP2 | 58:DA:3296:HOH:O | 2.05 | 0.74 |
| 26:DE:111:GLU:OE2 | 26:DE:114:ARG:NH1 | 2.21 | 0.74 |
| 11:AK:38:GLN:O | 11:AK:40:ASN:ND2 | 2.21 | 0.74 |
| 29:BH:117:LEU:HD11 | 29:BH:122:LEU:HD12 | 1.69 | 0.74 |
| 22:DA:2502:G:OP2 | 58:DA:3491:HOH:O | 2.03 | 0.74 |
| 1:AA:1422:G:O3' | 32:BK:49:ARG:NH2 | 2.18 | 0.74 |
| 22:BA:1604:C:OP2 | 58:BA:3411:HOH:O | 2.04 | 0.74 |
| 22:DA:581:C:OP2 | 38:DQ:33:ARG:NH1 | 2.21 | 0.74 |
| 42:DU:9:ASP:OD2 | 42:DU:10:GLU:N | 2.20 | 0.74 |
| 22:BA:622:G:OP2 | 58:BA:3292:HOH:O | 2.06 | 0.74 |
| 22:BA:1124:G:N7 | 58:BA:3607:HOH:O | 2.19 | 0.74 |
| 1:CA:1067:A:N1 | 1:CA:1108:G:O2' | 2.19 | 0.74 |
| 4:AD:3:ARG:CZ | 4:AD:115:ARG:HD3 | 2.18 | 0.74 |
| 9:CI:12:ARG:NH1 | 9:CI:107:ASP:OD2 | 2.21 | 0.74 |
| 12:CL:57:LEU:O | 12:CL:60:GLY:N | 2.20 | 0.74 |
| 27:DF:122:PHE:O | 27:DF:124:GLY:N | 2.21 | 0.74 |
| 1:AA:411:A:OP1 | 4:AD:26:ARG:NH2 | 2.20 | 0.74 |
| 5:AE:104:GLY:O | 5:AE:105:ILE:HG22 | 1.87 | 0.74 |
| 4:AD:59:GLN:O | 4:AD:63:ARG:HG2 | 1.87 | 0.74 |
| 9:AI:57:MET:SD | 9:AI:58:VAL:N | 2.61 | 0.74 |
| 23:DB:29:A:O2' | 23:DB:58:A:N1 | 2.21 | 0.74 |
| 22:BA:653:U:OP2 | 22:BA:653:U:C6 | 2.41 | 0.74 |
| 22:BA:1179:G:C4 | 22:BA:1180:U:H1' | 2.22 | 0.74 |
| 22:BA:1922:G:N2 | 22:BA:1923:U:H1' | 2.03 | 0.74 |
| 1:CA:374:A:H5'' | 1:CA:452:A:N1 | 2.03 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:CM:10:PRO:O | 13:CM:11:ASP:HB2 | 1.87 | 0.74 |
| 1:CA:1108:G:O6 | 58:CA:1857:HOH:O | 2.04 | 0.73 |
| 22:DA:1973:G:OP1 | 58:DA:3462:HOH:O | 2.05 | 0.73 |
| 1:AA:1181:G:O2' | 1:AA:1182:G:C5 | 2.41 | 0.73 |
| 22:BA:1917:U:C4 | 22:BA:1918:A:C6 | 2.75 | 0.73 |
| 20:CT:44:LYS:NZ | 20:CT:86:LEU:O | 2.18 | 0.73 |
| 22:BA:2728:U:O2' | 22:BA:2729:G:OP2 | 2.06 | 0.73 |
| 1:CA:266:G:H3' | 17:CQ:69:LYS:HB2 | 1.70 | 0.73 |
| 22:DA:1995:U:OP1 | 58:DA:3807:HOH:O | 2.04 | 0.73 |
| 17:AQ:16:LYS:C | 17:AQ:17:MET:SD | 2.67 | 0.73 |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:N | 2.03 | 0.73 |
| 22:DA:2127:G:O2' | 22:DA:2173:A:N3 | 2.21 | 0.73 |
| 1:AA:1370:G:O5' | 9:AI:111:VAL:HG21 | 1.88 | 0.73 |
| 21:AU:36:GLU:O | 21:AU:37:PHE:HB2 | 1.87 | 0.73 |
| 28:BG:104:ASN:ND2 | 28:BG:114:ASP:OD1 | 2.21 | 0.73 |
| 32:DK:34:GLY:O | 32:DK:36:GLY:N | 2.22 | 0.73 |
| 22:BA:2291:U:H2' | 22:BA:2292:U:C6 | 2.23 | 0.73 |
| 22:BA:2346:A:H4' | 22:BA:2347:C:OP2 | 1.88 | 0.73 |
| 16:AP:79:ASN:O | 16:AP:80:LYS:HB2 | 1.88 | 0.73 |
| 1:CA:403:C:OP1 | 4:CD:134:SER:OG | 2.03 | 0.73 |
| 4:CD:100:ASN:OD1 | 4:CD:111:ARG:NH1 | 2.21 | 0.73 |
| 5:CE:80:THR:OG1 | 5:CE:122:ASN:ND2 | 2.21 | 0.73 |
| 21:CU:18:ARG:O | 21:CU:21:ARG:N | 2.21 | 0.73 |
| 22:DA:777:G:C2 | 22:DA:778:G:C8 | 2.77 | 0.73 |
| 46:BY:34:SER:O | 46:BY:36:GLN:N | 2.22 | 0.73 |
| 1:CA:485:U:O2' | 1:CA:486:U:OP1 | 2.05 | 0.73 |
| 4:CD:26:ARG:HG3 | 4:CD:27:ALA:N | 2.03 | 0.73 |
| 22:DA:242:G:O2' | 22:DA:254:G:O6 | 2.05 | 0.73 |
| 1:AA:1198:G:N7 | 58:AA:1787:HOH:O | 2.21 | 0.73 |
| 10:CJ:63:ASP:OD1 | 14:CN:85:ARG:NH1 | 2.22 | 0.73 |
| 50:D2:44:VAL:O | 50:D2:45:SER:OG | 2.07 | 0.73 |
| 2:AB:87:CYS:O | 2:AB:89:GLN:N | 2.22 | 0.73 |
| 49:D1:15:ALA:O | 49:D1:17:THR:N | 2.22 | 0.73 |
| 2:AB:82:ASP:O | 2:AB:85:LEU:N | 2.22 | 0.72 |
| 3:AC:36:ASP:OD1 | 3:AC:59:ARG:NH1 | 2.22 | 0.72 |
| 11:AK:76:GLU:C | 22:BA:2141:G:OP1 | 2.27 | 0.72 |
| 1:CA:1124:G:O2' | 1:CA:1145:A:N6 | 2.21 | 0.72 |
| 22:DA:2091:C:H3' | 22:DA:2092:U:H5'' | 1.69 | 0.72 |
| 22:DA:2355:G:OP1 | 44:DW:25:ARG:NH2 | 2.22 | 0.72 |
| 1:CA:376:G:H5' | 16:CP:5:ARG:HB3 | 1.69 | 0.72 |
| 1:CA:1181:G:O2' | 1:CA:1182:G:N7 | 2.21 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 24:DC:258:ARG:NH1 | 24:DC:264:ASP:OD2 | 2.22 | 0.72 |
| 1:AA:131:A:H2' | 1:AA:132:C:C6 | 2.23 | 0.72 |
| 1:AA:1225:A:H2' | 1:AA:1226:C:C5 | 2.25 | 0.72 |
| 14:AN:46:LEU:O | 14:AN:48:LEU:N | 2.22 | 0.72 |
| 20:AT:59:ASP:OD1 | 20:AT:76:LYS:NZ | 2.19 | 0.72 |
| 21:AU:34:ARG:CZ | 21:AU:35:ARG:HB2 | 2.19 | 0.72 |
| 22:DA:1141:U:OP2 | 31:DJ:65:THR:OG1 | 2.05 | 0.72 |
| 22:BA:509:C:O3' | 58:BA:3771:HOH:O | 2.07 | 0.72 |
| 1:CA:1308:U:OP1 | 13:CM:97:VAL:N | 2.22 | 0.72 |
| 22:DA:79:C:O2' | 22:DA:346:A:N3 | 2.21 | 0.72 |
| 1:AA:800:G:O6 | 58:AA:1812:HOH:O | 2.07 | 0.72 |
| 22:BA:587:C:OP2 | 33:BL:21:ARG:NH1 | 2.23 | 0.72 |
| 1:CA:688:G:O2' | 1:CA:704:A:N1 | 2.19 | 0.72 |
| 22:DA:70:G:N2 | 22:DA:71:A:N1 | 2.37 | 0.72 |
| 22:BA:404:A:O2' | 22:BA:405:U:OP2 | 2.07 | 0.72 |
| 22:BA:826:U:OP1 | 58:BA:3699:HOH:O | 2.08 | 0.72 |
| 22:BA:944:C:OP2 | 58:BA:3260:HOH:O | 2.06 | 0.72 |
| 1:CA:8:A:N6 | 4:CD:54:GLN:OE1 | 2.21 | 0.72 |
| 22:DA:2504:U:C5 | 56:DA:3001:DOL:H161 | 2.25 | 0.72 |
| 22:DA:2707:U:O2 | 35:DN:71:ARG:NH1 | 2.22 | 0.72 |
| 22:DA:2838:G:O2' | 35:DN:45:ARG:NH1 | 2.22 | 0.72 |
| 40:DS:66:ILE:O | 40:DS:68:ASP:N | 2.23 | 0.72 |
| 22:BA:2757:A:N1 | 28:BG:67:THR:HG21 | 2.03 | 0.72 |
| 22:DA:1440:U:O4 | 58:DA:3627:HOH:O | 2.06 | 0.72 |
| 2:AB:63:ARG:O | 2:AB:64:LYS:HB2 | 1.88 | 0.72 |
| 13:AM:73:ILE:O | 13:AM:76:SER:OG | 2.07 | 0.72 |
| 22:BA:757:G:N7 | 58:BA:3303:HOH:O | 2.23 | 0.72 |
| 22:BA:1057:A:N6 | 22:BA:1087:G:OP2 | 2.23 | 0.72 |
| 11:CK:17:SER:O | 11:CK:80:LYS:N | 2.23 | 0.72 |
| 1:AA:844:G:C6 | 1:AA:846:G:O2' | 2.43 | 0.71 |
| 2:AB:23:TRP:CH2 | 2:AB:25:PRO:HA | 2.25 | 0.71 |
| 27:BF:21:ASN:O | 27:BF:21:ASN:ND2 | 2.22 | 0.71 |
| 22:DA:2199:A:OP1 | 45:DX:37:ARG:NH1 | 2.23 | 0.71 |
| 1:AA:173:U:C2 | 1:AA:197:A:N1 | 2.58 | 0.71 |
| 1:AA:976:G:OP2 | 1:AA:1358:U:O2' | 2.09 | 0.71 |
| 7:AG:64:VAL:O | 7:AG:67:GLU:N | 2.23 | 0.71 |
| 20:AT:83:ILE:O | 20:AT:87:ALA:HB3 | 1.90 | 0.71 |
| 22:DA:2343:U:O2' | 22:DA:2373:G:O2' | 2.07 | 0.71 |
| 27:BF:40:VAL:O | 27:BF:42:GLU:N | 2.23 | 0.71 |
| 29:DH:31:VAL:HB | 29:DH:32:PRO:CD | 2.20 | 0.71 |
| 23:BB:30:C:OP1 | 36:BO:3:LYS:NZ | 2.23 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 23:BB:91:C:OP2 | 34:BM:18:ARG:HG2 | 1.91 | 0.71 |
| 51:B3:31:HIS:CD2 | 51:B3:32:ILE:HG13 | 2.26 | 0.71 |
| 22:DA:593:U:H2' | 22:DA:594:U:C6 | 2.26 | 0.71 |
| 22:DA:668:A:C2 | 22:DA:670:A:C5 | 2.79 | 0.71 |
| 22:DA:776:G:O2' | 22:DA:2241:A:OP1 | 2.09 | 0.71 |
| 25:DD:149:ASN:OD1 | 25:DD:150:GLN:N | 2.24 | 0.71 |
| 22:BA:2125:G:N3 | 22:BA:2173:A:N6 | 2.39 | 0.71 |
| 53:B5:50:ILE:C | 53:B5:52:PRO:HD3 | 2.11 | 0.71 |
| 22:DA:52:A:N3 | 22:DA:178:G:N2 | 2.39 | 0.71 |
| 22:BA:2189:U:H2' | 22:BA:2190:G:C1' | 2.19 | 0.71 |
| 56:BA:3001:DOL:H421 | 56:BA:3001:DOL:N5 | 2.06 | 0.71 |
| 9:CI:57:MET:SD | 9:CI:58:VAL:N | 2.64 | 0.71 |
| 22:DA:46:G:C2 | 22:DA:47:C:C5 | 2.78 | 0.71 |
| 22:DA:1153:C:OP1 | 58:DA:3359:HOH:O | 2.08 | 0.71 |
| 22:DA:1154:G:OP2 | 38:DQ:58:ARG:NH1 | 2.24 | 0.71 |
| 22:DA:2407:A:OP1 | 58:DA:3560:HOH:O | 2.08 | 0.71 |
| 1:AA:993:G:O2' | 1:AA:994:A:N7 | 2.23 | 0.71 |
| 39:BR:49:ILE:HG22 | 39:BR:53:PHE:CA | 2.20 | 0.71 |
| 22:DA:1335:C:N4 | 58:DA:3392:HOH:O | 2.22 | 0.71 |
| 22:DA:2115:G:O2' | 22:DA:2117:A:N6 | 2.23 | 0.71 |
| 22:BA:181:A:H2' | 22:BA:182:A:C8 | 2.26 | 0.71 |
| 22:BA:1061:U:HO2' | 22:BA:1062:G:P | 2.13 | 0.71 |
| 24:BC:143:ASN:OD1 | 24:BC:152:GLY:HA3 | 1.90 | 0.71 |
| 22:DA:2788:C:O2' | 22:DA:2809:A:N3 | 2.22 | 0.71 |
| 22:DA:827:U:OP2 | 58:DA:3696:HOH:O | 2.08 | 0.71 |
| 10:CJ:87:LEU:HD13 | 10:CJ:88:MET:N | 2.06 | 0.70 |
| 22:BA:566:U:OP1 | 33:BL:29:LYS:HD2 | 1.91 | 0.70 |
| 24:DC:45:ASN:OD1 | 24:DC:46:ASN:N | 2.24 | 0.70 |
| 1:AA:683:G:N2 | 11:AK:39:GLY:O | 2.24 | 0.70 |
| 1:CA:537:G:OP1 | 12:CL:110:ARG:NH2 | 2.24 | 0.70 |
| 22:DA:277:G:H3' | 22:DA:277:G:N3 | 2.06 | 0.70 |
| 1:AA:652:U:O4 | 1:AA:752:G:O2' | 2.05 | 0.70 |
| 56:BA:3001:DOL:H421 | 56:BA:3001:DOL:C6 | 2.22 | 0.70 |
| 42:BU:49:VAL:CG2 | 42:BU:49:VAL:O | 2.39 | 0.70 |
| 22:DA:686:U:OP2 | 58:DA:3717:HOH:O | 2.09 | 0.70 |
| 24:DC:70:ASN:O | 24:DC:72:ASP:N | 2.23 | 0.70 |
| 1:AA:254:G:OP1 | 17:AQ:70:THR:HB | 1.91 | 0.70 |
| 4:AD:78:GLU:OE1 | 4:AD:81:ARG:NH1 | 2.24 | 0.70 |
| 17:AQ:69:LYS:O | 17:AQ:70:THR:CB | 2.39 | 0.70 |
| 20:AT:6:SER:OG | 20:AT:7:ALA:N | 2.23 | 0.70 |
| 22:BA:1179:G:N7 | 22:BA:1180:U:C6 | 2.59 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:BA:2192:U:H2' | 22:BA:2193:G:H5' | 1.72 | 0.70 |
| 2:CB:83:ALA:O | 2:CB:86:SER:OG | 2.09 | 0.70 |
| 2:CB:203:ASN:OD1 | 2:CB:204:ASP:N | 2.23 | 0.70 |
| 22:DA:2609:U:H2' | 54:D6:7:004:HA | 1.71 | 0.70 |
| 29:BH:94:ILE:HG22 | 29:BH:99:ILE:HG13 | 1.72 | 0.70 |
| 1:CA:679:C:O2 | 1:CA:712:A:C2 | 2.45 | 0.70 |
| 22:DA:388:G:N7 | 22:DA:390:U:H2' | 2.05 | 0.70 |
| 22:DA:1603:A:OP1 | 58:DA:3409:HOH:O | 2.10 | 0.70 |
| 56:DA:3001:DOL:C43 | 56:DA:3001:DOL:HC1 | 2.22 | 0.70 |
| 22:BA:1450:G:C6 | 22:BA:1451:C:N4 | 2.60 | 0.70 |
| 28:BG:80:THR:HG22 | 28:BG:81:GLU:N | 2.07 | 0.70 |
| 1:CA:802:A:C2 | 1:CA:803:G:H1' | 2.26 | 0.70 |
| 12:CL:25:GLU:O | 12:CL:26:ALA:C | 2.27 | 0.70 |
| 22:DA:2199:A:C5 | 22:DA:2225:A:C6 | 2.80 | 0.70 |
| 22:DA:2289:G:HO2' | 22:DA:2383:G:HO2' | 1.35 | 0.70 |
| 54:D6:6:MHV:HE1 | 54:D6:7:004:HNA | 1.55 | 0.70 |
| 16:AP:46:LYS:HD3 | 16:AP:47:GLU:N | 2.07 | 0.70 |
| 12:CL:21:VAL:O | 12:CL:23:ALA:N | 2.25 | 0.70 |
| 22:DA:1340:U:C5 | 22:DA:1603:A:C8 | 2.80 | 0.70 |
| 2:AB:21:ARG:HA | 2:AB:21:ARG:CZ | 2.22 | 0.70 |
| 1:CA:1204:A:OP2 | 58:CA:1848:HOH:O | 2.09 | 0.70 |
| 22:DA:116:C:O2' | 22:DA:126:A:O2' | 2.06 | 0.70 |
| 22:DA:377:G:C6 | 22:DA:378:C:C4 | 2.80 | 0.70 |
| 2:AB:50:PHE:HA | 2:AB:213:TYR:OH | 1.92 | 0.69 |
| 22:BA:2057:G:OP2 | 58:BA:3489:HOH:O | 2.10 | 0.69 |
| 12:CL:25:GLU:O | 12:CL:27:CYS:N | 2.24 | 0.69 |
| 22:DA:564:C:O4' | 38:DQ:37:GLN:NE2 | 2.24 | 0.69 |
| 22:DA:616:A:H4' | 26:DE:101:TYR:CZ | 2.26 | 0.69 |
| 22:DA:1109:C:H5'' | 22:DA:1110:G:OP2 | 1.92 | 0.69 |
| 35:DN:107:ASN:ND2 | 35:DN:107:ASN:O | 2.24 | 0.69 |
| 22:BA:301:G:OP2 | 42:BU:82:ARG:NH1 | 2.26 | 0.69 |
| 22:BA:2061:G:O6 | 56:BA:3001:DOL:H162 | 1.93 | 0.69 |
| 35:BN:65:LEU:HD11 | 35:BN:69:ARG:NH2 | 2.06 | 0.69 |
| 39:BR:49:ILE:HB | 39:BR:52:PRO:C | 2.13 | 0.69 |
| 22:DA:1475:G:O2' | 22:DA:1476:U:P | 2.49 | 0.69 |
| 41:DT:21:SER:O | 41:DT:23:ALA:N | 2.24 | 0.69 |
| 1:CA:875:U:O2' | 8:CH:15:ARG:NH1 | 2.24 | 0.69 |
| 1:AA:109:A:H2' | 1:AA:326:G:N2 | 2.06 | 0.69 |
| 22:BA:2380:C:OP1 | 36:BO:17:LYS:NZ | 2.25 | 0.69 |
| 28:DG:118:PRO:CG | 28:DG:144:VAL:HG21 | 2.22 | 0.69 |
| 1:CA:533:A:O2' | 1:CA:535:A:OP2 | 2.10 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CA:858:G:O6 | 1:CA:869:G:H3' | 1.92 | 0.69 |
| 22:DA:453:A:OP1 | 58:DA:3242:HOH:O | 2.09 | 0.69 |
| 6:AF:91:ARG:C | 6:AF:92:THR:HG1 | 1.91 | 0.69 |
| 22:BA:528:A:C2 | 22:BA:2043:C:H4' | 2.27 | 0.69 |
| 22:BA:2886:A:C5 | 22:BA:2887:A:C8 | 2.81 | 0.69 |
| 1:CA:1211:U:O2' | 1:CA:1212:U:OP2 | 2.11 | 0.69 |
| 2:CB:21:ARG:HA | 2:CB:21:ARG:CZ | 2.22 | 0.69 |
| 22:DA:749:A:C5 | 22:DA:750:A:N7 | 2.61 | 0.69 |
| 22:DA:1973:G:C6 | 22:DA:1974:C:C4 | 2.80 | 0.69 |
| 2:CB:206:ALA:O | 2:CB:208:ARG:N | 2.25 | 0.69 |
| 5:CE:155:ALA:HB1 | 8:CH:66:PHE:CD2 | 2.27 | 0.69 |
| 11:CK:27:PHE:CZ | 11:CK:89:PRO:HG2 | 2.27 | 0.69 |
| 22:DA:247:G:H4' | 22:DA:386:G:C5 | 2.27 | 0.69 |
| 5:AE:82:GLN:NE2 | 5:AE:150:PRO:HD3 | 2.08 | 0.69 |
| 5:CE:101:GLU:O | 5:CE:101:GLU:CD | 2.31 | 0.69 |
| 23:DB:48:U:H4' | 36:DO:100:HIS:CD2 | 2.28 | 0.69 |
| 4:AD:27:ALA:O | 4:AD:31:LYS:NZ | 2.26 | 0.69 |
| 22:BA:1073:A:H3' | 22:BA:1074:G:H5' | 1.74 | 0.69 |
| 22:BA:1584:U:O2 | 22:BA:1584:U:H2' | 1.92 | 0.69 |
| 22:BA:1922:G:N3 | 22:BA:1922:G:H2' | 2.06 | 0.69 |
| 1:CA:562:U:OP2 | 12:CL:14:ARG:NE | 2.26 | 0.69 |
| 18:CR:20:GLU:N | 18:CR:55:LEU:HD12 | 2.08 | 0.69 |
| 1:AA:965:U:OP2 | 58:AA:1831:HOH:O | 2.10 | 0.69 |
| 22:BA:2308:G:O6 | 22:BA:2311:A:N7 | 2.26 | 0.69 |
| 9:CI:19:VAL:HG21 | 9:CI:82:GLY:HA3 | 1.75 | 0.69 |
| 22:DA:866:A:O4' | 22:DA:914:G:N2 | 2.26 | 0.69 |
| 22:DA:1313:U:H4' | 22:DA:1332:G:H4' | 1.74 | 0.69 |
| 1:AA:81:A:H2' | 1:AA:82:G:H5'' | 1.75 | 0.68 |
| 1:AA:792:A:H4' | 1:AA:793:U:O5' | 1.92 | 0.68 |
| 23:BB:91:C:OP2 | 34:BM:18:ARG:NH2 | 2.26 | 0.68 |
| 1:CA:674:G:OP1 | 6:CF:86:ARG:NH2 | 2.26 | 0.68 |
| 22:DA:1259:G:H2' | 22:DA:1260:A:C8 | 2.27 | 0.68 |
| 22:DA:1525:A:C2 | 22:DA:1526:C:C2 | 2.80 | 0.68 |
| 22:DA:1677:A:N7 | 58:DA:3765:HOH:O | 2.26 | 0.68 |
| 22:DA:2006:C:OP2 | 58:DA:3382:HOH:O | 2.10 | 0.68 |
| 1:AA:144:G:C4 | 1:AA:179:A:C2 | 2.81 | 0.68 |
| 1:AA:1018:G:C2 | 1:AA:1019:A:C8 | 2.81 | 0.68 |
| 22:BA:1901:A:OP2 | 24:BC:253:LYS:NZ | 2.22 | 0.68 |
| 35:DN:1:MET:HE2 | 35:DN:1:MET:H1 | 1.58 | 0.68 |
| 22:BA:1379:U:C6 | 22:BA:1379:U:OP1 | 2.47 | 0.68 |
| 22:BA:1917:U:C4 | 22:BA:1918:A:C5 | 2.81 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BH:117:LEU:O | 29:BH:121:VAL:HG22 | 1.93 | 0.68 |
| 22:DA:698:C:O2' | 22:DA:734:A:N6 | 2.26 | 0.68 |
| 22:DA:1237:A:H4' | 22:DA:1238:G:OP1 | 1.92 | 0.68 |
| 22:DA:2585:U:O2' | 54:D6:3:DBB:HG2 | 1.93 | 0.68 |
| 1:AA:111:G:O6 | 1:AA:330:C:N4 | 2.27 | 0.68 |
| 1:AA:645:G:N7 | 58:AA:1748:HOH:O | 2.27 | 0.68 |
| 1:AA:1236:A:H2' | 1:AA:1237:C:C6 | 2.29 | 0.68 |
| 22:BA:1182:G:H2' | 22:BA:1183:U:O4' | 1.94 | 0.68 |
| 25:BD:133:THR:HG23 | 25:BD:134:HIS:N | 2.08 | 0.68 |
| 6:CF:91:ARG:O | 6:CF:92:THR:OG1 | 2.10 | 0.68 |
| 22:DA:185:G:C6 | 22:DA:212:G:C2 | 2.81 | 0.68 |
| 22:DA:810:U:OP1 | 58:DA:3333:HOH:O | 2.10 | 0.68 |
| 22:DA:2594:C:N4 | 22:DA:2595:G:O6 | 2.26 | 0.68 |
| 11:AK:29:ASN:OD1 | 11:AK:30:THR:N | 2.26 | 0.68 |
| 22:BA:2499:C:OP2 | 58:BA:3685:HOH:O | 2.12 | 0.68 |
| 46:BY:9:LYS:O | 46:BY:12:GLU:N | 2.26 | 0.68 |
| 14:CN:21:PHE:O | 14:CN:23:LYS:N | 2.26 | 0.68 |
| 22:DA:118:A:C8 | 22:DA:119:A:C8 | 2.82 | 0.68 |
| 22:DA:2226:C:H2' | 22:DA:2227:A:O4' | 1.93 | 0.68 |
| 34:DM:19:GLY:O | 34:DM:38:ARG:NH1 | 2.27 | 0.68 |
| 40:DS:67:ASP:OD1 | 40:DS:67:ASP:N | 2.25 | 0.68 |
| 1:AA:130:A:N1 | 1:AA:233:C:O2' | 2.23 | 0.68 |
| 24:BC:15:HIS:O | 24:BC:204:VAL:HG21 | 1.93 | 0.68 |
| 1:AA:203:G:O2' | 1:AA:465:A:N1 | 2.25 | 0.68 |
| 22:DA:1094:U:H2' | 22:DA:1096:A:OP2 | 1.94 | 0.68 |
| 22:DA:2200:C:O2 | 22:DA:2226:C:N4 | 2.27 | 0.68 |
| 22:DA:2655:G:O2' | 22:DA:2656:U:P | 2.51 | 0.68 |
| 1:AA:1006:G:OP1 | 1:AA:1037:C:O2' | 2.12 | 0.68 |
| 22:BA:1915:U:C2 | 22:BA:1916:A:C8 | 2.82 | 0.68 |
| 43:BV:32:GLY:O | 43:BV:93:ARG:NH1 | 2.27 | 0.68 |
| 22:DA:2306:C:OP2 | 22:DA:2307:G:O2' | 2.10 | 0.68 |
| 1:AA:728:A:OP1 | 15:AO:54:ARG:NH2 | 2.27 | 0.68 |
| 22:BA:276:U:O2' | 22:BA:278:A:N7 | 2.27 | 0.68 |
| 22:BA:1266:G:OP1 | 48:B0:16:ARG:NE | 2.25 | 0.68 |
| 22:BA:1474:U:H2' | 22:BA:1475:G:H5' | 1.74 | 0.68 |
| 22:BA:2325:G:C6 | 22:BA:2326:C:N4 | 2.62 | 0.68 |
| 1:CA:1297:G:O2' | 7:CG:114:LYS:NZ | 2.22 | 0.68 |
| 17:CQ:21:ILE:N | 17:CQ:48:ASP:OD1 | 2.27 | 0.68 |
| 22:DA:1260:A:N6 | 58:DA:3277:HOH:O | 2.27 | 0.68 |
| 22:DA:1411:U:H2' | 22:DA:1412:U:O4' | 1.94 | 0.68 |
| 22:DA:2886:A:C2 | 22:DA:2887:A:H1' | 2.29 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:28:A:C5 | 22:BA:29:U:C5 | 2.81 | 0.67 |
| 25:BD:104:VAL:O | 25:BD:105:LYS:HB2 | 1.94 | 0.67 |
| 39:BR:39:LEU:HA | 39:BR:49:ILE:CG2 | 2.24 | 0.67 |
| 24:DC:237:GLY:O | 24:DC:239:ASN:N | 2.27 | 0.67 |
| 22:BA:572:A:C2 | 22:BA:2033:A:C2 | 2.83 | 0.67 |
| 1:CA:1525:G:O6 | 58:CA:1891:HOH:O | 2.09 | 0.67 |
| 22:DA:152:A:C2 | 22:DA:175:G:C2 | 2.83 | 0.67 |
| 22:DA:856:G:N2 | 22:DA:922:C:C2 | 2.62 | 0.67 |
| 12:AL:44:LYS:CB | 12:AL:45:PRO:CD | 2.72 | 0.67 |
| 22:BA:983:A:C6 | 22:BA:984:A:C2 | 2.83 | 0.67 |
| 22:BA:2189:U:H2' | 22:BA:2190:G:C8 | 2.29 | 0.67 |
| 22:BA:2520:C:C6 | 22:BA:2567:G:H1' | 2.30 | 0.67 |
| 22:DA:192:C:OP2 | 58:DA:3739:HOH:O | 2.11 | 0.67 |
| 22:DA:1715:G:O2' | 22:DA:1743:G:O6 | 2.13 | 0.67 |
| 22:BA:1187:G:H5'' | 39:BR:83:TYR:CE2 | 2.30 | 0.67 |
| 29:BH:122:LEU:HD23 | 29:BH:123:ARG:N | 2.10 | 0.67 |
| 39:BR:49:ILE:CG2 | 39:BR:53:PHE:N | 2.57 | 0.67 |
| 1:CA:1124:G:N2 | 1:CA:1127:G:C2 | 2.63 | 0.67 |
| 1:CA:1279:G:H2' | 1:CA:1279:G:N3 | 2.09 | 0.67 |
| 24:DC:204:VAL:O | 24:DC:206:GLY:N | 2.27 | 0.67 |
| 25:DD:56:LYS:O | 25:DD:58:ASN:N | 2.27 | 0.67 |
| 42:DU:38:GLY:HA2 | 42:DU:41:LEU:CD2 | 2.23 | 0.67 |
| 49:D1:5:ILE:O | 49:D1:28:ARG:NH1 | 2.27 | 0.67 |
| 13:AM:114:LYS:CB | 13:AM:115:PRO:HD3 | 2.23 | 0.67 |
| 17:AQ:14:SER:HB3 | 17:AQ:22:VAL:CG1 | 2.25 | 0.67 |
| 22:BA:361:G:O2' | 22:BA:362:A:O5' | 2.09 | 0.67 |
| 24:BC:71:LYS:NZ | 24:BC:98:ASP:OD2 | 2.27 | 0.67 |
| 25:BD:101:PHE:O | 25:BD:103:ASP:N | 2.27 | 0.67 |
| 22:DA:694:U:C2' | 22:DA:695:G:H5'' | 2.24 | 0.67 |
| 22:DA:1342:A:OP2 | 58:DA:3711:HOH:O | 2.12 | 0.67 |
| 22:DA:1603:A:OP2 | 58:DA:3407:HOH:O | 2.13 | 0.67 |
| 17:AQ:81:LYS:O | 17:AQ:83:VAL:N | 2.28 | 0.67 |
| 22:BA:1494:A:C2' | 22:BA:1495:A:O5' | 2.42 | 0.67 |
| 22:BA:2800:A:C2 | 22:BA:2895:G:H1' | 2.30 | 0.67 |
| 37:BP:53:ARG:CG | 37:BP:53:ARG:HH11 | 2.08 | 0.67 |
| 4:CD:174:ASP:O | 4:CD:175:ALA:CB | 2.42 | 0.67 |
| 22:DA:78:U:H2' | 22:DA:79:C:O4' | 1.94 | 0.67 |
| 22:BA:747:U:C4 | 22:BA:2613:U:C5 | 2.83 | 0.67 |
| 37:BP:90:GLY:O | 37:BP:113:ARG:NH1 | 2.26 | 0.67 |
| 1:CA:1006:G:H2' | 1:CA:1007:U:C6 | 2.30 | 0.67 |
| 22:BA:747:U:OP2 | 54:B6:8:MHT:H5 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:BJ:114:LEU:HG | 31:BJ:118:MET:CE | 2.25 | 0.67 |
| 37:BP:103:ARG:CG | 37:BP:103:ARG:HH11 | 2.08 | 0.67 |
| 39:BR:39:LEU:HA | 39:BR:49:ILE:HG23 | 1.76 | 0.67 |
| 48:B0:55:ILE:O | 48:B0:56:ALA:CB | 2.43 | 0.67 |
| 1:CA:31:G:O4' | 1:CA:306:A:C2 | 2.47 | 0.67 |
| 12:CL:47:SER:O | 12:CL:48:ALA:CB | 2.43 | 0.67 |
| 22:DA:2451:A:C4 | 56:DA:3001:DOL:HC12 | 2.30 | 0.67 |
| 23:DB:78:A:C5 | 23:DB:99:A:C8 | 2.83 | 0.67 |
| 42:DU:7:ARG:HG3 | 42:DU:8:ASP:N | 2.10 | 0.67 |
| 1:AA:1018:G:N3 | 1:AA:1018:G:H2' | 2.10 | 0.67 |
| 22:BA:2799:A:O2' | 22:BA:2800:A:O5' | 2.12 | 0.67 |
| 30:BI:19:ASN:N | 30:BI:20:PRO:CD | 2.58 | 0.67 |
| 22:DA:1141:U:H4' | 22:DA:1142:A:O4' | 1.95 | 0.67 |
| 22:DA:2058:A:N6 | 22:DA:2059:A:N6 | 2.43 | 0.67 |
| 30:DI:58:VAL:HG12 | 30:DI:59:ILE:N | 2.10 | 0.67 |
| 46:DY:56:LEU:O | 46:DY:57:LEU:CB | 2.43 | 0.67 |
| 1:AA:203:G:N2 | 1:AA:215:C:C2 | 2.63 | 0.67 |
| 1:AA:381:C:H2' | 1:AA:382:A:O4' | 1.95 | 0.67 |
| 2:AB:154:MET:O | 2:AB:156:GLY:N | 2.28 | 0.67 |
| 22:BA:1065:U:O4 | 22:BA:1074:G:O2' | 2.13 | 0.67 |
| 22:BA:1394:U:P | 58:BA:3407:HOH:O | 2.52 | 0.67 |
| 29:BH:27:ARG:O | 29:BH:28:ASN:HB2 | 1.95 | 0.67 |
| 46:BY:18:LEU:O | 46:BY:22:LEU:HB2 | 1.95 | 0.67 |
| 1:CA:552:U:C4 | 1:CA:553:A:N7 | 2.63 | 0.67 |
| 1:CA:1302:C:C4 | 13:CM:17:ILE:HD13 | 2.30 | 0.67 |
| 1:AA:89:U:O2' | 1:AA:90:C:C5' | 2.43 | 0.66 |
| 1:AA:1406:U:C5 | 1:AA:1407:C:C5 | 2.83 | 0.66 |
| 29:BH:91:PHE:O | 1:CA:55:A:C6 | 2.48 | 0.66 |
| 1:CA:70:U:H2' | 1:CA:94:G:N7 | 2.10 | 0.66 |
| 1:CA:1072:G:C6 | 1:CA:1073:U:C4 | 2.83 | 0.66 |
| 22:DA:981:A:OP2 | 22:DA:982:C:N4 | 2.27 | 0.66 |
| 22:DA:1378:A:O3' | 58:DA:3751:HOH:O | 2.13 | 0.66 |
| 22:DA:2507:C:OP1 | 58:DA:3708:HOH:O | 2.12 | 0.66 |
| 22:DA:2609:U:H6 | 54:D6:7:004:HA | 1.59 | 0.66 |
| 47:DZ:52:SER:OG | 47:DZ:53:PHE:N | 2.26 | 0.66 |
| 1:AA:1493:A:C8 | 1:AA:1493:A:OP2 | 2.49 | 0.66 |
| 5:AE:69:ARG:O | 5:AE:71:MET:N | 2.27 | 0.66 |
| 13:AM:95:LEU:HB3 | 13:AM:96:PRO:HD2 | 1.77 | 0.66 |
| 22:BA:1717:A:H2' | 22:BA:1718:G:O5' | 1.94 | 0.66 |
| 28:BG:121:ILE:HD12 | 28:BG:141:ILE:HG22 | 1.77 | 0.66 |
| 1:CA:1316:G:N1 | 1:CA:1319:A:OP2 | 2.28 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:1737:G:C6 | 22:DA:1738:G:N1 | 2.64 | 0.66 |
| 22:DA:2241:A:N7 | 58:DA:3502:HOH:O | 2.27 | 0.66 |
| 28:DG:111:HIS:ND1 | 28:DG:111:HIS:O | 2.28 | 0.66 |
| 1:AA:650:G:C2' | 1:AA:651:C:H5' | 2.26 | 0.66 |
| 22:BA:1288:G:C4 | 22:BA:1327:A:C2 | 2.82 | 0.66 |
| 22:BA:1371:G:N7 | 58:BA:3401:HOH:O | 2.28 | 0.66 |
| 1:CA:154:U:C2' | 1:CA:155:A:H5' | 2.25 | 0.66 |
| 1:CA:533:A:OP1 | 58:CA:1763:HOH:O | 2.13 | 0.66 |
| 22:DA:2505:G:OP2 | 56:DA:3001:DOL:HC17 | 1.95 | 0.66 |
| 22:DA:2751:G:OP1 | 28:DG:3:ARG:NH1 | 2.29 | 0.66 |
| 41:DT:17:SER:O | 41:DT:19:LYS:N | 2.28 | 0.66 |
| 2:AB:24:ASN:O | 2:AB:26:LYS:N | 2.29 | 0.66 |
| 11:AK:34:ILE:HB | 11:AK:74:VAL:HG11 | 1.78 | 0.66 |
| 13:AM:4:ILE:O | 13:AM:6:GLY:N | 2.28 | 0.66 |
| 13:AM:64:VAL:O | 13:AM:64:VAL:HG12 | 1.94 | 0.66 |
| 22:BA:142:A:C5 | 22:BA:143:C:C4 | 2.83 | 0.66 |
| 22:BA:2591:C:OP1 | 24:BC:238:ARG:NH1 | 2.27 | 0.66 |
| 29:BH:94:ILE:CG2 | 29:BH:99:ILE:HG13 | 2.26 | 0.66 |
| 10:CJ:91:ASP:N | 10:CJ:91:ASP:OD1 | 2.29 | 0.66 |
| 22:DA:1581:G:C5 | 22:DA:1582:C:C4 | 2.84 | 0.66 |
| 22:DA:2339:C:H2' | 22:DA:2340:A:C8 | 2.30 | 0.66 |
| 33:DL:38:GLN:O | 33:DL:40:SER:N | 2.28 | 0.66 |
| 22:BA:265:A:H4' | 22:BA:266:G:OP1 | 1.96 | 0.66 |
| 22:BA:744:U:OP1 | 58:BA:3654:HOH:O | 2.12 | 0.66 |
| 30:BI:97:LYS:CG | 30:BI:139:VAL:HG22 | 2.25 | 0.66 |
| 22:DA:223:A:C5 | 22:DA:422:A:C8 | 2.83 | 0.66 |
| 22:DA:1855:U:C5 | 22:DA:1856:U:C5 | 2.83 | 0.66 |
| 22:DA:1875:G:O2' | 22:DA:1876:A:OP2 | 2.14 | 0.66 |
| 50:D2:29:GLN:O | 50:D2:33:ARG:NH2 | 2.27 | 0.66 |
| 22:BA:620:G:H4' | 22:BA:621:A:O5' | 1.95 | 0.66 |
| 22:BA:1384:A:H1' | 22:BA:1405:U:H1' | 1.78 | 0.66 |
| 22:BA:1869:G:H3' | 22:BA:1870:C:H5' | 1.78 | 0.66 |
| 22:BA:1952:A:C6 | 22:BA:1953:A:N1 | 2.64 | 0.66 |
| 39:BR:24:LYS:HA | 39:BR:94:THR:HG23 | 1.77 | 0.66 |
| 5:CE:137:VAL:O | 5:CE:138:ARG:HG2 | 1.95 | 0.66 |
| 22:DA:444:C:OP1 | 26:DE:40:ARG:NH1 | 2.28 | 0.66 |
| 22:DA:1627:G:C2 | 22:DA:1628:G:N7 | 2.64 | 0.66 |
| 22:DA:2261:C:C2 | 22:DA:2280:G:N2 | 2.64 | 0.66 |
| 30:DI:69:PHE:N | 30:DI:69:PHE:CD1 | 2.64 | 0.66 |
| 35:DN:90:ARG:CZ | 35:DN:116:VAL:HG11 | 2.25 | 0.66 |
| 1:AA:209:U:H4' | 1:AA:210:C:OP2 | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:345:C:O2' | 32:BK:116:ILE:HD11 | 1.95 | 0.66 |
| 4:AD:32:CYS:O | 4:AD:33:LYS:HB2 | 1.95 | 0.66 |
| 22:BA:2582:G:C2 | 22:BA:2583:G:C8 | 2.83 | 0.66 |
| 1:CA:1005:A:O3' | 1:CA:1037:C:O2' | 2.13 | 0.66 |
| 1:CA:1460:C:N4 | 1:CA:1461:G:C6 | 2.64 | 0.66 |
| 22:DA:362:A:C5 | 22:DA:363:G:C8 | 2.84 | 0.66 |
| 1:AA:262:A:C6 | 1:AA:263:A:C6 | 2.84 | 0.66 |
| 15:AO:63:ARG:HG2 | 15:AO:67:LEU:HD12 | 1.76 | 0.66 |
| 22:BA:1509:A:O2' | 22:BA:1510:G:P | 2.54 | 0.66 |
| 1:CA:1004:A:O2' | 1:CA:1036:A:N1 | 2.28 | 0.66 |
| 1:CA:1408:A:C2 | 1:CA:1494:G:C4 | 2.84 | 0.66 |
| 22:DA:352:A:H2' | 22:DA:353:C:O4' | 1.96 | 0.66 |
| 22:DA:931:U:OP1 | 47:DZ:30:ARG:NH1 | 2.29 | 0.66 |
| 22:DA:1826:G:C5 | 22:DA:1827:U:C5 | 2.84 | 0.66 |
| 22:DA:2415:G:C6 | 22:DA:2416:C:C4 | 2.84 | 0.66 |
| 22:DA:2636:C:H2' | 22:DA:2637:U:C6 | 2.31 | 0.66 |
| 26:DE:149:ILE:CD1 | 26:DE:172:ALA:HA | 2.26 | 0.66 |
| 32:DK:76:VAL:HG12 | 37:DP:73:VAL:HG22 | 1.77 | 0.66 |
| 9:AI:91:ASP:OD2 | 9:AI:93:SER:N | 2.29 | 0.66 |
| 1:CA:1108:G:H5'' | 3:CC:176:HIS:CD2 | 2.31 | 0.66 |
| 22:DA:395:U:H4' | 22:DA:396:G:OP1 | 1.96 | 0.66 |
| 22:DA:1006:C:OP2 | 58:DA:3779:HOH:O | 2.14 | 0.66 |
| 22:DA:2061:G:O6 | 56:DA:3001:DOL:H162 | 1.96 | 0.66 |
| 22:DA:2874:C:H2' | 22:DA:2875:C:C6 | 2.31 | 0.66 |
| 43:DV:51:GLN:HB3 | 43:DV:56:PHE:CG | 2.31 | 0.66 |
| 22:DA:1010:A:OP2 | 58:DA:3776:HOH:O | 2.14 | 0.66 |
| 22:DA:1120:G:C6 | 22:DA:1121:C:C4 | 2.84 | 0.66 |
| 22:DA:2146:C:H5'' | 22:DA:2147:A:OP1 | 1.95 | 0.66 |
| 35:DN:87:PHE:O | 35:DN:90:ARG:N | 2.29 | 0.66 |
| 1:AA:67:C:O2' | 1:AA:171:A:N3 | 2.29 | 0.65 |
| 22:BA:1494:A:C2 | 22:BA:1495:A:C4 | 2.84 | 0.65 |
| 22:BA:1925:C:H4' | 22:BA:1926:U:OP1 | 1.95 | 0.65 |
| 23:BB:116:G:H4' | 36:BO:54:VAL:HG13 | 1.78 | 0.65 |
| 29:BH:14:SER:O | 29:BH:15:LEU:HB2 | 1.95 | 0.65 |
| 1:CA:154:U:H2' | 1:CA:155:A:H5' | 1.77 | 0.65 |
| 22:DA:226:A:N6 | 22:DA:227:A:N1 | 2.44 | 0.65 |
| 22:DA:2164:C:H2' | 22:DA:2165:C:C6 | 2.32 | 0.65 |
| 14:AN:21:PHE:HA | 14:AN:25:ALA:HB3 | 1.77 | 0.65 |
| 22:DA:425:G:C2 | 22:DA:426:C:C4 | 2.84 | 0.65 |
| 22:DA:1359:A:C8 | 22:DA:1373:A:C2 | 2.83 | 0.65 |
| 22:DA:2407:A:OP2 | 58:DA:3558:HOH:O | 2.13 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:68:G:C5 | 1:AA:69:G:H1' | 2.31 | 0.65 |
| 1:AA:1304:G:N1 | 1:AA:1305:G:N2 | 2.45 | 0.65 |
| 22:BA:819:A:C4 | 22:BA:1189:A:C2 | 2.84 | 0.65 |
| 22:BA:1922:G:H22 | 22:BA:1923:U:H1' | 1.62 | 0.65 |
| 1:CA:1077:G:N2 | 1:CA:1080:A:OP2 | 2.28 | 0.65 |
| 22:DA:2063:C:H4' | 56:DA:3001:DOL:H343 | 1.77 | 0.65 |
| 56:DA:3001:DOL:HC1 | 56:DA:3001:DOL:H431 | 1.77 | 0.65 |
| 42:DU:36:VAL:O | 42:DU:38:GLY:N | 2.29 | 0.65 |
| 22:BA:2430:A:H5' | 22:BA:2431:U:OP2 | 1.96 | 0.65 |
| 5:CE:146:ASN:N | 5:CE:146:ASN:OD1 | 2.26 | 0.65 |
| 20:CT:15:GLU:OE2 | 20:CT:18:ARG:NH2 | 2.29 | 0.65 |
| 22:DA:125:A:OP2 | 50:D2:19:ARG:NH2 | 2.30 | 0.65 |
| 22:DA:250:G:OP2 | 51:D3:13:ARG:NH1 | 2.28 | 0.65 |
| 22:DA:1430:G:H2' | 22:DA:1431:A:O4' | 1.97 | 0.65 |
| 25:DD:104:VAL:O | 25:DD:105:LYS:CB | 2.44 | 0.65 |
| 4:AD:11:LEU:CD2 | 4:AD:63:ARG:HD3 | 2.27 | 0.65 |
| 11:AK:26:SER:O | 11:AK:28:ASN:N | 2.29 | 0.65 |
| 29:BH:139:PHE:O | 29:BH:140:ALA:CB | 2.44 | 0.65 |
| 12:CL:57:LEU:O | 12:CL:59:ASN:N | 2.29 | 0.65 |
| 22:DA:301:G:O4' | 22:DA:317:G:N2 | 2.29 | 0.65 |
| 22:DA:948:C:O2 | 22:DA:984:A:O2' | 2.15 | 0.65 |
| 22:DA:1581:G:C5 | 22:DA:1582:C:N4 | 2.65 | 0.65 |
| 22:DA:1638:C:H5'' | 22:DA:2710:C:O2' | 1.97 | 0.65 |
| 22:DA:1676:A:H2' | 22:DA:1677:A:O4' | 1.97 | 0.65 |
| 22:DA:2334:U:C4 | 36:DO:16:ARG:HD3 | 2.32 | 0.65 |
| 22:BA:997:G:OP1 | 38:BQ:92:ARG:HG2 | 1.96 | 0.65 |
| 22:BA:2749:A:OP1 | 28:BG:2:SER:N | 2.30 | 0.65 |
| 29:BH:114:GLU:HB3 | 29:BH:133:GLN:O | 1.97 | 0.65 |
| 1:CA:706:A:C5 | 1:CA:707:U:C5 | 2.85 | 0.65 |
| 1:CA:1490:U:H2' | 1:CA:1491:G:O4' | 1.96 | 0.65 |
| 4:CD:173:VAL:O | 4:CD:174:ASP:HB3 | 1.97 | 0.65 |
| 12:CL:44:LYS:O | 12:CL:46:ASN:N | 2.30 | 0.65 |
| 18:CR:33:ILE:HA | 18:CR:40:VAL:HG23 | 1.79 | 0.65 |
| 22:DA:2032:G:H1' | 25:DD:150:GLN:NE2 | 2.11 | 0.65 |
| 22:DA:2603:G:C6 | 22:DA:2604:U:C4 | 2.84 | 0.65 |
| 1:AA:16:A:O2' | 1:AA:17:U:H5' | 1.97 | 0.65 |
| 10:AJ:33:GLY:O | 10:AJ:34:ALA:CB | 2.45 | 0.65 |
| 22:BA:84:A:N1 | 22:BA:98:G:O2' | 2.23 | 0.65 |
| 22:BA:142:A:N7 | 22:BA:143:C:N4 | 2.45 | 0.65 |
| 22:BA:747:U:C4 | 22:BA:2613:U:C4 | 2.84 | 0.65 |
| 22:BA:1141:U:H4' | 22:BA:1142:A:O4' | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BS:63:GLY:O | 40:BS:64:ALA:CB | 2.45 | 0.65 |
| 1:CA:73:C:O2' | 1:CA:74:A:O5' | 2.14 | 0.65 |
| 1:CA:268:U:H2' | 1:CA:269:C:C6 | 2.30 | 0.65 |
| 1:CA:378:G:C2 | 1:CA:386:C:O2 | 2.50 | 0.65 |
| 22:DA:1317:G:C2 | 22:DA:1336:A:C2 | 2.84 | 0.65 |
| 22:DA:1801:A:C5 | 24:DC:262:ARG:NH2 | 2.65 | 0.65 |
| 22:DA:1938:A:C6 | 22:DA:2590:A:H1' | 2.32 | 0.65 |
| 25:DD:12:THR:OG1 | 25:DD:13:ARG:N | 2.29 | 0.65 |
| 2:AB:151:ILE:HD12 | 2:AB:154:MET:SD | 2.36 | 0.65 |
| 8:AH:10:MET:HE1 | 8:AH:33:LYS:HB3 | 1.78 | 0.65 |
| 17:AQ:69:LYS:O | 17:AQ:70:THR:HB | 1.96 | 0.65 |
| 1:CA:734:G:C2 | 1:CA:735:C:C6 | 2.84 | 0.65 |
| 22:DA:527:C:OP1 | 58:DA:3247:HOH:O | 2.14 | 0.65 |
| 22:DA:2297:A:C2 | 22:DA:2298:A:C8 | 2.84 | 0.65 |
| 34:DM:2:LEU:O | 34:DM:3:GLN:HB3 | 1.96 | 0.65 |
| 1:AA:536:C:OP1 | 58:AA:1884:HOH:O | 2.13 | 0.65 |
| 2:AB:184:PHE:CZ | 2:AB:198:PHE:CD2 | 2.85 | 0.65 |
| 22:BA:973:A:O4' | 22:BA:1188:U:C6 | 2.50 | 0.65 |
| 22:BA:2321:U:H5' | 22:BA:2322:A:OP2 | 1.95 | 0.65 |
| 22:BA:2728:U:O2' | 22:BA:2729:G:P | 2.55 | 0.65 |
| 33:BL:82:LEU:HD23 | 33:BL:83:ALA:N | 2.12 | 0.65 |
| 41:BT:1:MET:O | 41:BT:2:ILE:HG13 | 1.96 | 0.65 |
| 1:CA:1356:G:H2' | 1:CA:1357:A:C8 | 2.31 | 0.65 |
| 22:DA:1097:U:C5 | 22:DA:1098:A:H1' | 2.32 | 0.65 |
| 22:DA:1197:G:H2' | 22:DA:1198:U:C6 | 2.32 | 0.65 |
| 34:DM:76:LYS:NZ | 34:DM:85:GLY:O | 2.30 | 0.65 |
| 1:AA:597:G:C2 | 1:AA:644:U:C2 | 2.84 | 0.65 |
| 1:AA:684:U:O2' | 11:AK:40:ASN:O | 2.14 | 0.65 |
| 1:AA:715:A:OP1 | 1:AA:805:C:O2' | 2.10 | 0.65 |
| 13:AM:114:LYS:HB2 | 13:AM:115:PRO:HD3 | 1.78 | 0.65 |
| 22:BA:684:G:OP1 | 50:B2:21:ARG:NH1 | 2.30 | 0.65 |
| 24:BC:141:VAL:HG11 | 24:BC:190:ALA:HB1 | 1.77 | 0.65 |
| 22:DA:2056:G:O6 | 22:DA:2612:C:N3 | 2.29 | 0.65 |
| 22:DA:2612:C:H5'' | 22:DA:2613:U:OP1 | 1.97 | 0.65 |
| 1:AA:89:U:O2' | 1:AA:90:C:H5'' | 1.96 | 0.64 |
| 12:AL:21:VAL:HG23 | 12:AL:95:TYR:CE1 | 2.32 | 0.64 |
| 22:BA:455:C:N3 | 22:BA:472:A:H2' | 2.11 | 0.64 |
| 24:BC:6:CYS:SG | 24:BC:18:LYS:HD2 | 2.37 | 0.64 |
| 29:BH:122:LEU:C | 29:BH:123:ARG:HG2 | 2.17 | 0.64 |
| 1:CA:604:G:H2' | 1:CA:605:U:O4' | 1.97 | 0.64 |
| 22:DA:247:G:H4' | 22:DA:386:G:C4 | 2.32 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:443:A:N7 | 26:DE:40:ARG:HG3 | 2.12 | 0.64 |
| 22:DA:583:G:C6 | 22:DA:584:C:C4 | 2.85 | 0.64 |
| 22:DA:694:U:H2' | 22:DA:695:G:H5'' | 1.79 | 0.64 |
| 22:DA:788:A:OP1 | 22:DA:791:C:N4 | 2.30 | 0.64 |
| 22:DA:1566:A:C2 | 24:DC:213:TRP:CD2 | 2.85 | 0.64 |
| 22:DA:2147:A:H2' | 22:DA:2148:G:O4' | 1.97 | 0.64 |
| 26:DE:108:ILE:HD13 | 26:DE:181:ILE:CG1 | 2.27 | 0.64 |
| 48:D0:55:ILE:O | 48:D0:56:ALA:CB | 2.45 | 0.64 |
| 1:AA:202:G:N2 | 1:AA:216:U:O2 | 2.29 | 0.64 |
| 4:AD:58:LYS:HG3 | 4:AD:59:GLN:N | 2.11 | 0.64 |
| 19:AS:22:ALA:O | 19:AS:26:GLY:N | 2.30 | 0.64 |
| 52:B4:37:GLN:HG2 | 52:B4:37:GLN:O | 1.96 | 0.64 |
| 22:DA:53:A:N3 | 22:DA:179:C:H4' | 2.11 | 0.64 |
| 22:DA:160:A:N3 | 22:DA:2208:C:O2' | 2.29 | 0.64 |
| 22:DA:1361:G:C2 | 22:DA:1362:C:C6 | 2.85 | 0.64 |
| 22:DA:2498:C:OP2 | 58:DA:3681:HOH:O | 2.15 | 0.64 |
| 1:AA:338:A:N1 | 1:AA:351:G:O6 | 2.31 | 0.64 |
| 11:AK:13:ARG:NE | 22:BA:2142:A:OP1 | 2.30 | 0.64 |
| 22:BA:136:G:N2 | 22:BA:144:A:C5 | 2.65 | 0.64 |
| 22:BA:1607:C:N4 | 22:BA:1622:G:N7 | 2.45 | 0.64 |
| 30:BI:39:CYS:HA | 30:BI:42:PHE:CB | 2.28 | 0.64 |
| 2:CB:134:ALA:O | 2:CB:138:THR:OG1 | 2.11 | 0.64 |
| 13:CM:98:ARG:O | 13:CM:100:GLN:N | 2.30 | 0.64 |
| 14:CN:80:SER:O | 14:CN:82:ILE:N | 2.29 | 0.64 |
| 22:DA:49:A:C8 | 22:DA:51:G:N2 | 2.66 | 0.64 |
| 22:DA:1438:U:C5 | 22:DA:1552:A:C2 | 2.86 | 0.64 |
| 22:DA:2820:A:C8 | 25:DD:196:ALA:HB1 | 2.32 | 0.64 |
| 1:AA:31:G:O2' | 1:AA:48:C:N4 | 2.30 | 0.64 |
| 1:AA:484:G:H4' | 1:AA:485:U:OP1 | 1.97 | 0.64 |
| 4:AD:11:LEU:HD22 | 4:AD:63:ARG:HD3 | 1.79 | 0.64 |
| 22:BA:983:A:N6 | 22:BA:984:A:N1 | 2.45 | 0.64 |
| 34:BM:42:THR:HG22 | 34:BM:93:VAL:HG12 | 1.78 | 0.64 |
| 1:CA:716:A:N3 | 11:CK:119:ASN:O | 2.30 | 0.64 |
| 1:CA:1151:A:C2 | 1:CA:1152:A:C5 | 2.85 | 0.64 |
| 5:CE:24:THR:HA | 5:CE:29:ARG:HA | 1.79 | 0.64 |
| 20:CT:67:ILE:O | 20:CT:67:ILE:CG2 | 2.44 | 0.64 |
| 22:DA:1027:A:C6 | 22:DA:1126:A:N3 | 2.66 | 0.64 |
| 22:DA:1606:C:C2' | 22:DA:1607:C:OP2 | 2.44 | 0.64 |
| 8:AH:42:GLU:OE1 | 8:AH:42:GLU:N | 2.30 | 0.64 |
| 12:AL:72:HIS:ND1 | 12:AL:72:HIS:O | 2.30 | 0.64 |
| 22:BA:395:U:O2' | 22:BA:396:G:N7 | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1056:G:H5'' | 22:BA:1057:A:O4' | 1.98 | 0.64 |
| 6:CF:32:ALA:O | 6:CF:34:GLY:N | 2.29 | 0.64 |
| 22:DA:192:C:N4 | 22:DA:193:U:O2 | 2.31 | 0.64 |
| 22:DA:1210:G:O6 | 22:DA:1237:A:O2' | 2.12 | 0.64 |
| 22:DA:2590:A:O3' | 24:DC:238:ARG:NH1 | 2.31 | 0.64 |
| 22:DA:2824:C:N4 | 22:DA:2825:G:N7 | 2.46 | 0.64 |
| 25:DD:97:SER:O | 25:DD:99:GLU:N | 2.30 | 0.64 |
| 34:DM:136:MET:O | 43:DV:79:ARG:NH2 | 2.31 | 0.64 |
| 1:AA:1304:G:OP2 | 58:AA:1795:HOH:O | 2.15 | 0.64 |
| 22:BA:1924:C:C2' | 22:BA:1925:C:H5'' | 2.27 | 0.64 |
| 41:BT:49:LYS:HD3 | 41:BT:49:LYS:N | 2.13 | 0.64 |
| 1:CA:505:G:C6 | 1:CA:535:A:C2 | 2.86 | 0.64 |
| 1:CA:1069:C:C2' | 1:CA:1070:U:O5' | 2.46 | 0.64 |
| 22:DA:341:C:H2' | 22:DA:342:A:C8 | 2.31 | 0.64 |
| 22:DA:1753:G:C2 | 22:DA:1756:G:N2 | 2.66 | 0.64 |
| 17:AQ:12:VAL:HG12 | 17:AQ:13:VAL:N | 2.12 | 0.64 |
| 22:BA:500:G:N2 | 22:BA:502:A:H3' | 2.13 | 0.64 |
| 22:BA:1800:C:H3' | 24:BC:146:MET:HE1 | 1.78 | 0.64 |
| 5:CE:41:ASP:OD1 | 5:CE:43:ASN:N | 2.31 | 0.64 |
| 20:CT:67:ILE:O | 20:CT:67:ILE:HG22 | 1.98 | 0.64 |
| 22:DA:1251:C:OP2 | 38:DQ:6:ARG:NH2 | 2.30 | 0.64 |
| 26:DE:21:ARG:NH1 | 26:DE:103:GLY:O | 2.31 | 0.64 |
| 28:DG:11:VAL:O | 28:DG:48:ASN:ND2 | 2.31 | 0.64 |
| 1:AA:736:C:OP1 | 18:AR:61:ARG:NH1 | 2.31 | 0.64 |
| 22:BA:1717:A:C2' | 22:BA:1718:G:O5' | 2.46 | 0.64 |
| 1:CA:1012:A:C2 | 1:CA:1018:G:C2 | 2.86 | 0.64 |
| 1:CA:1069:C:H2' | 1:CA:1070:U:O5' | 1.97 | 0.64 |
| 22:DA:276:U:O2 | 22:DA:276:U:H2' | 1.98 | 0.64 |
| 22:DA:1208:C:C4 | 22:DA:1209:U:C4 | 2.86 | 0.64 |
| 22:BA:1066:U:O2 | 22:BA:1069:A:N7 | 2.30 | 0.64 |
| 22:BA:1079:C:C5 | 22:BA:1088:A:C2 | 2.86 | 0.64 |
| 22:BA:1924:C:H2' | 22:BA:1925:C:C5' | 2.28 | 0.64 |
| 22:BA:2188:U:H2' | 22:BA:2189:U:C6 | 2.33 | 0.64 |
| 22:BA:2258:C:O2' | 22:BA:2427:C:OP2 | 2.12 | 0.64 |
| 22:BA:2419:U:O2' | 22:BA:2420:C:H5' | 1.98 | 0.64 |
| 53:B5:213:VAL:O | 53:B5:214:TYR:CB | 2.45 | 0.64 |
| 22:DA:682:G:N2 | 22:DA:683:U:C2 | 2.66 | 0.64 |
| 22:DA:1469:A:C2 | 22:DA:1470:A:C6 | 2.86 | 0.64 |
| 23:DB:87:U:O2' | 23:DB:88:C:H5' | 1.97 | 0.64 |
| 3:AC:64:ILE:HG23 | 3:AC:99:ALA:HB2 | 1.80 | 0.64 |
| 4:AD:46:PRO:O | 4:AD:48:LEU:N | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1073:A:H3' | 22:BA:1074:G:H5'' | 1.79 | 0.64 |
| 22:BA:2191:A:H2' | 22:BA:2192:U:C6 | 2.33 | 0.64 |
| 39:BR:66:HIS:ND1 | 39:BR:94:THR:HG22 | 2.13 | 0.64 |
| 1:CA:1147:C:O2 | 9:CI:18:ARG:NH2 | 2.31 | 0.64 |
| 22:DA:2111:U:C5 | 22:DA:2145:C:H2' | 2.32 | 0.64 |
| 22:DA:2182:U:H2' | 22:DA:2183:A:C8 | 2.32 | 0.64 |
| 25:DD:208:LYS:O | 25:DD:209:ALA:CB | 2.46 | 0.64 |
| 1:AA:604:G:C2 | 1:AA:635:A:C2 | 2.86 | 0.63 |
| 1:AA:1204:A:OP1 | 58:AA:1781:HOH:O | 2.14 | 0.63 |
| 22:BA:1917:U:C2' | 22:BA:1918:A:H5' | 2.28 | 0.63 |
| 39:BR:14:VAL:CG1 | 39:BR:98:ILE:HG13 | 2.28 | 0.63 |
| 1:CA:706:A:O2' | 11:CK:31:ILE:HD11 | 1.98 | 0.63 |
| 1:CA:791:G:C6 | 1:CA:792:A:N7 | 2.65 | 0.63 |
| 16:CP:14:ARG:N | 16:CP:15:PRO:CD | 2.61 | 0.63 |
| 22:DA:1607:C:O2 | 22:DA:1621:U:C4 | 2.50 | 0.63 |
| 22:DA:2816:G:N3 | 22:DA:2883:A:O2' | 2.29 | 0.63 |
| 29:DH:117:LEU:CD1 | 29:DH:130:VAL:HG22 | 2.28 | 0.63 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.34 | 0.63 |
| 1:AA:1299:A:H2' | 1:AA:1299:A:N3 | 2.13 | 0.63 |
| 2:AB:160:ALA:O | 2:AB:161:LEU:HB2 | 1.98 | 0.63 |
| 22:BA:1668:A:O2' | 22:BA:1674:G:N7 | 2.21 | 0.63 |
| 22:BA:1915:U:C2' | 22:BA:1916:A:H5' | 2.28 | 0.63 |
| 1:CA:811:C:O2' | 1:CA:901:A:N1 | 2.29 | 0.63 |
| 3:CC:74:GLY:O | 3:CC:78:GLY:N | 2.32 | 0.63 |
| 18:CR:22:ASP:OD1 | 18:CR:23:TYR:N | 2.31 | 0.63 |
| 22:DA:271:G:H4' | 22:DA:272:A:OP1 | 1.98 | 0.63 |
| 22:DA:1826:G:C6 | 22:DA:1827:U:C4 | 2.86 | 0.63 |
| 22:DA:2001:C:H4' | 22:DA:2689:U:H2' | 1.79 | 0.63 |
| 22:DA:2121:G:N2 | 22:DA:2177:C:O2 | 2.31 | 0.63 |
| 37:DP:29:LYS:HB3 | 37:DP:40:LEU:HD21 | 1.79 | 0.63 |
| 5:AE:137:VAL:O | 5:AE:138:ARG:HB2 | 1.98 | 0.63 |
| 20:AT:3:ASN:C | 20:AT:3:ASN:OD1 | 2.35 | 0.63 |
| 53:B5:121:MET:CB | 53:B5:143:ALA:HB1 | 2.29 | 0.63 |
| 1:CA:1521:C:N3 | 1:CA:1522:U:C5 | 2.66 | 0.63 |
| 22:DA:1364:G:H2' | 22:DA:1365:A:H5' | 1.79 | 0.63 |
| 35:DN:71:ARG:HH21 | 35:DN:71:ARG:CG | 2.12 | 0.63 |
| 22:BA:2286:G:H5'' | 22:BA:2287:A:O4' | 1.99 | 0.63 |
| 40:BS:84:ARG:HB2 | 40:BS:96:ILE:CG1 | 2.29 | 0.63 |
| 1:CA:1219:A:N6 | 1:CA:1220:G:O6 | 2.32 | 0.63 |
| 1:CA:1225:A:H2' | 1:CA:1226:C:C5 | 2.32 | 0.63 |
| 4:CD:95:GLU:OE2 | 4:CD:100:ASN:ND2 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 4:CD:174:ASP:OD1 | 4:CD:175:ALA:N | 2.30 | 0.63 |
| 22:DA:2622:U:O2' | 22:DA:2825:G:N7 | 2.31 | 0.63 |
| 17:AQ:16:LYS:N | 17:AQ:17:MET:SD | 2.72 | 0.63 |
| 22:BA:2189:U:H2' | 22:BA:2190:G:N9 | 2.12 | 0.63 |
| 1:CA:499:A:C6 | 1:CA:547:A:C8 | 2.86 | 0.63 |
| 1:CA:801:U:H2' | 1:CA:802:A:H8 | 1.63 | 0.63 |
| 15:CO:17:ARG:O | 15:CO:18:ASP:HB3 | 1.98 | 0.63 |
| 22:DA:19:A:C2 | 22:DA:522:A:C2 | 2.86 | 0.63 |
| 23:DB:78:A:C6 | 23:DB:99:A:C8 | 2.86 | 0.63 |
| 29:DH:117:LEU:HG | 29:DH:120:GLY:O | 1.98 | 0.63 |
| 33:DL:93:ASN:OD1 | 33:DL:94:THR:N | 2.31 | 0.63 |
| 22:BA:2191:A:C6 | 22:BA:2192:U:O4 | 2.52 | 0.63 |
| 27:BF:176:PRO:O | 27:BF:177:PHE:CG | 2.52 | 0.63 |
| 1:CA:64:G:C8 | 1:CA:99:C:N4 | 2.67 | 0.63 |
| 1:CA:718:A:C5 | 11:CK:118:HIS:CD2 | 2.86 | 0.63 |
| 2:CB:21:ARG:O | 2:CB:23:TRP:N | 2.31 | 0.63 |
| 1:AA:328:C:O2 | 1:AA:328:C:H2' | 1.98 | 0.63 |
| 1:AA:468:A:C2 | 1:AA:469:C:C4 | 2.85 | 0.63 |
| 2:AB:149:GLY:O | 2:AB:151:ILE:N | 2.32 | 0.63 |
| 22:BA:2061:G:C2 | 56:BA:3001:DOL:HC22 | 2.34 | 0.63 |
| 22:BA:2211:A:H1' | 22:BA:2212:A:OP1 | 1.99 | 0.63 |
| 22:BA:2444:G:P | 26:BE:63:LYS:HD3 | 2.39 | 0.63 |
| 25:BD:125:TRP:CD2 | 25:BD:160:LYS:HD2 | 2.33 | 0.63 |
| 51:B3:27:ALA:O | 51:B3:28:ASN:HB2 | 1.99 | 0.63 |
| 4:CD:32:CYS:SG | 4:CD:33:LYS:N | 2.72 | 0.63 |
| 6:CF:45:ARG:O | 6:CF:56:LYS:HA | 1.99 | 0.63 |
| 22:DA:771:G:C2 | 22:DA:772:C:C6 | 2.87 | 0.63 |
| 22:DA:1075:C:H2' | 22:DA:1076:C:C6 | 2.34 | 0.63 |
| 22:DA:1707:G:N2 | 22:DA:1752:C:C2 | 2.67 | 0.63 |
| 22:DA:2688:G:N1 | 22:DA:2720:U:OP2 | 2.27 | 0.63 |
| 3:AC:139:GLN:O | 3:AC:141:ALA:N | 2.31 | 0.63 |
| 5:AE:99:ALA:O | 5:AE:101:GLU:N | 2.31 | 0.63 |
| 22:BA:1921:G:C2 | 22:BA:1922:G:C8 | 2.87 | 0.63 |
| 27:BF:85:ILE:O | 27:BF:85:ILE:CG1 | 2.47 | 0.63 |
| 22:DA:2353:G:H2' | 22:DA:2354:C:O4' | 1.99 | 0.63 |
| 22:DA:2563:U:C1' | 22:DA:2566:A:N6 | 2.61 | 0.63 |
| 1:AA:1118:U:H1' | 1:AA:1179:A:C4 | 2.33 | 0.63 |
| 12:AL:25:GLU:O | 12:AL:26:ALA:C | 2.38 | 0.63 |
| 13:AM:46:SER:O | 13:AM:47:GLU:HB3 | 1.98 | 0.63 |
| 14:AN:51:LEU:O | 14:AN:53:ARG:N | 2.32 | 0.63 |
| 1:CA:182:A:C5 | 1:CA:184:G:N7 | 2.67 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:254:G:O2' | 17:CQ:18:GLU:O | 2.15 | 0.63 |
| 2:CB:58:ASN:ND2 | 2:CB:220:THR:O | 2.32 | 0.63 |
| 22:DA:481:G:C4 | 22:DA:507:A:C2 | 2.87 | 0.63 |
| 22:DA:2128:G:N3 | 22:DA:2173:A:O2' | 2.32 | 0.63 |
| 22:DA:2790:U:H5' | 22:DA:2893:A:N7 | 2.13 | 0.63 |
| 35:DN:69:ARG:O | 35:DN:71:ARG:N | 2.31 | 0.63 |
| 1:AA:773:G:H2' | 1:AA:774:G:O4' | 1.98 | 0.62 |
| 7:AG:40:GLU:HB2 | 7:AG:44:TYR:CE2 | 2.35 | 0.62 |
| 22:BA:2033:A:P | 58:BA:3478:HOH:O | 2.57 | 0.62 |
| 22:BA:2128:G:H2' | 22:BA:2129:C:O4' | 1.98 | 0.62 |
| 24:BC:70:ASN:O | 24:BC:71:LYS:C | 2.37 | 0.62 |
| 2:CB:96:TRP:CE2 | 2:CB:172:ALA:HB2 | 2.33 | 0.62 |
| 52:D4:36:ARG:HG2 | 52:D4:37:GLN:N | 2.14 | 0.62 |
| 9:AI:43:THR:O | 9:AI:44:ALA:HB3 | 1.99 | 0.62 |
| 22:BA:70:G:H4' | 22:BA:71:A:OP1 | 1.98 | 0.62 |
| 22:BA:245:G:O6 | 51:B3:8:ARG:HD3 | 1.99 | 0.62 |
| 22:BA:324:A:N6 | 22:BA:338:G:O2' | 2.32 | 0.62 |
| 22:BA:1176:U:C4 | 22:BA:1177:G:O6 | 2.53 | 0.62 |
| 32:BK:78:ARG:NH1 | 37:BP:71:GLU:OE2 | 2.31 | 0.62 |
| 12:CL:21:VAL:N | 12:CL:22:PRO:HD3 | 2.14 | 0.62 |
| 22:DA:287:G:C2 | 22:DA:354:A:C2 | 2.87 | 0.62 |
| 22:DA:2271:G:O6 | 58:DA:3508:HOH:O | 2.10 | 0.62 |
| 22:DA:2854:G:C2 | 22:DA:2864:G:C2 | 2.86 | 0.62 |
| 39:DR:49:ILE:HG22 | 39:DR:54:VAL:N | 2.14 | 0.62 |
| 30:BI:117:MET:HE3 | 30:BI:129:ILE:HD11 | 1.81 | 0.62 |
| 1:CA:790:A:C6 | 1:CA:791:G:C6 | 2.87 | 0.62 |
| 1:CA:801:U:H2' | 1:CA:802:A:C8 | 2.34 | 0.62 |
| 18:CR:24:LYS:O | 18:CR:26:ILE:N | 2.31 | 0.62 |
| 21:CU:21:ARG:N | 21:CU:21:ARG:HD3 | 2.13 | 0.62 |
| 22:DA:503:A:C2 | 22:DA:506:G:C4 | 2.88 | 0.62 |
| 22:DA:1875:G:C2' | 22:DA:1876:A:OP2 | 2.46 | 0.62 |
| 4:AD:84:GLY:O | 4:AD:89:ASN:ND2 | 2.33 | 0.62 |
| 22:BA:1816:C:C5 | 24:BC:62:TYR:CE1 | 2.87 | 0.62 |
| 2:CB:167:ASP:O | 2:CB:168:HIS:CB | 2.46 | 0.62 |
| 22:BA:2190:G:C6 | 22:BA:2191:A:C5 | 2.87 | 0.62 |
| 22:BA:2846:G:OP2 | 37:BP:52:ASN:HB2 | 1.99 | 0.62 |
| 26:BE:149:ILE:HD11 | 26:BE:172:ALA:HA | 1.81 | 0.62 |
| 27:BF:2:ALA:O | 27:BF:3:LYS:C | 2.38 | 0.62 |
| 1:CA:992:U:C4 | 1:CA:1043:G:C8 | 2.87 | 0.62 |
| 3:CC:168:TYR:OH | 5:CE:55:GLU:OE1 | 2.16 | 0.62 |
| 22:DA:1088:A:N6 | 30:DI:135:SER:OG | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1378:A:C2' | 22:DA:1380:G:N7 | 2.62 | 0.62 |
| 22:DA:1973:G:C5 | 22:DA:1974:C:C5 | 2.88 | 0.62 |
| 22:DA:1993:U:H4' | 25:DD:133:THR:HG22 | 1.80 | 0.62 |
| 1:AA:1539:C:H5'' | 21:AU:18:ARG:CG | 2.30 | 0.62 |
| 20:AT:58:VAL:CG1 | 20:AT:72:ALA:HB1 | 2.30 | 0.62 |
| 22:BA:871:U:H2' | 22:BA:872:U:C6 | 2.35 | 0.62 |
| 22:BA:1178:C:H2' | 22:BA:1179:G:N7 | 2.14 | 0.62 |
| 22:BA:2503:A:N3 | 22:BA:2503:A:H5' | 2.14 | 0.62 |
| 1:CA:920:U:H2' | 1:CA:921:U:C6 | 2.34 | 0.62 |
| 1:CA:1092:A:C6 | 1:CA:1183:U:O2 | 2.53 | 0.62 |
| 22:DA:990:A:N1 | 39:DR:78:ARG:NH1 | 2.48 | 0.62 |
| 22:DA:2467:C:N4 | 22:DA:2468:A:C6 | 2.68 | 0.62 |
| 25:DD:35:THR:O | 25:DD:36:GLN:CB | 2.47 | 0.62 |
| 5:AE:81:LEU:HA | 5:AE:147:MET:HE1 | 1.80 | 0.62 |
| 7:AG:120:LEU:HD13 | 7:AG:124:LEU:HD23 | 1.82 | 0.62 |
| 22:BA:265:A:N1 | 22:BA:427:U:O2' | 2.28 | 0.62 |
| 22:BA:572:A:H5'' | 22:BA:573:U:OP2 | 1.99 | 0.62 |
| 22:BA:1277:G:H5' | 35:BN:20:MET:CE | 2.30 | 0.62 |
| 22:BA:1528:A:H2' | 22:BA:1529:G:O4' | 2.00 | 0.62 |
| 23:BB:33:G:O2' | 23:BB:34:A:H5' | 2.00 | 0.62 |
| 24:BC:252:THR:O | 24:BC:253:LYS:C | 2.38 | 0.62 |
| 14:CN:52:PRO:O | 14:CN:53:ARG:CB | 2.47 | 0.62 |
| 22:DA:196:A:O2' | 22:DA:805:G:O6 | 2.08 | 0.62 |
| 22:DA:858:G:C4 | 22:DA:2268:A:C2 | 2.87 | 0.62 |
| 22:DA:998:C:OP2 | 38:DQ:58:ARG:NH2 | 2.33 | 0.62 |
| 22:DA:1300:G:O6 | 22:DA:1626:A:O2' | 2.18 | 0.62 |
| 22:DA:1844:C:O3' | 24:DC:256:LYS:NZ | 2.32 | 0.62 |
| 22:DA:2262:U:OP1 | 44:DW:41:ARG:NH2 | 2.33 | 0.62 |
| 53:B5:174:ALA:O | 53:B5:175:PRO:CB | 2.47 | 0.62 |
| 22:DA:608:A:H2' | 22:DA:609:A:C8 | 2.35 | 0.62 |
| 22:DA:674:G:H1' | 26:DE:69:ARG:NE | 2.15 | 0.62 |
| 22:DA:1187:G:H5'' | 39:DR:83:TYR:CE2 | 2.35 | 0.62 |
| 22:DA:1444:G:C2 | 22:DA:1548:A:C2 | 2.88 | 0.62 |
| 22:DA:1465:G:C5 | 22:DA:1466:U:C4 | 2.88 | 0.62 |
| 22:DA:1649:G:C6 | 22:DA:2009:A:C6 | 2.87 | 0.62 |
| 1:AA:995:C:N3 | 1:AA:1046:A:O2' | 2.31 | 0.62 |
| 11:AK:125:LYS:O | 11:AK:126:LYS:O | 2.18 | 0.62 |
| 22:BA:1923:U:O2' | 22:BA:1924:C:C5' | 2.48 | 0.62 |
| 48:B0:33:THR:HG22 | 48:B0:33:THR:O | 2.00 | 0.62 |
| 1:CA:1007:U:H2' | 1:CA:1008:U:C5' | 2.28 | 0.62 |
| 2:CB:219:ALA:O | 2:CB:220:THR:HB | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:53:A:N7 | 22:DA:54:G:C4 | 2.68 | 0.62 |
| 22:DA:590:A:C6 | 22:DA:591:U:C4 | 2.88 | 0.62 |
| 22:DA:2408:U:O4 | 58:DA:3559:HOH:O | 2.14 | 0.62 |
| 22:DA:2531:A:H5' | 28:DG:157:TYR:CZ | 2.35 | 0.62 |
| 4:AD:99:ASP:OD2 | 4:AD:115:ARG:NH2 | 2.33 | 0.62 |
| 7:AG:56:LYS:O | 7:AG:57:SER:CB | 2.47 | 0.62 |
| 11:AK:13:ARG:N | 22:BA:2141:G:H4' | 2.13 | 0.62 |
| 22:BA:1188:U:C2' | 22:BA:1189:A:H5' | 2.30 | 0.62 |
| 22:BA:2547:A:H2' | 22:BA:2548:U:C6 | 2.34 | 0.62 |
| 33:BL:68:SER:O | 33:BL:69:ARG:HB2 | 2.00 | 0.62 |
| 1:CA:38:G:C2 | 1:CA:397:A:C2 | 2.88 | 0.62 |
| 4:CD:59:GLN:OE1 | 4:CD:59:GLN:HA | 2.00 | 0.62 |
| 22:DA:1806:C:C5 | 22:DA:1807:G:N7 | 2.68 | 0.62 |
| 52:D4:22:VAL:O | 52:D4:24:ARG:N | 2.33 | 0.62 |
| 22:BA:555:G:O2' | 22:BA:556:A:OP2 | 2.16 | 0.61 |
| 22:BA:1433:A:O2' | 22:BA:1434:A:H5' | 2.00 | 0.61 |
| 22:BA:1605:C:C2' | 22:BA:1606:C:H5' | 2.30 | 0.61 |
| 22:BA:1731:G:C6 | 22:BA:1733:G:C5 | 2.88 | 0.61 |
| 1:CA:692:U:O2' | 1:CA:694:A:N7 | 2.29 | 0.61 |
| 21:CU:8:GLU:HB3 | 21:CU:12:PHE:CD2 | 2.35 | 0.61 |
| 22:DA:300:A:O2' | 22:DA:318:C:O2' | 2.07 | 0.61 |
| 29:DH:32:PRO:O | 29:DH:33:GLN:CB | 2.48 | 0.61 |
| 1:AA:1157:A:N7 | 1:AA:1180:A:N6 | 2.47 | 0.61 |
| 1:AA:1161:C:H2' | 1:AA:1162:C:C6 | 2.35 | 0.61 |
| 1:AA:1278:G:H4' | 1:AA:1279:G:C8 | 2.35 | 0.61 |
| 16:AP:22:ALA:HA | 16:AP:33:ILE:HG13 | 1.80 | 0.61 |
| 22:BA:528:A:H2 | 22:BA:2043:C:H5' | 1.65 | 0.61 |
| 1:CA:527:G:C6 | 1:CA:528:C:C5 | 2.88 | 0.61 |
| 1:CA:801:U:C2 | 1:CA:802:A:C8 | 2.88 | 0.61 |
| 21:CU:12:PHE:O | 21:CU:13:ASP:HB2 | 2.00 | 0.61 |
| 22:DA:629:G:N3 | 22:DA:639:U:O2' | 2.32 | 0.61 |
| 22:DA:699:A:N6 | 22:DA:733:G:O2' | 2.33 | 0.61 |
| 23:DB:7:G:H5' | 36:DO:29:HIS:CE1 | 2.35 | 0.61 |
| 1:AA:627:G:OP1 | 16:AP:51:ARG:NH2 | 2.33 | 0.61 |
| 22:BA:1327:A:N6 | 22:BA:1328:A:C2 | 2.68 | 0.61 |
| 25:BD:140:HIS:CE1 | 58:BD:303:HOH:O | 2.44 | 0.61 |
| 1:CA:577:G:C8 | 1:CA:816:A:C6 | 2.87 | 0.61 |
| 1:CA:582:C:N3 | 1:CA:760:G:C6 | 2.68 | 0.61 |
| 4:CD:30:THR:C | 4:CD:31:LYS:HD3 | 2.21 | 0.61 |
| 15:CO:42:HIS:O | 15:CO:45:GLU:O | 2.18 | 0.61 |
| 22:DA:450:G:N1 | 22:DA:454:A:OP2 | 2.28 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:776:G:N7 | 22:DA:793:A:C4 | 2.68 | 0.61 |
| 22:DA:1360:G:C2 | 22:DA:1361:G:H1' | 2.35 | 0.61 |
| 22:DA:2142:A:C2 | 22:DA:2150:C:N3 | 2.69 | 0.61 |
| 22:DA:2162:G:C4' | 22:DA:2163:A:OP1 | 2.48 | 0.61 |
| 42:DU:53:ASN:O | 42:DU:53:ASN:ND2 | 2.33 | 0.61 |
| 1:AA:71:A:O2' | 1:AA:72:A:P | 2.58 | 0.61 |
| 11:AK:16:VAL:O | 11:AK:17:SER:OG | 2.16 | 0.61 |
| 22:BA:1232:G:C5 | 22:BA:1233:C:C5 | 2.88 | 0.61 |
| 53:B5:180:SER:CB | 53:B5:188:ASP:CB | 2.79 | 0.61 |
| 21:CU:37:PHE:CD2 | 21:CU:41:PRO:HG3 | 2.36 | 0.61 |
| 22:DA:30:G:O2' | 22:DA:1214:A:N3 | 2.33 | 0.61 |
| 25:DD:151:THR:O | 25:DD:152:PRO:C | 2.38 | 0.61 |
| 30:DI:114:ALA:O | 30:DI:115:ALA:CB | 2.48 | 0.61 |
| 38:DQ:25:TYR:CD2 | 38:DQ:26:GLY:N | 2.67 | 0.61 |
| 22:BA:1779:U:H5 | 22:BA:1784:A:N7 | 1.99 | 0.61 |
| 25:BD:62:LYS:HB2 | 25:BD:63:PRO:HD3 | 1.82 | 0.61 |
| 34:BM:69:PRO:O | 34:BM:70:ASP:CG | 2.39 | 0.61 |
| 35:BN:79:LEU:O | 35:BN:80:PHE:HB2 | 2.01 | 0.61 |
| 40:BS:29:VAL:HG13 | 40:BS:55:ILE:HD11 | 1.82 | 0.61 |
| 53:B5:68:GLY:O | 53:B5:70:GLY:N | 2.33 | 0.61 |
| 2:CB:15:HIS:O | 2:CB:17:GLY:N | 2.34 | 0.61 |
| 4:CD:4:TYR:O | 4:CD:5:LEU:HB2 | 1.99 | 0.61 |
| 4:CD:34:ILE:O | 4:CD:35:GLU:CB | 2.48 | 0.61 |
| 5:CE:154:ALA:HA | 5:CE:157:ARG:HB3 | 1.82 | 0.61 |
| 2:AB:187:VAL:HG23 | 2:AB:187:VAL:O | 2.01 | 0.61 |
| 22:BA:18:U:OP1 | 38:BQ:30:ARG:NH2 | 2.33 | 0.61 |
| 23:BB:60:C:N4 | 58:BB:303:HOH:O | 2.33 | 0.61 |
| 30:BI:62:TYR:O | 30:BI:63:ALA:CB | 2.49 | 0.61 |
| 53:B5:50:ILE:O | 53:B5:203:GLU:CB | 2.48 | 0.61 |
| 1:CA:1211:U:C2' | 1:CA:1212:U:OP2 | 2.49 | 0.61 |
| 4:CD:35:GLU:O | 4:CD:38:PRO:HD3 | 2.00 | 0.61 |
| 22:DA:26:G:C6 | 22:DA:27:G:N1 | 2.69 | 0.61 |
| 22:DA:1096:A:H2' | 22:DA:1097:U:O4' | 2.00 | 0.61 |
| 22:DA:1359:A:C8 | 22:DA:1373:A:N1 | 2.68 | 0.61 |
| 22:DA:1951:U:H2' | 22:DA:1953:A:OP2 | 2.01 | 0.61 |
| 23:DB:37:C:C5 | 23:DB:38:C:C5 | 2.88 | 0.61 |
| 24:DC:108:LYS:N | 24:DC:194:GLU:O | 2.33 | 0.61 |
| 29:DH:83:LYS:H | 29:DH:149:GLU:HG2 | 1.64 | 0.61 |
| 31:DJ:77:HIS:HA | 31:DJ:83:GLY:O | 2.00 | 0.61 |
| 1:AA:64:G:C8 | 1:AA:99:C:N4 | 2.68 | 0.61 |
| 1:AA:807:A:C5 | 1:AA:808:C:C5 | 2.88 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:AD:70:ARG:O | 4:AD:74:ASN:ND2 | 2.34 | 0.61 |
| 17:AQ:53:CYS:SG | 17:AQ:75:LEU:HD23 | 2.41 | 0.61 |
| 22:BA:482:A:H5'' | 22:BA:483:A:OP1 | 2.01 | 0.61 |
| 22:BA:588:U:H2' | 22:BA:589:U:C6 | 2.35 | 0.61 |
| 22:BA:1429:G:O2' | 22:BA:1430:G:H5' | 2.00 | 0.61 |
| 22:BA:2897:U:H2' | 22:BA:2898:U:C6 | 2.35 | 0.61 |
| 31:BJ:31:GLU:HG3 | 31:BJ:142:ILE:HD11 | 1.82 | 0.61 |
| 38:BQ:76:TYR:OH | 38:BQ:92:ARG:NH1 | 2.33 | 0.61 |
| 43:BV:80:HIS:CE1 | 43:BV:83:LYS:CG | 2.83 | 0.61 |
| 1:CA:994:A:N3 | 1:CA:994:A:H2' | 2.15 | 0.61 |
| 3:CC:139:GLN:O | 3:CC:141:ALA:N | 2.34 | 0.61 |
| 4:CD:166:GLU:O | 4:CD:167:LYS:HB2 | 1.99 | 0.61 |
| 22:DA:53:A:C8 | 22:DA:54:G:C8 | 2.89 | 0.61 |
| 22:DA:126:A:N7 | 22:DA:127:A:C2 | 2.69 | 0.61 |
| 22:DA:511:U:H5'' | 22:DA:1235:G:H4' | 1.83 | 0.61 |
| 22:DA:864:G:C6 | 22:DA:865:C:N4 | 2.69 | 0.61 |
| 22:DA:1827:U:C2' | 22:DA:1828:G:O5' | 2.48 | 0.61 |
| 22:DA:2418:A:OP1 | 51:D3:45:ARG:NH1 | 2.34 | 0.61 |
| 22:DA:2725:A:C4 | 22:DA:2727:A:C8 | 2.88 | 0.61 |
| 22:DA:2744:G:C6 | 22:DA:2761:A:N6 | 2.69 | 0.61 |
| 30:DI:6:GLN:O | 30:DI:7:ALA:CB | 2.49 | 0.61 |
| 1:AA:1446:A:H2' | 1:AA:1447:A:H5' | 1.83 | 0.61 |
| 15:AO:2:SER:O | 15:AO:3:LEU:CB | 2.48 | 0.61 |
| 22:BA:142:A:H2' | 22:BA:143:C:C6 | 2.36 | 0.61 |
| 22:BA:1590:A:H2' | 22:BA:1591:A:C8 | 2.35 | 0.61 |
| 2:CB:21:ARG:HA | 2:CB:21:ARG:NH1 | 2.15 | 0.61 |
| 12:CL:88:LYS:HG3 | 12:CL:88:LYS:O | 2.01 | 0.61 |
| 22:DA:104:A:N7 | 22:DA:105:C:C4 | 2.69 | 0.61 |
| 22:DA:192:C:C5 | 22:DA:193:U:C2 | 2.88 | 0.61 |
| 22:DA:684:G:OP1 | 50:D2:16:HIS:ND1 | 2.34 | 0.61 |
| 22:DA:740:C:H5' | 22:DA:1784:A:H3' | 1.82 | 0.61 |
| 22:DA:2061:G:H2' | 22:DA:2501:C:O2' | 2.00 | 0.61 |
| 22:DA:2788:C:H2' | 22:DA:2789:C:C6 | 2.35 | 0.61 |
| 1:AA:232:G:H2' | 1:AA:233:C:O4' | 2.01 | 0.61 |
| 1:AA:1492:A:O2' | 22:BA:1913:A:N1 | 2.31 | 0.61 |
| 1:AA:1528:U:O3' | 1:AA:1529:G:H3' | 2.01 | 0.61 |
| 9:AI:23:PRO:HA | 9:AI:61:LEU:HA | 1.82 | 0.61 |
| 22:BA:1250:G:C5' | 38:BQ:6:ARG:HD3 | 2.30 | 0.61 |
| 14:CN:61:ARG:O | 14:CN:62:ASN:HB2 | 2.00 | 0.61 |
| 22:DA:67:U:C2 | 22:DA:68:G:C8 | 2.89 | 0.61 |
| 22:DA:353:C:H2' | 22:DA:354:A:C8 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:724:U:H2' | 22:DA:725:G:O4' | 2.01 | 0.61 |
| 22:DA:2330:G:N2 | 22:DA:2386:A:C2 | 2.68 | 0.61 |
| 32:DK:107:LEU:O | 32:DK:109:SER:N | 2.34 | 0.61 |
| 35:DN:1:MET:H1 | 35:DN:1:MET:CE | 2.13 | 0.61 |
| 1:AA:887:G:H2' | 1:AA:888:G:H5' | 1.83 | 0.61 |
| 1:AA:1429:A:C2 | 1:AA:1430:A:C8 | 2.88 | 0.61 |
| 4:AD:174:ASP:OD2 | 4:AD:176:GLY:N | 2.34 | 0.61 |
| 22:BA:357:C:H2' | 22:BA:358:U:C6 | 2.35 | 0.61 |
| 22:BA:1936:A:C2 | 22:BA:1945:G:C8 | 2.89 | 0.61 |
| 22:BA:2502:G:H5' | 22:BA:2503:A:H5'' | 1.82 | 0.61 |
| 1:CA:72:A:N6 | 1:CA:73:C:N4 | 2.48 | 0.61 |
| 1:CA:1376:U:O4 | 7:CG:10:ARG:NH1 | 2.33 | 0.61 |
| 1:CA:1381:U:C2' | 1:CA:1382:C:O5' | 2.49 | 0.61 |
| 22:DA:54:G:C2 | 22:DA:55:G:C8 | 2.88 | 0.61 |
| 22:DA:2571:U:C4 | 22:DA:2574:G:C8 | 2.89 | 0.61 |
| 26:DE:108:ILE:HD11 | 26:DE:180:LEU:CB | 2.31 | 0.61 |
| 1:AA:1160:G:O6 | 1:AA:1181:G:C6 | 2.54 | 0.60 |
| 1:AA:1352:C:H2' | 1:AA:1353:G:C8 | 2.36 | 0.60 |
| 12:AL:24:LEU:O | 12:AL:25:GLU:C | 2.37 | 0.60 |
| 23:BB:30:C:H2' | 23:BB:31:C:H5' | 1.83 | 0.60 |
| 24:BC:230:HIS:CD2 | 24:BC:247:PRO:HA | 2.36 | 0.60 |
| 1:CA:960:U:C5 | 1:CA:1225:A:C8 | 2.89 | 0.60 |
| 1:CA:994:A:C8 | 1:CA:1216:A:H4' | 2.36 | 0.60 |
| 1:CA:1521:C:C4 | 1:CA:1522:U:C5 | 2.88 | 0.60 |
| 5:CE:133:PRO:O | 5:CE:137:VAL:HG12 | 2.00 | 0.60 |
| 7:CG:74:GLU:O | 7:CG:88:PRO:HA | 2.01 | 0.60 |
| 22:DA:38:A:H2' | 22:DA:39:G:O4' | 2.00 | 0.60 |
| 22:DA:616:A:C2 | 22:DA:617:G:O4' | 2.54 | 0.60 |
| 22:DA:2720:U:OP1 | 37:DP:53:ARG:NH2 | 2.34 | 0.60 |
| 32:DK:87:LEU:HD22 | 32:DK:92:GLU:HA | 1.82 | 0.60 |
| 39:DR:82:HIS:O | 39:DR:82:HIS:CG | 2.54 | 0.60 |
| 50:D2:44:VAL:HG13 | 50:D2:45:SER:N | 2.16 | 0.60 |
| 1:AA:108:G:N3 | 1:AA:108:G:H5' | 2.15 | 0.60 |
| 1:AA:154:U:C2 | 1:AA:168:G:N2 | 2.69 | 0.60 |
| 2:AB:49:MET:O | 2:AB:53:ALA:CB | 2.49 | 0.60 |
| 5:AE:90:THR:HG22 | 5:AE:91:GLY:N | 2.16 | 0.60 |
| 5:AE:109:GLY:O | 5:AE:110:ALA:CB | 2.49 | 0.60 |
| 22:BA:137:U:H2' | 22:BA:140:C:C2 | 2.36 | 0.60 |
| 22:BA:142:A:C5 | 22:BA:143:C:N4 | 2.69 | 0.60 |
| 29:BH:121:VAL:N | 29:BH:122:LEU:HB2 | 2.16 | 0.60 |
| 41:BT:2:ILE:CA | 41:BT:3:ARG:HB2 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:109:A:C6 | 1:CA:327:A:C6 | 2.89 | 0.60 |
| 1:CA:115:G:H4' | 1:CA:116:A:O5' | 2.01 | 0.60 |
| 1:CA:945:G:C2 | 1:CA:946:A:C8 | 2.88 | 0.60 |
| 9:CI:15:SER:OG | 9:CI:69:GLY:O | 2.12 | 0.60 |
| 12:CL:20:ASN:N | 12:CL:20:ASN:OD1 | 2.34 | 0.60 |
| 20:CT:43:ASP:HB3 | 20:CT:46:ALA:HB3 | 1.83 | 0.60 |
| 22:DA:88:G:C2 | 22:DA:89:A:C8 | 2.88 | 0.60 |
| 22:DA:187:G:C2 | 22:DA:210:C:C2 | 2.89 | 0.60 |
| 22:DA:497:A:H2' | 22:DA:498:G:O4' | 2.01 | 0.60 |
| 22:DA:1179:G:C5 | 22:DA:1180:U:H1' | 2.36 | 0.60 |
| 22:DA:2146:C:C5' | 22:DA:2147:A:OP1 | 2.49 | 0.60 |
| 30:DI:80:LEU:HD13 | 30:DI:136:MET:SD | 2.41 | 0.60 |
| 35:DN:24:MET:HE3 | 35:DN:44:LEU:HD13 | 1.83 | 0.60 |
| 1:AA:701:U:H4' | 1:AA:702:A:H5'' | 1.83 | 0.60 |
| 1:AA:1074:G:OP1 | 5:AE:69:ARG:NH2 | 2.34 | 0.60 |
| 22:BA:475:C:C4 | 22:BA:481:G:O6 | 2.55 | 0.60 |
| 26:BE:149:ILE:CD1 | 26:BE:172:ALA:HA | 2.31 | 0.60 |
| 29:BH:100:ALA:HB1 | 29:BH:112:LYS:HA | 1.83 | 0.60 |
| 5:CE:89:HIS:CE1 | 5:CE:90:THR:HG1 | 2.19 | 0.60 |
| 19:CS:66:MET:SD | 19:CS:74:PHE:CZ | 2.94 | 0.60 |
| 23:DB:4:C:C2 | 23:DB:117:G:N2 | 2.69 | 0.60 |
| 35:DN:49:GLU:N | 35:DN:50:PRO:CD | 2.65 | 0.60 |
| 1:AA:673:A:H2' | 1:AA:674:G:C8 | 2.36 | 0.60 |
| 5:AE:83:HIS:HB2 | 5:AE:84:PRO:HD2 | 1.83 | 0.60 |
| 9:AI:63:LEU:N | 9:AI:63:LEU:HD23 | 2.17 | 0.60 |
| 11:AK:16:VAL:O | 11:AK:17:SER:CB | 2.49 | 0.60 |
| 23:BB:28:C:OP1 | 36:BO:31:THR:HG21 | 2.01 | 0.60 |
| 33:BL:68:SER:O | 33:BL:69:ARG:CB | 2.50 | 0.60 |
| 35:BN:58:ASP:OD1 | 35:BN:63:ARG:NH2 | 2.35 | 0.60 |
| 38:BQ:88:VAL:HG13 | 39:BR:49:ILE:HD11 | 1.82 | 0.60 |
| 40:BS:83:LYS:O | 40:BS:84:ARG:HD3 | 2.00 | 0.60 |
| 1:CA:475:C:H2' | 1:CA:476:U:C6 | 2.36 | 0.60 |
| 1:CA:485:U:OP2 | 1:CA:485:U:H4' | 2.00 | 0.60 |
| 6:CF:98:GLU:O | 6:CF:99:ALA:HB3 | 2.00 | 0.60 |
| 22:DA:749:A:C4 | 22:DA:750:A:C8 | 2.89 | 0.60 |
| 22:DA:1355:G:H2' | 22:DA:1356:G:H5' | 1.84 | 0.60 |
| 22:DA:1735:A:N1 | 22:DA:1736:U:C2 | 2.70 | 0.60 |
| 22:DA:1868:C:N4 | 22:DA:1869:G:O6 | 2.34 | 0.60 |
| 29:DH:126:GLY:O | 29:DH:146:VAL:HG23 | 2.00 | 0.60 |
| 30:DI:58:VAL:CG1 | 30:DI:59:ILE:N | 2.63 | 0.60 |
| 2:AB:123:ASP:N | 2:AB:123:ASP:OD1 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:417:C:H2' | 22:BA:418:C:H6 | 1.66 | 0.60 |
| 22:BA:636:G:C6 | 33:BL:111:ILE:HD11 | 2.36 | 0.60 |
| 22:BA:997:G:OP1 | 38:BQ:92:ARG:CG | 2.49 | 0.60 |
| 22:BA:1916:A:C6 | 22:BA:1917:U:C2 | 2.90 | 0.60 |
| 27:BF:119:ALA:HB2 | 27:BF:177:PHE:CD2 | 2.37 | 0.60 |
| 35:BN:73:ASN:HA | 35:BN:76:VAL:CG1 | 2.31 | 0.60 |
| 1:CA:227:G:H2' | 1:CA:228:A:O4' | 2.00 | 0.60 |
| 1:CA:409:U:OP1 | 4:CD:24:GLY:HA3 | 2.00 | 0.60 |
| 1:CA:495:A:C2 | 1:CA:496:A:N6 | 2.70 | 0.60 |
| 22:DA:324:A:N6 | 22:DA:338:G:O2' | 2.33 | 0.60 |
| 22:DA:528:A:N1 | 22:DA:2043:C:O5' | 2.34 | 0.60 |
| 22:DA:846:U:O2' | 22:DA:847:U:O5' | 2.19 | 0.60 |
| 22:DA:1127:A:C2' | 22:DA:1128:G:H5'' | 2.32 | 0.60 |
| 22:DA:1390:U:H2' | 22:DA:1391:U:H5' | 1.83 | 0.60 |
| 22:DA:2058:A:C6 | 22:DA:2059:A:N6 | 2.69 | 0.60 |
| 22:DA:2133:G:H2' | 22:DA:2157:G:N2 | 2.15 | 0.60 |
| 49:D1:21:TYR:CD1 | 49:D1:38:LYS:HD2 | 2.37 | 0.60 |
| 1:AA:188:C:O2 | 1:AA:188:C:H2' | 2.01 | 0.60 |
| 1:AA:327:A:O3' | 1:AA:328:C:H4' | 2.02 | 0.60 |
| 4:AD:174:ASP:OD2 | 4:AD:177:LYS:N | 2.35 | 0.60 |
| 22:BA:2786:U:OP1 | 25:BD:70:LYS:NZ | 2.28 | 0.60 |
| 27:BF:108:VAL:HG11 | 27:BF:176:PRO:HG2 | 1.82 | 0.60 |
| 1:CA:909:A:H2' | 1:CA:910:C:O4' | 2.01 | 0.60 |
| 9:CI:19:VAL:HG21 | 9:CI:82:GLY:CA | 2.32 | 0.60 |
| 22:DA:642:U:O2' | 22:DA:644:A:N7 | 2.29 | 0.60 |
| 22:DA:826:U:O2' | 33:DL:53:GLY:HA3 | 2.02 | 0.60 |
| 22:DA:1060:U:O4' | 22:DA:1062:G:H5' | 2.02 | 0.60 |
| 22:DA:1358:G:O2' | 22:DA:1359:A:H5' | 2.02 | 0.60 |
| 22:DA:1850:G:O6 | 22:DA:1892:C:N3 | 2.35 | 0.60 |
| 25:DD:151:THR:HG22 | 25:DD:152:PRO:CD | 2.31 | 0.60 |
| 26:DE:108:ILE:HD11 | 26:DE:180:LEU:HB2 | 1.83 | 0.60 |
| 4:AD:3:ARG:NE | 4:AD:115:ARG:HD3 | 2.16 | 0.60 |
| 22:BA:790:U:O2' | 22:BA:791:C:O5' | 2.19 | 0.60 |
| 22:BA:1688:U:N3 | 22:BA:1698:A:C2 | 2.70 | 0.60 |
| 53:B5:65:LEU:HD11 | 53:B5:191:ARG:CB | 2.32 | 0.60 |
| 2:CB:210:VAL:O | 2:CB:214:LEU:HB2 | 2.00 | 0.60 |
| 22:DA:400:G:N7 | 45:DX:57:ARG:NH1 | 2.50 | 0.60 |
| 22:DA:2328:A:H2' | 22:DA:2329:U:C6 | 2.37 | 0.60 |
| 23:DB:48:U:H2' | 23:DB:49:C:C6 | 2.37 | 0.60 |
| 22:BA:1078:U:H1' | 22:BA:1088:A:C2 | 2.37 | 0.60 |
| 22:BA:1132:U:H3' | 22:BA:1133:A:H5'' | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 22:BA:1269:A:OP2 | 58:BA:3385:HOH:O | 2.16 | 0.60 |
| 22:BA:1866:A:N1 | 22:BA:1876:A:C8 | 2.70 | 0.60 |
| 22:BA:2683:C:OP1 | 37:BP:51:ARG:NH2 | 2.34 | 0.60 |
| 29:BH:117:LEU:CD2 | 29:BH:121:VAL:HA | 2.31 | 0.60 |
| 33:BL:61:LEU:O | 51:B3:13:ARG:HD3 | 2.02 | 0.60 |
| 36:BO:53:THR:HB | 36:BO:65:THR:HG22 | 1.84 | 0.60 |
| 43:BV:13:GLY:O | 43:BV:17:SER:OG | 2.19 | 0.60 |
| 1:CA:1007:U:H2' | 1:CA:1008:U:H5' | 1.82 | 0.60 |
| 22:DA:39:G:C6 | 22:DA:40:U:C4 | 2.90 | 0.60 |
| 22:DA:271:G:C2 | 22:DA:367:G:C2 | 2.90 | 0.60 |
| 22:DA:363:G:H2' | 22:DA:364:C:C6 | 2.36 | 0.60 |
| 22:DA:2074:U:H2' | 22:DA:2075:U:C6 | 2.36 | 0.60 |
| 1:AA:495:A:C2 | 1:AA:496:A:N6 | 2.69 | 0.60 |
| 4:AD:68:LEU:HD22 | 4:AD:68:LEU:N | 2.17 | 0.60 |
| 22:BA:1179:G:C6 | 22:BA:1180:U:C2 | 2.90 | 0.60 |
| 22:BA:2094:A:C2 | 22:BA:2196:C:C2 | 2.90 | 0.60 |
| 22:BA:2187:U:H2' | 22:BA:2188:U:C1' | 2.32 | 0.60 |
| 22:BA:2318:G:C6 | 22:BA:2319:G:N1 | 2.70 | 0.60 |
| 26:BE:108:ILE:HD11 | 26:BE:180:LEU:HB3 | 1.84 | 0.60 |
| 27:BF:83:TYR:O | 27:BF:85:ILE:HG22 | 2.02 | 0.60 |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:H | 1.65 | 0.60 |
| 53:B5:56:ASP:OD2 | 53:B5:58:ASN:ND2 | 2.34 | 0.60 |
| 1:CA:73:C:C2 | 1:CA:74:A:C8 | 2.90 | 0.60 |
| 1:CA:1296:C:H4' | 1:CA:1302:C:N4 | 2.17 | 0.60 |
| 5:CE:56:VAL:N | 5:CE:57:PRO:HD2 | 2.17 | 0.60 |
| 5:CE:157:ARG:HD3 | 5:CE:158:GLY:N | 2.17 | 0.60 |
| 22:DA:269:C:O2 | 22:DA:269:C:H2' | 2.02 | 0.60 |
| 22:DA:680:C:H2' | 22:DA:681:G:C8 | 2.37 | 0.60 |
| 22:DA:1582:C:O2' | 22:DA:1585:C:N3 | 2.33 | 0.60 |
| 56:DA:3001:DOL:H483 | 56:DA:3001:DOL:C46 | 2.24 | 0.60 |
| 1:AA:859:G:H2' | 1:AA:860:A:C8 | 2.36 | 0.60 |
| 1:AA:1378:C:C5 | 1:AA:1379:G:C8 | 2.90 | 0.60 |
| 9:AI:114:LYS:HG2 | 9:AI:120:LYS:HA | 1.82 | 0.60 |
| 22:BA:1916:A:P | 22:BA:1917:U:OP2 | 2.60 | 0.60 |
| 30:BI:39:CYS:HA | 30:BI:42:PHE:HB3 | 1.83 | 0.60 |
| 1:CA:949:A:C2 | 1:CA:1233:G:N3 | 2.70 | 0.60 |
| 1:CA:992:U:C4 | 1:CA:1043:G:N7 | 2.70 | 0.60 |
| 5:CE:106:ILE:HD11 | 5:CE:124:LEU:HD23 | 1.83 | 0.60 |
| 11:CK:126:LYS:O | 11:CK:127:ARG:HB2 | 2.01 | 0.60 |
| 22:DA:1351:C:H2' | 22:DA:1352:U:O4' | 2.01 | 0.60 |
| 22:DA:1709:U:H2' | 22:DA:1710:G:C8 | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DB:29:A:H2' | 23:DB:30:C:C6 | 2.37 | 0.60 |
| 26:DE:149:ILE:HD12 | 26:DE:172:ALA:HA | 1.83 | 0.60 |
| 1:AA:1491:G:H2' | 1:AA:1492:A:O4' | 2.01 | 0.59 |
| 14:AN:41:ARG:O | 14:AN:43:ASN:N | 2.35 | 0.59 |
| 19:AS:64:ASP:O | 19:AS:65:GLU:HB3 | 2.02 | 0.59 |
| 22:BA:1735:A:C2 | 22:BA:1736:U:C1' | 2.85 | 0.59 |
| 24:BC:204:VAL:O | 24:BC:205:LEU:HB2 | 2.01 | 0.59 |
| 31:BJ:30:THR:HG22 | 31:BJ:31:GLU:N | 2.17 | 0.59 |
| 1:CA:734:G:N3 | 1:CA:735:C:C6 | 2.70 | 0.59 |
| 1:CA:1201:A:H4' | 1:CA:1202:U:O5' | 2.01 | 0.59 |
| 5:CE:78:ASN:OD1 | 5:CE:79:GLY:N | 2.35 | 0.59 |
| 9:CI:120:LYS:HG3 | 9:CI:123:ARG:HB3 | 1.82 | 0.59 |
| 22:DA:120:U:H1' | 22:DA:149:A:C8 | 2.37 | 0.59 |
| 22:DA:1369:G:C2 | 22:DA:1370:C:C6 | 2.90 | 0.59 |
| 22:DA:2757:A:N1 | 28:DG:67:THR:HG21 | 2.17 | 0.59 |
| 22:BA:28:A:C4 | 22:BA:29:U:C6 | 2.89 | 0.59 |
| 22:BA:350:G:H2' | 22:BA:351:C:O4' | 2.02 | 0.59 |
| 22:BA:2418:A:C5 | 22:BA:2419:U:C5 | 2.89 | 0.59 |
| 27:BF:158:THR:O | 58:BF:201:HOH:O | 2.17 | 0.59 |
| 1:CA:66:A:C6 | 1:CA:67:C:C5 | 2.90 | 0.59 |
| 1:CA:1167:A:N7 | 1:CA:1169:A:C5 | 2.70 | 0.59 |
| 1:CA:1190:G:H5' | 3:CC:176:HIS:CE1 | 2.37 | 0.59 |
| 1:CA:1365:G:H2' | 1:CA:1366:C:O4' | 2.02 | 0.59 |
| 3:CC:42:TYR:CE1 | 3:CC:90:VAL:HG21 | 2.36 | 0.59 |
| 21:CU:47:ARG:HA | 21:CU:47:ARG:HE | 1.66 | 0.59 |
| 22:DA:1668:A:O4' | 22:DA:1669:A:C2 | 2.55 | 0.59 |
| 22:DA:2889:C:N4 | 22:DA:2890:G:C6 | 2.70 | 0.59 |
| 24:DC:9:THR:O | 24:DC:10:SER:CB | 2.49 | 0.59 |
| 22:BA:1922:G:N2 | 22:BA:1923:U:C1' | 2.65 | 0.59 |
| 27:BF:132:VAL:HG22 | 27:BF:152:LEU:HB3 | 1.83 | 0.59 |
| 28:BG:60:ASP:OD2 | 58:BG:201:HOH:O | 2.17 | 0.59 |
| 29:BH:94:ILE:HG22 | 29:BH:99:ILE:CG1 | 2.32 | 0.59 |
| 29:BH:123:ARG:HH22 | 1:CA:367:U:P | 2.25 | 0.59 |
| 39:BR:51:VAL:HG23 | 39:BR:52:PRO:HD2 | 1.84 | 0.59 |
| 43:BV:48:MET:SD | 43:BV:86:LEU:HD12 | 2.43 | 0.59 |
| 53:B5:99:GLU:O | 53:B5:103:LYS:CB | 2.51 | 0.59 |
| 1:CA:1089:G:C5 | 1:CA:1090:U:C5 | 2.91 | 0.59 |
| 22:DA:362:A:C4 | 22:DA:363:G:C8 | 2.90 | 0.59 |
| 22:DA:777:G:N7 | 22:DA:793:A:H2 | 1.99 | 0.59 |
| 22:DA:1395:A:O2' | 22:DA:1397:U:C6 | 2.54 | 0.59 |
| 22:DA:1790:C:O2' | 24:DC:208:ALA:HB2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2079:U:H2' | 22:DA:2080:A:O4' | 2.01 | 0.59 |
| 22:DA:2815:C:O2' | 48:D0:41:HIS:ND1 | 2.35 | 0.59 |
| 5:AE:45:ARG:HG2 | 5:AE:73:ASN:HB3 | 1.84 | 0.59 |
| 9:AI:45:ARG:HG2 | 9:AI:46:MET:SD | 2.43 | 0.59 |
| 22:BA:746:U:O2' | 54:B6:8:MHT:H8A | 2.02 | 0.59 |
| 22:BA:1131:G:OP1 | 31:BJ:82:GLY:HA2 | 2.02 | 0.59 |
| 24:BC:91:ILE:HD12 | 24:BC:103:TYR:CD1 | 2.37 | 0.59 |
| 29:BH:99:ILE:HB | 29:BH:115:VAL:HG11 | 1.84 | 0.59 |
| 1:CA:388:G:O2' | 1:CA:389:A:OP1 | 2.17 | 0.59 |
| 1:CA:1141:C:O2' | 1:CA:1142:G:O5' | 2.19 | 0.59 |
| 2:CB:93:ASN:OD1 | 2:CB:94:HIS:N | 2.36 | 0.59 |
| 2:CB:184:PHE:CE1 | 2:CB:198:PHE:CD2 | 2.91 | 0.59 |
| 11:CK:23:ILE:HG21 | 11:CK:96:THR:HG21 | 1.84 | 0.59 |
| 17:CQ:48:ASP:N | 17:CQ:48:ASP:OD2 | 2.35 | 0.59 |
| 21:CU:8:GLU:HB3 | 21:CU:12:PHE:CE2 | 2.38 | 0.59 |
| 22:DA:118:A:N7 | 22:DA:119:A:C8 | 2.70 | 0.59 |
| 41:DT:89:GLU:O | 41:DT:91:GLN:N | 2.35 | 0.59 |
| 1:AA:205:A:OP1 | 1:AA:205:A:H4' | 2.01 | 0.59 |
| 22:BA:2000:C:O2' | 22:BA:2001:C:H5' | 2.03 | 0.59 |
| 29:BH:1:MET:O | 29:BH:20:ASN:ND2 | 2.35 | 0.59 |
| 53:B5:87:ALA:HB2 | 53:B5:153:ILE:CB | 2.32 | 0.59 |
| 22:DA:945:A:C8 | 22:DA:2448:A:C2 | 2.89 | 0.59 |
| 22:DA:2110:G:O2' | 22:DA:2120:G:OP2 | 2.14 | 0.59 |
| 41:DT:82:LYS:HG2 | 41:DT:83:ALA:N | 2.18 | 0.59 |
| 1:AA:131:A:O2' | 1:AA:262:A:N3 | 2.32 | 0.59 |
| 1:AA:1211:U:HO2' | 1:AA:1212:U:P | 2.24 | 0.59 |
| 1:AA:1306:A:C4 | 1:AA:1307:U:C6 | 2.91 | 0.59 |
| 2:AB:49:MET:O | 2:AB:53:ALA:HB2 | 2.03 | 0.59 |
| 3:AC:25:ASN:O | 3:AC:27:LYS:N | 2.35 | 0.59 |
| 9:AI:6:TYR:HB3 | 9:AI:89:GLU:HG2 | 1.84 | 0.59 |
| 13:AM:3:ARG:O | 13:AM:4:ILE:HG12 | 2.03 | 0.59 |
| 17:AQ:6:ARG:O | 17:AQ:7:THR:HG23 | 2.02 | 0.59 |
| 22:BA:264:C:O2' | 22:BA:265:A:H2' | 2.02 | 0.59 |
| 22:BA:1952:A:C5 | 32:BK:22:ILE:HG21 | 2.37 | 0.59 |
| 48:B0:55:ILE:HG22 | 48:B0:56:ALA:N | 2.17 | 0.59 |
| 1:CA:1302:C:C5 | 13:CM:17:ILE:HD13 | 2.38 | 0.59 |
| 1:CA:1364:U:O2 | 1:CA:1364:U:H2' | 2.03 | 0.59 |
| 8:CH:18:GLN:NE2 | 8:CH:70:ALA:HB1 | 2.18 | 0.59 |
| 15:CO:53:ARG:O | 15:CO:56:LEU:N | 2.35 | 0.59 |
| 26:DE:196:VAL:O | 26:DE:196:VAL:HG12 | 2.01 | 0.59 |
| 28:DG:118:PRO:HG3 | 28:DG:144:VAL:HG21 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DY:18:LEU:O | 46:DY:22:LEU:HB3 | 2.03 | 0.59 |
| 1:AA:984:C:N4 | 58:AA:1836:HOH:O | 2.35 | 0.59 |
| 5:AE:108:GLY:O | 5:AE:109:GLY:C | 2.41 | 0.59 |
| 9:AI:57:MET:CG | 9:AI:58:VAL:H | 2.14 | 0.59 |
| 12:AL:76:GLU:O | 12:AL:77:HIS:HB2 | 2.03 | 0.59 |
| 14:AN:21:PHE:HA | 14:AN:25:ALA:CB | 2.33 | 0.59 |
| 16:AP:10:GLY:HA3 | 16:AP:15:PRO:HA | 1.83 | 0.59 |
| 22:BA:2182:U:O4 | 22:BA:2183:A:N6 | 2.36 | 0.59 |
| 22:BA:2192:U:C2' | 22:BA:2193:G:H5' | 2.32 | 0.59 |
| 26:BE:48:THR:O | 26:BE:50:ALA:N | 2.35 | 0.59 |
| 46:BY:18:LEU:O | 46:BY:22:LEU:N | 2.34 | 0.59 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:N7 | 2.71 | 0.59 |
| 2:CB:119:THR:O | 2:CB:120:GLN:HB2 | 2.01 | 0.59 |
| 6:CF:97:THR:O | 6:CF:98:GLU:HB3 | 2.03 | 0.59 |
| 7:CG:68:ASN:O | 7:CG:138:ARG:NH2 | 2.35 | 0.59 |
| 7:CG:92:ARG:HB3 | 7:CG:93:PRO:HD2 | 1.84 | 0.59 |
| 22:DA:1410:G:C2 | 22:DA:1411:U:C4 | 2.91 | 0.59 |
| 22:DA:1668:A:C4 | 22:DA:1674:G:N7 | 2.70 | 0.59 |
| 22:DA:1798:U:O2' | 22:DA:1802:A:N3 | 2.33 | 0.59 |
| 22:DA:2038:G:H2' | 22:DA:2039:U:O4' | 2.02 | 0.59 |
| 22:DA:2250:G:OP1 | 22:DA:2275:C:O2' | 2.13 | 0.59 |
| 22:DA:2293:G:H2' | 22:DA:2294:G:O4' | 2.03 | 0.59 |
| 23:DB:84:G:N2 | 23:DB:93:C:C2 | 2.70 | 0.59 |
| 29:DH:126:GLY:O | 29:DH:146:VAL:N | 2.35 | 0.59 |
| 31:DJ:105:VAL:HG12 | 31:DJ:109:LEU:HD12 | 1.84 | 0.59 |
| 1:AA:178:C:OP2 | 20:AT:60:ARG:NH2 | 2.35 | 0.59 |
| 1:AA:582:C:C2 | 1:AA:583:A:C8 | 2.91 | 0.59 |
| 1:AA:872:A:C5 | 1:AA:874:G:C8 | 2.91 | 0.59 |
| 1:AA:1377:A:C4 | 7:AG:7:ILE:HD11 | 2.38 | 0.59 |
| 11:AK:35:THR:OG1 | 11:AK:41:ALA:N | 2.35 | 0.59 |
| 22:BA:616:A:C2 | 22:BA:617:G:H1' | 2.38 | 0.59 |
| 22:BA:734:A:C5 | 22:BA:735:A:C8 | 2.90 | 0.59 |
| 22:BA:1935:G:C6 | 22:BA:1962:C:C5 | 2.91 | 0.59 |
| 22:BA:2685:G:OP1 | 32:BK:78:ARG:NH2 | 2.34 | 0.59 |
| 1:CA:803:G:C5 | 1:CA:804:U:C4 | 2.90 | 0.59 |
| 22:DA:237:C:C4 | 22:DA:238:C:C5 | 2.90 | 0.59 |
| 22:DA:583:G:C5 | 22:DA:584:C:C5 | 2.91 | 0.59 |
| 22:DA:2262:U:OP2 | 44:DW:16:SER:HB2 | 2.03 | 0.59 |
| 30:DI:58:VAL:O | 30:DI:69:PHE:HB3 | 2.03 | 0.59 |
| 1:AA:4:U:O2 | 1:AA:4:U:H2' | 2.03 | 0.59 |
| 5:AE:65:GLU:OE1 | 5:AE:66:LYS:N | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:AJ:80:THR:O | 10:AJ:83:THR:N | 2.35 | 0.59 |
| 22:BA:538:A:H5'' | 31:BJ:7:LYS:HE3 | 1.85 | 0.59 |
| 1:CA:206:C:H2' | 1:CA:207:C:H5' | 1.85 | 0.59 |
| 1:CA:1439:G:C2 | 1:CA:1463:U:O2 | 2.56 | 0.59 |
| 2:CB:54:LEU:HA | 2:CB:57:LEU:HB3 | 1.84 | 0.59 |
| 4:CD:105:MET:SD | 4:CD:143:VAL:HG13 | 2.43 | 0.59 |
| 22:DA:332:A:O2' | 22:DA:334:C:OP2 | 2.11 | 0.59 |
| 22:DA:1447:C:H2' | 22:DA:1448:G:C8 | 2.37 | 0.59 |
| 22:DA:2305:U:C4 | 22:DA:2306:C:C4 | 2.91 | 0.59 |
| 22:DA:2645:G:H3' | 22:DA:2646:C:H5' | 1.85 | 0.59 |
| 35:DN:55:ALA:HA | 35:DN:80:PHE:CE1 | 2.37 | 0.59 |
| 46:DY:56:LEU:O | 46:DY:57:LEU:HB2 | 2.03 | 0.59 |
| 1:AA:151:A:H2' | 1:AA:152:A:O4' | 2.03 | 0.59 |
| 1:AA:212:G:C2 | 1:AA:213:G:C4 | 2.90 | 0.59 |
| 30:BI:96:ASP:OD1 | 30:BI:97:LYS:N | 2.36 | 0.59 |
| 39:BR:16:GLU:OE1 | 39:BR:100:GLY:HA2 | 2.03 | 0.59 |
| 42:BU:12:ILE:HG21 | 42:BU:80:ALA:HB2 | 1.85 | 0.59 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:C8 | 2.38 | 0.59 |
| 3:CC:77:ILE:HA | 3:CC:84:VAL:CG2 | 2.33 | 0.59 |
| 14:CN:52:PRO:O | 14:CN:53:ARG:HB3 | 2.03 | 0.59 |
| 20:CT:55:GLN:N | 20:CT:56:PRO:CD | 2.65 | 0.59 |
| 22:DA:82:U:C2 | 22:DA:83:A:C8 | 2.90 | 0.59 |
| 22:DA:1203:U:H1' | 33:DL:4:ASN:HB3 | 1.85 | 0.59 |
| 39:DR:38:VAL:HG11 | 39:DR:57:GLY:HA3 | 1.83 | 0.59 |
| 1:AA:69:G:O6 | 1:AA:98:A:N6 | 2.36 | 0.58 |
| 1:AA:90:C:C2 | 1:AA:91:U:C6 | 2.91 | 0.58 |
| 1:AA:1134:G:C2 | 1:AA:1135:U:C2 | 2.89 | 0.58 |
| 22:BA:1008:A:N6 | 22:BA:1136:G:C6 | 2.71 | 0.58 |
| 22:BA:1935:G:C6 | 22:BA:1962:C:C6 | 2.91 | 0.58 |
| 1:CA:243:A:H4' | 1:CA:244:U:H5'' | 1.83 | 0.58 |
| 2:CB:141:LEU:O | 2:CB:145:GLU:N | 2.34 | 0.58 |
| 22:DA:841:G:N2 | 22:DA:937:C:O2 | 2.32 | 0.58 |
| 22:DA:1439:A:N7 | 22:DA:1552:A:C2 | 2.71 | 0.58 |
| 22:DA:2189:U:H2' | 22:DA:2190:G:H5' | 1.84 | 0.58 |
| 22:DA:2845:U:H2' | 22:DA:2846:G:O4' | 2.03 | 0.58 |
| 30:DI:76:ALA:CB | 30:DI:129:ILE:HG23 | 2.33 | 0.58 |
| 1:AA:701:U:H4' | 1:AA:702:A:C5' | 2.33 | 0.58 |
| 2:AB:222:ARG:HB3 | 2:AB:222:ARG:CZ | 2.34 | 0.58 |
| 8:AH:111:MET:HE1 | 8:AH:116:ALA:HA | 1.84 | 0.58 |
| 24:BC:117:GLN:N | 24:BC:128:ASN:OD1 | 2.35 | 0.58 |
| 46:BY:45:GLN:O | 46:BY:46:VAL:HB | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:B5:50:ILE:HB | 53:B5:52:PRO:HD3 | 1.85 | 0.58 |
| 22:DA:85:G:OP2 | 42:DU:28:VAL:HG12 | 2.03 | 0.58 |
| 23:DB:22:U:O4 | 58:DB:302:HOH:O | 2.15 | 0.58 |
| 2:AB:200:ILE:O | 2:AB:201:PRO:O | 2.21 | 0.58 |
| 4:AD:58:LYS:NZ | 4:AD:69:GLU:OE2 | 2.32 | 0.58 |
| 7:AG:13:LEU:O | 7:AG:15:ASP:N | 2.37 | 0.58 |
| 10:AJ:48:ARG:NH1 | 10:AJ:66:GLU:OE1 | 2.35 | 0.58 |
| 13:AM:10:PRO:O | 13:AM:11:ASP:HB3 | 2.04 | 0.58 |
| 16:AP:51:ARG:HG2 | 16:AP:51:ARG:HH11 | 1.67 | 0.58 |
| 17:AQ:12:VAL:O | 17:AQ:13:VAL:HG12 | 2.03 | 0.58 |
| 22:BA:1355:G:O2' | 22:BA:1356:G:H5' | 2.03 | 0.58 |
| 27:BF:174:ASP:O | 27:BF:175:PHE:O | 2.21 | 0.58 |
| 39:BR:52:PRO:O | 39:BR:53:PHE:O | 2.21 | 0.58 |
| 1:CA:1245:C:C4 | 1:CA:1246:A:N7 | 2.71 | 0.58 |
| 2:CB:15:HIS:O | 2:CB:15:HIS:CG | 2.55 | 0.58 |
| 22:DA:1068:G:H2' | 22:DA:1068:G:N3 | 2.17 | 0.58 |
| 22:DA:1544:A:N1 | 22:DA:1545:A:C2 | 2.71 | 0.58 |
| 22:DA:1605:C:H2' | 22:DA:1606:C:H5' | 1.85 | 0.58 |
| 22:DA:1808:A:N1 | 45:DX:28:ARG:HD2 | 2.17 | 0.58 |
| 24:DC:34:LEU:O | 24:DC:35:GLU:HB3 | 2.03 | 0.58 |
| 32:DK:18:ARG:HB2 | 32:DK:45:GLU:HB3 | 1.84 | 0.58 |
| 36:DO:33:ARG:O | 36:DO:34:HIS:CB | 2.50 | 0.58 |
| 21:AU:10:GLU:CG | 21:AU:11:PRO:HD3 | 2.33 | 0.58 |
| 1:CA:913:A:H4' | 1:CA:914:A:OP1 | 2.02 | 0.58 |
| 1:CA:1127:G:H5' | 1:CA:1280:A:O2' | 2.02 | 0.58 |
| 7:CG:5:ARG:NE | 7:CG:5:ARG:HA | 2.18 | 0.58 |
| 1:AA:119:A:OP2 | 1:AA:288:A:N6 | 2.35 | 0.58 |
| 2:AB:145:GLU:O | 2:AB:149:GLY:N | 2.37 | 0.58 |
| 5:AE:101:GLU:HB3 | 5:AE:122:ASN:HB2 | 1.84 | 0.58 |
| 22:BA:811:U:C2 | 22:BA:1251:C:C5 | 2.91 | 0.58 |
| 22:BA:1421:G:C2 | 22:BA:1422:G:C8 | 2.92 | 0.58 |
| 30:BI:82:LYS:O | 30:BI:83:ALA:HB2 | 2.04 | 0.58 |
| 1:CA:618:C:H5'' | 1:CA:619:U:H5'' | 1.84 | 0.58 |
| 2:CB:119:THR:O | 2:CB:120:GLN:CB | 2.50 | 0.58 |
| 15:CO:18:ASP:OD1 | 15:CO:20:ASN:HB2 | 2.03 | 0.58 |
| 22:DA:129:C:H2' | 22:DA:130:C:C6 | 2.39 | 0.58 |
| 22:DA:636:G:N1 | 33:DL:76:GLU:OE2 | 2.36 | 0.58 |
| 42:DU:18:ASP:OD2 | 42:DU:18:ASP:N | 2.36 | 0.58 |
| 1:AA:722:G:H3' | 1:AA:722:G:N3 | 2.18 | 0.58 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C5 | 2.39 | 0.58 |
| 1:AA:1492:A:OP1 | 12:AL:44:LYS:N | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:BA:545:U:H3' | 22:BA:546:U:H4' | 1.86 | 0.58 |
| 22:BA:1916:A:H2' | 22:BA:1917:U:C1' | 2.34 | 0.58 |
| 22:BA:2358:A:N1 | 33:BL:54:GLN:NE2 | 2.50 | 0.58 |
| 42:BU:18:ASP:O | 42:BU:19:LYS:C | 2.41 | 0.58 |
| 4:CD:35:GLU:HG3 | 4:CD:36:GLN:N | 2.18 | 0.58 |
| 17:CQ:46:VAL:HG21 | 17:CQ:61:ILE:CD1 | 2.34 | 0.58 |
| 22:DA:607:U:N3 | 22:DA:620:G:O4' | 2.36 | 0.58 |
| 22:DA:720:U:H2' | 22:DA:721:A:C8 | 2.38 | 0.58 |
| 22:DA:1099:G:N7 | 22:DA:1100:C:N4 | 2.52 | 0.58 |
| 22:DA:1344:U:O2' | 22:DA:1345:C:P | 2.62 | 0.58 |
| 29:DH:34:GLY:O | 29:DH:35:LYS:CB | 2.51 | 0.58 |
| 1:AA:1394:A:N1 | 1:AA:1500:A:O2' | 2.32 | 0.58 |
| 2:AB:186:ILE:HA | 2:AB:200:ILE:O | 2.04 | 0.58 |
| 4:AD:32:CYS:O | 4:AD:33:LYS:CB | 2.52 | 0.58 |
| 9:AI:9:THR:HG22 | 9:AI:10:GLY:N | 2.18 | 0.58 |
| 16:AP:42:ILE:O | 16:AP:43:ALA:C | 2.41 | 0.58 |
| 22:BA:1417:C:H2' | 22:BA:1418:G:O4' | 2.03 | 0.58 |
| 22:BA:1439:A:OP2 | 58:BA:3636:HOH:O | 2.17 | 0.58 |
| 24:BC:141:VAL:HG12 | 24:BC:142:HIS:N | 2.19 | 0.58 |
| 28:BG:124:GLU:OE1 | 28:BG:125:CYS:N | 2.37 | 0.58 |
| 28:BG:174:ALA:O | 28:BG:175:LYS:CB | 2.51 | 0.58 |
| 29:BH:31:VAL:N | 29:BH:32:PRO:HD2 | 2.19 | 0.58 |
| 37:BP:91:ALA:HB2 | 37:BP:113:ARG:HA | 1.84 | 0.58 |
| 1:CA:815:A:N7 | 1:CA:1509:C:O2' | 2.28 | 0.58 |
| 22:DA:1351:C:H2' | 22:DA:1352:U:C1' | 2.34 | 0.58 |
| 22:DA:1360:G:N1 | 22:DA:1361:G:H1' | 2.18 | 0.58 |
| 22:DA:1510:G:H2' | 22:DA:1511:G:O4' | 2.03 | 0.58 |
| 22:DA:2266:A:C2 | 22:DA:2272:U:C5 | 2.91 | 0.58 |
| 4:AD:120:HIS:O | 4:AD:121:LYS:C | 2.41 | 0.58 |
| 22:BA:1674:G:N2 | 22:BA:1677:A:N1 | 2.49 | 0.58 |
| 22:BA:2517:C:C5 | 22:BA:2542:A:C5 | 2.92 | 0.58 |
| 22:BA:2534:A:H2' | 22:BA:2535:G:O5' | 2.04 | 0.58 |
| 39:BR:68:ARG:HD3 | 39:BR:92:TRP:CZ2 | 2.39 | 0.58 |
| 1:CA:190:A:C8 | 1:CA:191:G:H1' | 2.39 | 0.58 |
| 6:CF:86:ARG:CG | 6:CF:86:ARG:HH11 | 2.17 | 0.58 |
| 11:CK:125:LYS:O | 21:CU:34:ARG:NE | 2.35 | 0.58 |
| 22:DA:1648:U:H2' | 22:DA:1649:G:O4' | 2.03 | 0.58 |
| 22:DA:2061:G:C6 | 56:DA:3001:DOL:HC19 | 2.39 | 0.58 |
| 22:DA:2123:G:C2 | 22:DA:2176:A:C2 | 2.92 | 0.58 |
| 30:DI:10:LYS:HB2 | 30:DI:56:PRO:CB | 2.33 | 0.58 |
| 11:AK:69:ARG:CD | 22:BA:2146:C:N3 | 2.66 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:AR:47:THR:HG22 | 18:AR:48:ARG:O | 2.02 | 0.58 |
| 21:AU:4:ILE:N | 21:AU:20:LYS:HZ1 | 2.02 | 0.58 |
| 22:BA:544:C:H5' | 22:BA:545:U:OP2 | 2.04 | 0.58 |
| 42:BU:49:VAL:O | 42:BU:49:VAL:HG22 | 2.04 | 0.58 |
| 1:CA:1330:U:H4' | 13:CM:23:TYR:CE1 | 2.38 | 0.58 |
| 22:DA:223:A:C4 | 22:DA:408:G:H1' | 2.38 | 0.58 |
| 22:DA:306:U:O2 | 22:DA:312:G:N2 | 2.37 | 0.58 |
| 22:DA:425:G:N2 | 22:DA:426:C:C2 | 2.72 | 0.58 |
| 22:DA:622:G:H2' | 22:DA:623:C:C6 | 2.38 | 0.58 |
| 36:DO:33:ARG:O | 36:DO:34:HIS:HB2 | 2.04 | 0.58 |
| 1:AA:152:A:N6 | 1:AA:170:U:C2 | 2.71 | 0.58 |
| 1:AA:887:G:C2' | 1:AA:888:G:H5' | 2.34 | 0.58 |
| 1:AA:1337:G:C5' | 1:AA:1338:G:OP1 | 2.51 | 0.58 |
| 3:AC:7:PRO:HG2 | 3:AC:184:TYR:CD1 | 2.39 | 0.58 |
| 20:AT:58:VAL:HG12 | 20:AT:59:ASP:N | 2.18 | 0.58 |
| 22:BA:1020:A:C2 | 22:BA:1141:U:C2 | 2.92 | 0.58 |
| 22:BA:1695:G:H1' | 24:BC:8:PRO:O | 2.04 | 0.58 |
| 22:BA:1786:A:C4 | 22:BA:1938:A:C6 | 2.91 | 0.58 |
| 22:BA:2665:A:C2 | 22:BA:2666:C:C6 | 2.91 | 0.58 |
| 5:CE:56:VAL:O | 5:CE:60:ILE:HG23 | 2.04 | 0.58 |
| 6:CF:8:PHE:CZ | 6:CF:60:VAL:HB | 2.38 | 0.58 |
| 6:CF:26:THR:O | 6:CF:30:THR:OG1 | 2.22 | 0.58 |
| 18:CR:63:ARG:HB3 | 18:CR:70:TYR:CE1 | 2.38 | 0.58 |
| 22:DA:182:A:H2' | 22:DA:183:C:C6 | 2.39 | 0.58 |
| 22:DA:454:A:H4' | 22:DA:455:C:OP2 | 2.02 | 0.58 |
| 22:DA:668:A:N6 | 22:DA:670:A:O2' | 2.37 | 0.58 |
| 22:DA:1802:A:C2 | 22:DA:1803:A:C4 | 2.92 | 0.58 |
| 22:DA:1809:A:H2' | 22:DA:1810:A:C8 | 2.39 | 0.58 |
| 22:DA:2563:U:H1' | 22:DA:2566:A:C6 | 2.39 | 0.58 |
| 1:AA:736:C:H2' | 1:AA:737:C:C6 | 2.39 | 0.57 |
| 1:AA:1311:A:C2 | 1:AA:1327:C:N3 | 2.72 | 0.57 |
| 2:AB:75:ALA:O | 2:AB:76:ALA:HB2 | 2.02 | 0.57 |
| 2:AB:219:ALA:O | 2:AB:220:THR:HB | 2.03 | 0.57 |
| 16:AP:75:ILE:HG22 | 16:AP:80:LYS:HE2 | 1.86 | 0.57 |
| 20:AT:67:ILE:HG13 | 20:AT:71:LYS:HG2 | 1.85 | 0.57 |
| 22:BA:1106:G:N2 | 22:BA:1107:G:H1' | 2.19 | 0.57 |
| 22:BA:1377:G:H5'' | 22:BA:1378:A:OP2 | 2.03 | 0.57 |
| 22:BA:1754:A:C6 | 22:BA:1755:A:C6 | 2.92 | 0.57 |
| 22:BA:2716:C:O2' | 22:BA:2717:C:H5' | 2.04 | 0.57 |
| 30:BI:69:PHE:O | 30:BI:69:PHE:CD1 | 2.57 | 0.57 |
| 1:CA:152:A:N6 | 1:CA:170:U:C2 | 2.72 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:765:G:C6 | 1:CA:812:G:C4 | 2.92 | 0.57 |
| 1:CA:977:A:H3' | 1:CA:977:A:N3 | 2.19 | 0.57 |
| 4:CD:32:CYS:O | 4:CD:33:LYS:CB | 2.51 | 0.57 |
| 6:CF:97:THR:O | 6:CF:98:GLU:CB | 2.51 | 0.57 |
| 9:CI:84:THR:HG21 | 9:CI:103:PHE:HB3 | 1.86 | 0.57 |
| 12:CL:44:LYS:CB | 12:CL:45:PRO:CD | 2.82 | 0.57 |
| 22:DA:396:G:C5' | 45:DX:13:VAL:HG21 | 2.34 | 0.57 |
| 22:DA:479:A:H4' | 22:DA:480:A:OP1 | 2.04 | 0.57 |
| 22:DA:1263:U:O4 | 40:DS:95:ARG:NH1 | 2.36 | 0.57 |
| 22:DA:1315:C:O2' | 22:DA:1392:A:N3 | 2.33 | 0.57 |
| 29:DH:108:VAL:O | 29:DH:110:VAL:N | 2.36 | 0.57 |
| 33:DL:55:MET:SD | 33:DL:59:ARG:HB3 | 2.43 | 0.57 |
| 1:AA:1299:A:C6 | 1:AA:1301:U:O2 | 2.57 | 0.57 |
| 4:AD:25:VAL:HG12 | 4:AD:26:ARG:N | 2.19 | 0.57 |
| 9:AI:47:VAL:HA | 9:AI:50:GLN:HB2 | 1.86 | 0.57 |
| 22:BA:580:U:H2' | 22:BA:581:C:H6 | 1.69 | 0.57 |
| 22:BA:826:U:O2' | 33:BL:53:GLY:HA3 | 2.04 | 0.57 |
| 22:BA:1563:U:H2' | 22:BA:1564:C:C6 | 2.39 | 0.57 |
| 22:BA:1965:C:OP1 | 22:BA:1966:A:O2' | 2.21 | 0.57 |
| 29:BH:123:ARG:NH2 | 1:CA:367:U:OP2 | 2.31 | 0.57 |
| 43:BV:48:MET:O | 43:BV:51:GLN:HG3 | 2.04 | 0.57 |
| 1:CA:1041:G:H2' | 1:CA:1042:A:C8 | 2.39 | 0.57 |
| 22:DA:27:G:HO2' | 22:DA:28:A:P | 2.27 | 0.57 |
| 22:DA:247:G:N7 | 22:DA:249:C:C2 | 2.72 | 0.57 |
| 22:DA:674:G:H1' | 26:DE:69:ARG:HE | 1.69 | 0.57 |
| 22:DA:842:U:N3 | 22:DA:843:G:N7 | 2.52 | 0.57 |
| 22:DA:1109:C:C4 | 22:DA:1110:G:C6 | 2.93 | 0.57 |
| 22:DA:1308:A:N6 | 22:DA:1309:G:C2 | 2.72 | 0.57 |
| 22:DA:2054:A:OP1 | 22:DA:2055:C:O2' | 2.22 | 0.57 |
| 22:DA:2234:G:C6 | 22:DA:2235:G:N7 | 2.72 | 0.57 |
| 29:DH:62:LEU:HD13 | 29:DH:62:LEU:C | 2.25 | 0.57 |
| 35:DN:63:ARG:NH1 | 35:DN:81:ASN:OD1 | 2.37 | 0.57 |
| 45:DX:52:SER:OG | 45:DX:55:GLY:N | 2.35 | 0.57 |
| 1:AA:1107:C:C4 | 1:AA:1108:G:N7 | 2.72 | 0.57 |
| 1:AA:1144:G:H5'' | 1:AA:1145:A:OP2 | 2.04 | 0.57 |
| 9:AI:49:ARG:NH2 | 9:AI:52:LEU:O | 2.38 | 0.57 |
| 10:AJ:73:LEU:O | 10:AJ:74:VAL:HB | 2.04 | 0.57 |
| 22:BA:278:A:C2 | 22:BA:362:A:C8 | 2.91 | 0.57 |
| 22:BA:585:G:N7 | 38:BQ:6:ARG:NH1 | 2.53 | 0.57 |
| 22:BA:927:A:H2' | 22:BA:928:A:C8 | 2.39 | 0.57 |
| 22:BA:1385:A:C4 | 22:BA:1386:C:C5 | 2.93 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2032:G:N7 | 58:BA:3534:HOH:O | 2.32 | 0.57 |
| 26:BE:119:ILE:HB | 26:BE:187:VAL:HG22 | 1.84 | 0.57 |
| 1:CA:412:A:O2' | 1:CA:413:G:O5' | 2.05 | 0.57 |
| 1:CA:496:A:C2 | 1:CA:497:G:C5 | 2.92 | 0.57 |
| 1:CA:527:G:C2 | 1:CA:528:C:C6 | 2.92 | 0.57 |
| 2:CB:47:VAL:HB | 2:CB:48:PRO:HD3 | 1.86 | 0.57 |
| 12:CL:90:LEU:CB | 12:CL:93:VAL:HG21 | 2.35 | 0.57 |
| 22:DA:142:A:C5 | 22:DA:143:C:N4 | 2.72 | 0.57 |
| 22:DA:1773:A:N7 | 22:DA:1829:A:H1' | 2.19 | 0.57 |
| 37:DP:93:ARG:O | 37:DP:94:LYS:CB | 2.52 | 0.57 |
| 1:AA:22:G:H4' | 1:AA:885:G:C8 | 2.39 | 0.57 |
| 10:AJ:92:LEU:O | 10:AJ:93:ALA:CB | 2.52 | 0.57 |
| 22:BA:645:C:O2' | 22:BA:646:U:H5'' | 2.04 | 0.57 |
| 22:BA:1189:A:H2' | 22:BA:1190:G:O4' | 2.04 | 0.57 |
| 22:BA:1413:A:H2' | 22:BA:1414:C:O4' | 2.05 | 0.57 |
| 22:BA:1669:A:OP2 | 58:BA:3722:HOH:O | 2.17 | 0.57 |
| 22:BA:1736:U:H2' | 22:BA:1737:G:O4' | 2.04 | 0.57 |
| 22:BA:1793:C:O2' | 22:BA:1794:A:H5' | 2.04 | 0.57 |
| 22:BA:2120:G:N2 | 22:BA:2179:C:O2 | 2.37 | 0.57 |
| 22:BA:2491:U:H4' | 22:BA:2492:U:OP1 | 2.04 | 0.57 |
| 43:BV:10:LYS:N | 43:BV:10:LYS:HE2 | 2.19 | 0.57 |
| 1:CA:405:U:OP2 | 4:CD:3:ARG:NH1 | 2.37 | 0.57 |
| 11:CK:126:LYS:O | 21:CU:34:ARG:CZ | 2.52 | 0.57 |
| 22:DA:53:A:N7 | 22:DA:54:G:C5 | 2.73 | 0.57 |
| 22:DA:106:C:O2' | 22:DA:294:A:O2' | 2.08 | 0.57 |
| 22:DA:533:G:H5' | 38:DQ:24:TYR:CE2 | 2.39 | 0.57 |
| 22:DA:563:A:C4 | 22:DA:2018:G:C2 | 2.93 | 0.57 |
| 22:DA:588:U:H1' | 26:DE:85:PHE:CD1 | 2.39 | 0.57 |
| 22:DA:1050:A:C2 | 22:DA:2751:G:C4 | 2.92 | 0.57 |
| 28:DG:176:LYS:O | 28:DG:177:LYS:HB2 | 2.03 | 0.57 |
| 29:DH:117:LEU:HB3 | 29:DH:120:GLY:O | 2.05 | 0.57 |
| 37:DP:91:ALA:HB2 | 37:DP:113:ARG:HA | 1.85 | 0.57 |
| 1:AA:657:U:O2 | 15:AO:22:THR:CG2 | 2.52 | 0.57 |
| 2:AB:67:ILE:O | 2:AB:68:LEU:CB | 2.51 | 0.57 |
| 9:AI:30:ILE:HD11 | 9:AI:38:TYR:CD2 | 2.39 | 0.57 |
| 10:AJ:17:LEU:HD23 | 10:AJ:17:LEU:C | 2.24 | 0.57 |
| 30:BI:82:LYS:O | 30:BI:83:ALA:CB | 2.52 | 0.57 |
| 38:BQ:9:ILE:O | 38:BQ:13:ARG:HG3 | 2.04 | 0.57 |
| 40:BS:84:ARG:HB2 | 40:BS:96:ILE:HG13 | 1.85 | 0.57 |
| 1:CA:938:A:N6 | 1:CA:939:G:C6 | 2.72 | 0.57 |
| 1:CA:957:U:O3' | 19:CS:79:THR:OG1 | 2.21 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:CO:17:ARG:O | 15:CO:18:ASP:CB | 2.51 | 0.57 |
| 22:DA:324:A:C2 | 22:DA:325:G:H1' | 2.39 | 0.57 |
| 31:DJ:35:ARG:HG2 | 31:DJ:40:HIS:CD2 | 2.40 | 0.57 |
| 39:DR:52:PRO:O | 39:DR:53:PHE:CG | 2.57 | 0.57 |
| 11:AK:51:GLY:O | 11:AK:52:PHE:O | 2.22 | 0.57 |
| 11:AK:128:ARG:HG2 | 11:AK:128:ARG:HH11 | 1.70 | 0.57 |
| 22:BA:618:G:N7 | 58:BA:3286:HOH:O | 2.32 | 0.57 |
| 22:BA:995:C:H5' | 22:BA:995:C:H6 | 1.70 | 0.57 |
| 22:BA:2808:G:N2 | 22:BA:2891:U:C6 | 2.73 | 0.57 |
| 32:BK:36:GLY:HA2 | 32:BK:62:VAL:O | 2.05 | 0.57 |
| 39:BR:51:VAL:HB | 39:BR:52:PRO:CD | 2.35 | 0.57 |
| 40:BS:55:ILE:CG2 | 40:BS:66:ILE:HG12 | 2.35 | 0.57 |
| 53:B5:184:GLU:O | 53:B5:185:LYS:CB | 2.53 | 0.57 |
| 1:CA:992:U:N3 | 1:CA:1043:G:N7 | 2.53 | 0.57 |
| 1:CA:1343:G:H2' | 1:CA:1344:C:C6 | 2.40 | 0.57 |
| 2:CB:16:PHE:CE1 | 2:CB:18:HIS:CE1 | 2.93 | 0.57 |
| 22:DA:613:A:HO2' | 22:DA:614:A:P | 2.25 | 0.57 |
| 22:DA:1181:U:H2' | 22:DA:1182:G:C8 | 2.39 | 0.57 |
| 22:DA:2091:C:H1' | 45:DX:34:HIS:CD2 | 2.39 | 0.57 |
| 22:DA:2615:U:C2 | 48:D0:4:GLN:HA | 2.39 | 0.57 |
| 26:DE:97:ASN:HB2 | 26:DE:100:MET:SD | 2.44 | 0.57 |
| 28:DG:169:VAL:O | 28:DG:169:VAL:HG12 | 2.04 | 0.57 |
| 38:DQ:10:ALA:O | 38:DQ:13:ARG:HG3 | 2.05 | 0.57 |
| 42:DU:74:ASN:ND2 | 42:DU:96:PHE:CD1 | 2.72 | 0.57 |
| 1:AA:77:A:N1 | 1:AA:91:U:O4 | 2.38 | 0.57 |
| 1:AA:108:G:N3 | 1:AA:108:G:C5' | 2.68 | 0.57 |
| 1:AA:614:C:H2' | 1:AA:615:G:O4' | 2.05 | 0.57 |
| 10:AJ:53:ILE:HG22 | 10:AJ:61:ALA:CB | 2.35 | 0.57 |
| 22:BA:1078:U:H1' | 22:BA:1088:A:N1 | 2.19 | 0.57 |
| 22:BA:1309:G:H4' | 50:B2:7:PRO:HB2 | 1.85 | 0.57 |
| 22:BA:1731:G:C6 | 22:BA:1733:G:C6 | 2.92 | 0.57 |
| 22:BA:2328:A:H2' | 22:BA:2329:U:C6 | 2.40 | 0.57 |
| 29:BH:132:PHE:CE2 | 29:BH:142:VAL:HG21 | 2.40 | 0.57 |
| 35:BN:25:ALA:CB | 35:BN:48:VAL:HG22 | 2.35 | 0.57 |
| 38:BQ:89:GLU:H | 39:BR:49:ILE:CD1 | 2.18 | 0.57 |
| 40:BS:63:GLY:O | 40:BS:64:ALA:HB3 | 2.05 | 0.57 |
| 1:CA:1151:A:N3 | 1:CA:1152:A:C5 | 2.72 | 0.57 |
| 1:CA:1217:C:H2' | 1:CA:1218:C:C6 | 2.40 | 0.57 |
| 5:CE:83:HIS:CD2 | 8:CH:96:MET:CE | 2.88 | 0.57 |
| 6:CF:9:MET:SD | 6:CF:59:TYR:CE1 | 2.98 | 0.57 |
| 7:CG:125:SER:O | 7:CG:127:ALA:N | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:12:U:O2 | 22:DA:12:U:H2' | 2.04 | 0.57 |
| 22:DA:46:G:C2 | 22:DA:47:C:C6 | 2.92 | 0.57 |
| 22:DA:1353:A:C8 | 22:DA:1378:A:N6 | 2.73 | 0.57 |
| 22:DA:1566:A:C2 | 24:DC:213:TRP:CE3 | 2.92 | 0.57 |
| 22:DA:1753:G:C2 | 22:DA:1756:G:C2 | 2.92 | 0.57 |
| 22:DA:1843:C:H4' | 24:DC:251:GLN:CD | 2.25 | 0.57 |
| 22:DA:2272:U:H5'' | 22:DA:2273:A:OP1 | 2.03 | 0.57 |
| 22:DA:2387:U:H1' | 44:DW:41:ARG:CD | 2.35 | 0.57 |
| 24:DC:16:VAL:HG22 | 24:DC:206:GLY:HA3 | 1.87 | 0.57 |
| 25:DD:140:HIS:NE2 | 58:DD:303:HOH:O | 2.32 | 0.57 |
| 29:DH:21:VAL:HG22 | 29:DH:22:LYS:N | 2.19 | 0.57 |
| 37:DP:103:ARG:HB3 | 37:DP:108:ALA:HB2 | 1.87 | 0.57 |
| 5:AE:101:GLU:HB3 | 5:AE:122:ASN:CB | 2.34 | 0.57 |
| 6:AF:18:VAL:N | 6:AF:19:PRO:HD2 | 2.20 | 0.57 |
| 15:AO:87:LEU:O | 15:AO:88:ARG:CB | 2.52 | 0.57 |
| 22:BA:1688:U:H1' | 22:BA:1701:A:C6 | 2.40 | 0.57 |
| 22:BA:2191:A:C2 | 22:BA:2192:U:C4 | 2.93 | 0.57 |
| 24:BC:167:ARG:O | 24:BC:168:ASP:HB2 | 2.04 | 0.57 |
| 26:BE:106:LYS:HG3 | 26:BE:200:LEU:HG | 1.85 | 0.57 |
| 41:BT:64:LYS:N | 41:BT:64:LYS:HD3 | 2.19 | 0.57 |
| 53:B5:125:GLY:O | 53:B5:126:SER:CB | 2.53 | 0.57 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.40 | 0.57 |
| 1:CA:563:A:H2' | 1:CA:567:G:C8 | 2.40 | 0.57 |
| 16:CP:39:PHE:CD1 | 16:CP:74:LEU:HD11 | 2.39 | 0.57 |
| 20:CT:68:HIS:C | 20:CT:69:LYS:HG3 | 2.24 | 0.57 |
| 22:DA:372:G:N2 | 22:DA:401:A:OP2 | 2.36 | 0.57 |
| 22:DA:744:U:H4' | 22:DA:1658:C:H4' | 1.87 | 0.57 |
| 22:DA:893:C:H2' | 22:DA:894:U:O4' | 2.05 | 0.57 |
| 22:DA:1272:A:C2 | 22:DA:1618:A:C4 | 2.92 | 0.57 |
| 22:DA:2199:A:C6 | 22:DA:2200:C:C2 | 2.93 | 0.57 |
| 22:DA:2882:A:H5' | 35:DN:96:ARG:HB2 | 1.86 | 0.57 |
| 31:DJ:41:LYS:O | 31:DJ:42:ALA:C | 2.42 | 0.57 |
| 32:DK:105:ARG:NH2 | 37:DP:34:GLU:OE2 | 2.37 | 0.57 |
| 37:DP:103:ARG:CB | 37:DP:108:ALA:HB2 | 2.35 | 0.57 |
| 49:D1:14:SER:OG | 49:D1:48:ILE:O | 2.11 | 0.57 |
| 1:AA:495:A:C2 | 1:AA:496:A:C6 | 2.93 | 0.57 |
| 3:AC:155:GLY:HA2 | 3:AC:163:ALA:HB1 | 1.87 | 0.57 |
| 9:AI:112:GLU:OE2 | 9:AI:115:LYS:NZ | 2.38 | 0.57 |
| 11:AK:16:VAL:HG22 | 11:AK:17:SER:N | 2.20 | 0.57 |
| 18:AR:26:ILE:O | 18:AR:30:LYS:HG3 | 2.05 | 0.57 |
| 22:BA:495:G:H1' | 40:BS:57:ASN:OD1 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:974:G:H8 | 22:BA:990:A:H62 | 1.51 | 0.57 |
| 22:BA:1283:G:N1 | 22:BA:1286:A:OP2 | 2.38 | 0.57 |
| 22:BA:2825:G:C2' | 22:BA:2826:A:H5' | 2.35 | 0.57 |
| 29:BH:95:GLY:HA2 | 29:BH:117:LEU:HD22 | 1.87 | 0.57 |
| 29:BH:117:LEU:HD21 | 29:BH:121:VAL:CA | 2.35 | 0.57 |
| 42:BU:99:ASN:C | 42:BU:99:ASN:OD1 | 2.43 | 0.57 |
| 1:CA:455:G:N2 | 1:CA:478:A:C2 | 2.72 | 0.57 |
| 3:CC:72:ARG:HB3 | 3:CC:75:ILE:HG23 | 1.86 | 0.57 |
| 22:DA:43:G:N2 | 22:DA:437:U:C6 | 2.73 | 0.57 |
| 22:DA:537:G:N1 | 22:DA:555:G:C2 | 2.73 | 0.57 |
| 22:DA:667:U:C4 | 22:DA:668:A:N7 | 2.73 | 0.57 |
| 22:DA:2800:A:C2 | 22:DA:2895:G:H1' | 2.40 | 0.57 |
| 35:DN:84:GLY:N | 35:DN:85:PRO:CD | 2.68 | 0.57 |
| 39:DR:52:PRO:O | 39:DR:53:PHE:CB | 2.53 | 0.57 |
| 1:AA:769:G:H4' | 1:AA:1513:A:H4' | 1.86 | 0.57 |
| 1:AA:1238:A:C2 | 1:AA:1303:C:H4' | 2.40 | 0.57 |
| 4:AD:174:ASP:O | 4:AD:175:ALA:HB3 | 2.04 | 0.57 |
| 22:BA:666:A:H4' | 33:BL:48:ARG:HD3 | 1.87 | 0.57 |
| 22:BA:851:C:H2' | 22:BA:852:U:C6 | 2.40 | 0.57 |
| 22:BA:1924:C:OP2 | 22:BA:1924:C:H3' | 2.05 | 0.57 |
| 22:BA:1926:U:O2 | 22:BA:1928:A:N7 | 2.38 | 0.57 |
| 22:BA:2086:U:H2' | 22:BA:2087:G:C8 | 2.40 | 0.57 |
| 1:CA:8:A:C5 | 4:CD:206:LYS:HB3 | 2.40 | 0.57 |
| 1:CA:160:A:H2' | 1:CA:161:A:O4' | 2.05 | 0.57 |
| 1:CA:269:C:H2' | 1:CA:270:A:C8 | 2.40 | 0.57 |
| 1:CA:412:A:HO2' | 1:CA:413:G:P | 2.26 | 0.57 |
| 1:CA:545:C:OP2 | 4:CD:59:GLN:NE2 | 2.36 | 0.57 |
| 22:DA:56:A:C2 | 22:DA:57:C:C2 | 2.92 | 0.57 |
| 22:DA:411:G:OP2 | 22:DA:2406:A:O2' | 2.15 | 0.57 |
| 22:DA:1125:G:C6 | 22:DA:1126:A:N6 | 2.72 | 0.57 |
| 22:DA:1343:G:H1' | 22:DA:1597:A:C4 | 2.40 | 0.57 |
| 22:DA:1509:A:O2' | 22:DA:1510:G:P | 2.63 | 0.57 |
| 22:DA:2293:G:OP1 | 22:DA:2377:A:N6 | 2.38 | 0.57 |
| 28:DG:176:LYS:O | 28:DG:177:LYS:CB | 2.52 | 0.57 |
| 1:AA:80:A:C2 | 1:AA:90:C:N3 | 2.73 | 0.56 |
| 1:AA:269:C:H2' | 1:AA:270:A:C8 | 2.40 | 0.56 |
| 22:BA:831:G:OP1 | 58:BA:3262:HOH:O | 2.17 | 0.56 |
| 22:BA:1179:G:C5 | 22:BA:1180:U:C1' | 2.88 | 0.56 |
| 22:BA:1605:C:H2' | 22:BA:1606:C:H5' | 1.87 | 0.56 |
| 30:BI:21:SER:N | 30:BI:22:PRO:CD | 2.68 | 0.56 |
| 1:CA:145:G:C2 | 1:CA:146:G:C8 | 2.92 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:214:C:H2' | 1:CA:215:C:C6 | 2.40 | 0.56 |
| 9:CI:116:VAL:CG2 | 10:CJ:62:ARG:HD3 | 2.35 | 0.56 |
| 22:DA:749:A:C5 | 22:DA:1618:A:C2 | 2.93 | 0.56 |
| 22:DA:1581:G:C6 | 22:DA:1582:C:C4 | 2.93 | 0.56 |
| 22:DA:2652:C:C4 | 22:DA:2653:U:C4 | 2.93 | 0.56 |
| 26:DE:84:THR:O | 26:DE:85:PHE:CG | 2.58 | 0.56 |
| 30:DI:77:ALA:HA | 30:DI:80:LEU:HD12 | 1.87 | 0.56 |
| 47:DZ:24:LEU:HD11 | 47:DZ:54:MET:CE | 2.35 | 0.56 |
| 50:D2:15:SER:OG | 50:D2:16:HIS:CE1 | 2.58 | 0.56 |
| 1:AA:560:A:H5' | 1:AA:566:G:N2 | 2.19 | 0.56 |
| 1:AA:1269:A:C2 | 1:AA:1313:U:O4' | 2.57 | 0.56 |
| 1:AA:1289:A:O3' | 7:AG:35:LYS:NZ | 2.38 | 0.56 |
| 1:AA:1493:A:O2' | 1:AA:1494:G:OP2 | 2.19 | 0.56 |
| 11:AK:76:GLU:O | 11:AK:77:TYR:CD1 | 2.58 | 0.56 |
| 20:AT:29:ARG:O | 20:AT:33:LYS:HG2 | 2.04 | 0.56 |
| 22:BA:1700:A:H5' | 22:BA:1701:A:OP2 | 2.05 | 0.56 |
| 24:BC:97:LYS:N | 24:BC:97:LYS:HD2 | 2.19 | 0.56 |
| 26:BE:54:GLY:O | 26:BE:74:LYS:CE | 2.53 | 0.56 |
| 32:BK:34:GLY:O | 32:BK:35:VAL:C | 2.44 | 0.56 |
| 39:BR:48:LYS:O | 39:BR:48:LYS:HG2 | 2.05 | 0.56 |
| 41:BT:48:GLN:O | 41:BT:52:GLU:HA | 2.04 | 0.56 |
| 4:CD:148:LYS:O | 4:CD:149:ALA:HB3 | 2.04 | 0.56 |
| 5:CE:25:VAL:N | 5:CE:28:GLY:O | 2.37 | 0.56 |
| 5:CE:153:VAL:O | 5:CE:157:ARG:N | 2.37 | 0.56 |
| 22:DA:13:A:N1 | 22:DA:525:U:H2' | 2.20 | 0.56 |
| 22:DA:30:G:H2' | 22:DA:31:C:O4' | 2.05 | 0.56 |
| 22:DA:305:C:H1' | 22:DA:313:G:N2 | 2.20 | 0.56 |
| 22:DA:310:A:O2' | 22:DA:311:A:P | 2.63 | 0.56 |
| 22:DA:618:G:N7 | 58:DA:3290:HOH:O | 2.33 | 0.56 |
| 22:DA:1091:G:N3 | 22:DA:1092:C:C5 | 2.73 | 0.56 |
| 22:DA:1737:G:O6 | 22:DA:1738:G:N1 | 2.37 | 0.56 |
| 22:DA:2209:G:C2 | 22:DA:2216:G:C2 | 2.94 | 0.56 |
| 22:DA:2725:A:C5 | 22:DA:2727:A:C8 | 2.93 | 0.56 |
| 22:DA:2747:G:O6 | 22:DA:2755:C:H5'' | 2.05 | 0.56 |
| 23:DB:81:G:C5 | 23:DB:82:U:C5 | 2.93 | 0.56 |
| 24:DC:31:ALA:N | 24:DC:32:PRO:HD2 | 2.19 | 0.56 |
| 31:DJ:78:THR:OG1 | 31:DJ:80:HIS:HB2 | 2.05 | 0.56 |
| 1:AA:616:G:C2 | 1:AA:617:G:C8 | 2.93 | 0.56 |
| 2:AB:119:THR:O | 2:AB:120:GLN:CB | 2.54 | 0.56 |
| 10:AJ:33:GLY:O | 10:AJ:34:ALA:HB3 | 2.06 | 0.56 |
| 11:AK:76:GLU:N | 11:AK:76:GLU:OE2 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:AO:63:ARG:HG2 | 15:AO:67:LEU:CD1 | 2.36 | 0.56 |
| 16:AP:38:PHE:CE2 | 16:AP:51:ARG:HB2 | 2.40 | 0.56 |
| 17:AQ:17:MET:O | 17:AQ:19:LYS:N | 2.39 | 0.56 |
| 22:BA:274:C:C4 | 22:BA:275:C:C4 | 2.94 | 0.56 |
| 22:BA:752:A:H3' | 50:B2:1:MET:SD | 2.46 | 0.56 |
| 22:BA:1073:A:C3' | 22:BA:1074:G:C5' | 2.80 | 0.56 |
| 22:BA:1494:A:H2' | 22:BA:1495:A:O5' | 2.04 | 0.56 |
| 22:BA:1932:A:H5'' | 22:BA:1933:G:OP2 | 2.05 | 0.56 |
| 22:BA:2064:C:H2' | 22:BA:2065:C:C6 | 2.39 | 0.56 |
| 23:BB:37:C:C5 | 23:BB:38:C:C4 | 2.93 | 0.56 |
| 24:BC:125:LYS:HG2 | 24:BC:128:ASN:ND2 | 2.20 | 0.56 |
| 26:BE:59:PRO:HD3 | 26:BE:71:GLY:O | 2.05 | 0.56 |
| 29:BH:117:LEU:CD2 | 29:BH:121:VAL:H | 2.08 | 0.56 |
| 36:BO:79:ALA:HB2 | 36:BO:110:ALA:HA | 1.87 | 0.56 |
| 37:BP:103:ARG:HH11 | 37:BP:103:ARG:HG3 | 1.70 | 0.56 |
| 51:B3:27:ALA:O | 51:B3:28:ASN:CB | 2.53 | 0.56 |
| 1:CA:106:C:O2 | 1:CA:379:C:H4' | 2.05 | 0.56 |
| 1:CA:919:A:C2 | 1:CA:920:U:C5 | 2.94 | 0.56 |
| 2:CB:35:ARG:O | 2:CB:38:VAL:HG12 | 2.06 | 0.56 |
| 2:CB:210:VAL:HG22 | 2:CB:211:THR:N | 2.19 | 0.56 |
| 22:DA:204:A:O4' | 22:DA:206:U:C6 | 2.58 | 0.56 |
| 22:DA:290:U:C4 | 22:DA:291:G:N7 | 2.73 | 0.56 |
| 22:DA:684:G:C2 | 22:DA:794:A:C2 | 2.93 | 0.56 |
| 22:DA:1313:U:O2 | 22:DA:1313:U:H2' | 2.05 | 0.56 |
| 22:DA:1327:A:H2' | 22:DA:1328:A:O4' | 2.06 | 0.56 |
| 22:DA:1973:G:C6 | 22:DA:1974:C:N4 | 2.73 | 0.56 |
| 22:DA:2199:A:O4' | 29:DH:28:ASN:ND2 | 2.39 | 0.56 |
| 22:DA:2550:G:O6 | 22:DA:2551:C:N4 | 2.37 | 0.56 |
| 22:DA:2599:G:N7 | 24:DC:236:GLU:HB3 | 2.19 | 0.56 |
| 1:AA:81:A:C2' | 1:AA:82:G:H5'' | 2.36 | 0.56 |
| 3:AC:192:THR:HG1 | 3:AC:193:TYR:HD2 | 1.50 | 0.56 |
| 6:AF:98:GLU:CG | 6:AF:99:ALA:N | 2.68 | 0.56 |
| 14:AN:43:ASN:OD1 | 14:AN:47:LYS:NZ | 2.38 | 0.56 |
| 17:AQ:45:HIS:CD2 | 17:AQ:70:THR:CG2 | 2.88 | 0.56 |
| 22:BA:627:A:C6 | 22:BA:637:A:C8 | 2.93 | 0.56 |
| 22:BA:1073:A:C3' | 22:BA:1074:G:H5'' | 2.35 | 0.56 |
| 22:BA:1786:A:H1' | 22:BA:1938:A:N6 | 2.21 | 0.56 |
| 22:BA:1912:A:C2 | 22:BA:1919:A:C5 | 2.93 | 0.56 |
| 1:CA:466:A:N1 | 1:CA:468:A:N7 | 2.53 | 0.56 |
| 1:CA:572:A:H5' | 1:CA:573:A:OP2 | 2.06 | 0.56 |
| 1:CA:1000:A:H2' | 1:CA:1001:C:O4' | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:CG:129:GLU:OE1 | 7:CG:129:GLU:N | 2.38 | 0.56 |
| 12:CL:18:LYS:HD2 | 12:CL:18:LYS:C | 2.25 | 0.56 |
| 22:DA:2032:G:N7 | 58:DA:3531:HOH:O | 2.33 | 0.56 |
| 22:DA:2839:G:C6 | 22:DA:2840:C:C4 | 2.93 | 0.56 |
| 24:DC:108:LYS:HA | 24:DC:196:GLY:HA3 | 1.86 | 0.56 |
| 29:DH:32:PRO:HB3 | 45:DX:39:TRP:HB3 | 1.87 | 0.56 |
| 29:DH:83:LYS:N | 29:DH:149:GLU:HG2 | 2.20 | 0.56 |
| 1:AA:1492:A:OP1 | 12:AL:44:LYS:HA | 2.05 | 0.56 |
| 10:AJ:34:ALA:O | 10:AJ:35:GLN:CB | 2.53 | 0.56 |
| 15:AO:63:ARG:CG | 15:AO:67:LEU:HD12 | 2.35 | 0.56 |
| 22:BA:655:A:H4' | 22:BA:656:G:OP1 | 2.05 | 0.56 |
| 22:BA:1585:C:C2' | 22:BA:1586:A:H5' | 2.35 | 0.56 |
| 22:BA:1916:A:C2 | 22:BA:1917:U:O2 | 2.59 | 0.56 |
| 23:BB:54:G:H21 | 27:BF:26:MET:HE2 | 1.71 | 0.56 |
| 26:BE:54:GLY:O | 26:BE:74:LYS:HE2 | 2.05 | 0.56 |
| 49:B1:51:GLU:OE2 | 49:B1:53:LYS:HD3 | 2.05 | 0.56 |
| 1:CA:8:A:C6 | 4:CD:206:LYS:HB3 | 2.40 | 0.56 |
| 1:CA:247:G:C6 | 1:CA:278:G:N1 | 2.72 | 0.56 |
| 1:CA:955:U:O2' | 1:CA:1227:A:N6 | 2.39 | 0.56 |
| 2:CB:85:LEU:HG | 2:CB:85:LEU:O | 2.05 | 0.56 |
| 22:DA:424:G:C2 | 22:DA:425:G:C8 | 2.93 | 0.56 |
| 22:DA:2112:G:H2' | 22:DA:2112:G:N3 | 2.21 | 0.56 |
| 22:DA:2499:C:N4 | 22:DA:2500:U:O4 | 2.38 | 0.56 |
| 22:DA:2521:C:C2 | 22:DA:2545:G:N2 | 2.74 | 0.56 |
| 22:DA:2820:A:C8 | 25:DD:196:ALA:CB | 2.89 | 0.56 |
| 33:DL:95:LEU:O | 33:DL:100:ILE:HG23 | 2.06 | 0.56 |
| 42:DU:54:GLN:N | 42:DU:55:PRO:HD3 | 2.21 | 0.56 |
| 1:AA:1101:A:H4' | 1:AA:1102:A:O5' | 2.05 | 0.56 |
| 5:AE:157:ARG:HD2 | 8:AH:43:GLU:O | 2.05 | 0.56 |
| 6:AF:9:MET:HE3 | 18:AR:65:LEU:HA | 1.88 | 0.56 |
| 13:AM:16:VAL:HG23 | 13:AM:41:GLU:O | 2.05 | 0.56 |
| 20:AT:44:LYS:CD | 20:AT:87:ALA:HA | 2.36 | 0.56 |
| 22:BA:819:A:OP2 | 22:BA:1187:G:N2 | 2.29 | 0.56 |
| 22:BA:1001:A:P | 58:BA:3735:HOH:O | 2.57 | 0.56 |
| 22:BA:1405:U:H2' | 22:BA:1406:U:C6 | 2.41 | 0.56 |
| 22:BA:1824:G:N3 | 24:BC:252:THR:HG21 | 2.20 | 0.56 |
| 22:BA:1941:C:O2 | 22:BA:1941:C:H2' | 2.05 | 0.56 |
| 46:BY:6:LEU:O | 46:BY:60:LYS:NZ | 2.34 | 0.56 |
| 1:CA:511:C:C2 | 1:CA:512:U:C5 | 2.93 | 0.56 |
| 1:CA:755:G:C2 | 1:CA:756:C:C5 | 2.93 | 0.56 |
| 1:CA:824:G:H1' | 8:CH:2:SER:N | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:294:A:N6 | 22:DA:345:A:C4 | 2.73 | 0.56 |
| 22:DA:847:U:O2 | 22:DA:847:U:H2' | 2.06 | 0.56 |
| 22:DA:1312:U:C2 | 22:DA:1603:A:N1 | 2.74 | 0.56 |
| 22:DA:1693:U:O2' | 24:DC:14:ARG:NH2 | 2.38 | 0.56 |
| 22:DA:1817:G:H2' | 22:DA:1818:U:H5' | 1.88 | 0.56 |
| 22:DA:2171:A:O2' | 22:DA:2173:A:OP1 | 2.23 | 0.56 |
| 22:DA:2262:U:H1' | 22:DA:2328:A:H1' | 1.88 | 0.56 |
| 23:DB:32:U:C2 | 23:DB:51:G:N2 | 2.74 | 0.56 |
| 30:DI:80:LEU:HA | 30:DI:84:ALA:CB | 2.35 | 0.56 |
| 39:DR:14:VAL:HG21 | 39:DR:98:ILE:HG13 | 1.87 | 0.56 |
| 1:AA:205:A:H2' | 1:AA:205:A:N3 | 2.21 | 0.56 |
| 17:AQ:16:LYS:HG3 | 17:AQ:16:LYS:O | 2.04 | 0.56 |
| 22:BA:644:A:H2' | 22:BA:645:C:O4' | 2.06 | 0.56 |
| 22:BA:947:A:O2' | 22:BA:984:A:C2 | 2.56 | 0.56 |
| 22:BA:1071:G:C8 | 22:BA:1089:A:N6 | 2.74 | 0.56 |
| 22:BA:1915:U:H2' | 22:BA:1916:A:H5' | 1.87 | 0.56 |
| 22:BA:1916:A:H2' | 22:BA:1917:U:O2' | 2.05 | 0.56 |
| 22:BA:2474:U:H5'' | 22:BA:2475:C:OP2 | 2.06 | 0.56 |
| 24:BC:86:ASN:N | 24:BC:86:ASN:OD1 | 2.38 | 0.56 |
| 29:BH:40:THR:OG1 | 29:BH:43:ASN:OD1 | 2.24 | 0.56 |
| 53:B5:50:ILE:HG22 | 53:B5:51:ASP:H | 1.71 | 0.56 |
| 1:CA:1348:U:H4' | 9:CI:122:ARG:HG3 | 1.88 | 0.56 |
| 1:CA:1491:G:C6 | 1:CA:1492:A:N1 | 2.74 | 0.56 |
| 4:CD:174:ASP:O | 4:CD:175:ALA:HB2 | 2.05 | 0.56 |
| 19:CS:55:ARG:NE | 19:CS:79:THR:HG22 | 2.20 | 0.56 |
| 21:CU:14:VAL:HG12 | 21:CU:16:LEU:HG | 1.88 | 0.56 |
| 22:DA:478:A:C2 | 22:DA:480:A:C4 | 2.94 | 0.56 |
| 22:DA:848:C:H2' | 22:DA:849:A:C8 | 2.41 | 0.56 |
| 22:DA:1436:G:N2 | 22:DA:1557:C:C2 | 2.74 | 0.56 |
| 22:DA:2053:G:H2' | 22:DA:2054:A:O4' | 2.06 | 0.56 |
| 32:DK:30:ARG:NH2 | 32:DK:37:ASP:OD1 | 2.39 | 0.56 |
| 41:DT:23:ALA:O | 41:DT:27:SER:N | 2.39 | 0.56 |
| 1:AA:683:G:N2 | 11:AK:40:ASN:HA | 2.21 | 0.56 |
| 1:AA:844:G:N3 | 1:AA:845:A:N7 | 2.54 | 0.56 |
| 1:AA:1319:A:C8 | 1:AA:1323:G:C6 | 2.94 | 0.56 |
| 1:AA:1322:C:OP1 | 19:AS:78:ARG:NH2 | 2.39 | 0.56 |
| 22:BA:776:G:H4' | 22:BA:777:G:O5' | 2.05 | 0.56 |
| 22:BA:953:G:H5'' | 34:BM:16:ARG:NH1 | 2.21 | 0.56 |
| 22:BA:1436:G:N2 | 22:BA:1557:C:C2 | 2.74 | 0.56 |
| 22:BA:2825:G:H2' | 22:BA:2826:A:H5' | 1.86 | 0.56 |
| 41:BT:63:VAL:O | 41:BT:79:ASP:HB3 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CA:620:C:C2 | 4:CD:132:ILE:HD13 | 2.41 | 0.56 |
| 1:CA:632:U:O2 | 1:CA:632:U:H2' | 2.06 | 0.56 |
| 1:CA:1093:A:C5 | 1:CA:1095:U:O4' | 2.58 | 0.56 |
| 6:CF:45:ARG:HD2 | 6:CF:59:TYR:CE2 | 2.41 | 0.56 |
| 22:DA:565:C:H4' | 22:DA:1253:A:N6 | 2.21 | 0.56 |
| 22:DA:868:U:C4 | 22:DA:869:G:N7 | 2.74 | 0.56 |
| 22:DA:1115:G:O2' | 22:DA:1116:G:OP2 | 2.18 | 0.56 |
| 22:DA:1530:G:C2 | 22:DA:1542:U:O2 | 2.58 | 0.56 |
| 22:DA:1907:G:C2 | 22:DA:1924:C:C2 | 2.94 | 0.56 |
| 22:DA:2024:G:OP2 | 22:DA:2034:U:H4' | 2.05 | 0.56 |
| 22:DA:2571:U:C4 | 22:DA:2574:G:H8 | 2.24 | 0.56 |
| 56:DA:3001:DOL:H463 | 56:DA:3001:DOL:C48 | 2.16 | 0.56 |
| 25:DD:187:LEU:CD2 | 25:DD:203:VAL:HG11 | 2.36 | 0.56 |
| 36:DO:100:HIS:CD2 | 36:DO:101:GLY:N | 2.74 | 0.56 |
| 1:AA:2:A:N6 | 1:AA:3:A:N1 | 2.53 | 0.56 |
| 1:AA:265:G:H4' | 17:AQ:67:LEU:O | 2.05 | 0.56 |
| 1:AA:429:U:H1' | 1:AA:430:A:H5'' | 1.87 | 0.56 |
| 1:AA:1031:C:H4' | 1:AA:1032:G:O5' | 2.06 | 0.56 |
| 2:AB:181:ILE:O | 2:AB:183:VAL:HG23 | 2.04 | 0.56 |
| 4:AD:26:ARG:CD | 4:AD:31:LYS:HD2 | 2.36 | 0.56 |
| 5:AE:157:ARG:C | 5:AE:159:LYS:N | 2.60 | 0.56 |
| 20:AT:58:VAL:CG1 | 20:AT:72:ALA:CB | 2.84 | 0.56 |
| 22:BA:1917:U:H2' | 22:BA:1918:A:H5' | 1.87 | 0.56 |
| 22:BA:2334:U:C4 | 36:BO:16:ARG:HD3 | 2.40 | 0.56 |
| 27:BF:42:GLU:O | 27:BF:42:GLU:HG2 | 2.06 | 0.56 |
| 32:BK:116:ILE:HG13 | 32:BK:117:SER:N | 2.21 | 0.56 |
| 1:CA:375:U:C2 | 1:CA:376:G:C8 | 2.94 | 0.56 |
| 1:CA:718:A:C8 | 1:CA:719:C:C5 | 2.94 | 0.56 |
| 5:CE:109:GLY:O | 5:CE:110:ALA:HB3 | 2.05 | 0.56 |
| 19:CS:80:TYR:O | 19:CS:81:ARG:CB | 2.54 | 0.56 |
| 20:CT:60:ARG:O | 20:CT:64:LYS:N | 2.36 | 0.56 |
| 22:DA:76:C:HO2' | 46:DY:55:THR:HG1 | 1.51 | 0.56 |
| 22:DA:1062:G:C5 | 22:DA:1088:A:H2' | 2.41 | 0.56 |
| 24:DC:57:GLY:HA3 | 24:DC:213:TRP:HA | 1.88 | 0.56 |
| 24:DC:80:ARG:NE | 24:DC:82:GLU:OE2 | 2.39 | 0.56 |
| 32:DK:121:GLU:O | 32:DK:122:VAL:O | 2.24 | 0.56 |
| 51:D3:26:HIS:CE1 | 51:D3:48:ALA:HB2 | 2.41 | 0.56 |
| 52:D4:36:ARG:CG | 52:D4:37:GLN:N | 2.68 | 0.56 |
| 1:AA:11:G:C5 | 1:AA:12:U:C5 | 2.93 | 0.56 |
| 17:AQ:48:ASP:C | 17:AQ:48:ASP:OD2 | 2.43 | 0.56 |
| 19:AS:5:LEU:O | 19:AS:7:LYS:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 22:BA:813:U:H2' | 22:BA:814:C:C6 | 2.41 | 0.56 |
| 22:BA:973:A:H5' | 22:BA:1188:U:H1' | 1.87 | 0.56 |
| 22:BA:2243:U:OP1 | 58:BA:3739:HOH:O | 2.17 | 0.56 |
| 37:BP:31:TRP:CE2 | 37:BP:40:LEU:CD1 | 2.89 | 0.56 |
| 52:B4:36:ARG:HG2 | 52:B4:37:GLN:N | 2.20 | 0.56 |
| 1:CA:337:G:H2' | 1:CA:338:A:C8 | 2.40 | 0.56 |
| 1:CA:664:G:N2 | 1:CA:666:G:C8 | 2.74 | 0.56 |
| 1:CA:991:U:C4 | 1:CA:1212:U:O4' | 2.59 | 0.56 |
| 1:CA:1004:A:C6 | 1:CA:1005:A:C6 | 2.93 | 0.56 |
| 21:CU:35:ARG:NH2 | 58:CU:101:HOH:O | 2.39 | 0.56 |
| 22:DA:546:U:O2' | 22:DA:547:A:O4' | 2.20 | 0.56 |
| 22:DA:1087:G:C2 | 22:DA:1089:A:C2 | 2.94 | 0.56 |
| 22:DA:1304:A:N1 | 22:DA:1305:C:C4 | 2.74 | 0.56 |
| 22:DA:2111:U:C4 | 22:DA:2145:C:H2' | 2.41 | 0.56 |
| 22:DA:2365:G:H4' | 44:DW:60:PHE:CE2 | 2.41 | 0.56 |
| 22:DA:2602:A:H4' | 22:DA:2603:G:H5' | 1.86 | 0.56 |
| 25:DD:16:THR:OG1 | 25:DD:18:ASP:OD2 | 2.12 | 0.56 |
| 45:DX:68:LEU:HD22 | 45:DX:78:TYR:CZ | 2.41 | 0.56 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.41 | 0.55 |
| 10:AJ:35:GLN:CG | 10:AJ:77:VAL:HB | 2.36 | 0.55 |
| 20:AT:70:ASN:OD1 | 20:AT:70:ASN:N | 2.28 | 0.55 |
| 22:BA:878:A:N6 | 22:BA:899:A:O2' | 2.39 | 0.55 |
| 22:BA:1009:A:OP2 | 31:BJ:39:LYS:NZ | 2.38 | 0.55 |
| 22:BA:1322:A:O3' | 40:BS:84:ARG:NH1 | 2.37 | 0.55 |
| 22:BA:2076:U:O2 | 22:BA:2076:U:O4' | 2.23 | 0.55 |
| 30:BI:116:ASP:O | 30:BI:117:MET:CB | 2.54 | 0.55 |
| 37:BP:52:ASN:O | 37:BP:53:ARG:HG2 | 2.06 | 0.55 |
| 40:BS:73:LYS:HB2 | 40:BS:106:VAL:HB | 1.87 | 0.55 |
| 1:CA:495:A:N1 | 1:CA:496:A:N6 | 2.53 | 0.55 |
| 1:CA:568:G:N2 | 1:CA:883:C:C2 | 2.74 | 0.55 |
| 1:CA:866:C:C5 | 1:CA:867:G:H1' | 2.41 | 0.55 |
| 1:CA:1029:U:O2 | 1:CA:1029:U:H2' | 2.05 | 0.55 |
| 1:CA:1417:G:C6 | 1:CA:1482:G:C6 | 2.94 | 0.55 |
| 12:CL:3:THR:HB | 12:CL:6:GLN:HG3 | 1.86 | 0.55 |
| 22:DA:158:U:O2 | 22:DA:169:G:C2 | 2.58 | 0.55 |
| 22:DA:301:G:H1' | 22:DA:302:C:C6 | 2.41 | 0.55 |
| 22:DA:532:A:N7 | 22:DA:2021:C:H2' | 2.20 | 0.55 |
| 22:DA:559:G:N3 | 38:DQ:56:GLN:NE2 | 2.55 | 0.55 |
| 22:DA:776:G:C8 | 22:DA:793:A:C4 | 2.94 | 0.55 |
| 22:DA:1627:G:C2 | 22:DA:1628:G:C8 | 2.94 | 0.55 |
| 22:DA:2550:G:C6 | 22:DA:2551:C:N4 | 2.75 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2726:A:O2' | 22:DA:2727:A:O5' | 2.24 | 0.55 |
| 30:DI:18:ALA:O | 30:DI:19:ASN:CB | 2.54 | 0.55 |
| 42:DU:54:GLN:N | 42:DU:55:PRO:CD | 2.69 | 0.55 |
| 1:AA:91:U:H2' | 1:AA:92:U:O4' | 2.07 | 0.55 |
| 1:AA:211:G:N2 | 1:AA:212:G:C8 | 2.74 | 0.55 |
| 1:AA:1426:G:H2' | 1:AA:1427:C:O4' | 2.06 | 0.55 |
| 2:AB:186:ILE:HA | 2:AB:200:ILE:HB | 1.88 | 0.55 |
| 5:AE:155:ALA:HB1 | 8:AH:66:PHE:CZ | 2.41 | 0.55 |
| 9:AI:40:GLY:O | 9:AI:41:ARG:CB | 2.55 | 0.55 |
| 22:BA:682:G:H5' | 50:B2:26:ASN:OD1 | 2.05 | 0.55 |
| 22:BA:686:U:H2' | 22:BA:788:A:N1 | 2.22 | 0.55 |
| 22:BA:1045:C:C3' | 22:BA:1046:A:H5' | 2.36 | 0.55 |
| 22:BA:1794:A:H2' | 22:BA:1795:C:H6 | 1.70 | 0.55 |
| 25:BD:151:THR:HG22 | 25:BD:152:PRO:CD | 2.36 | 0.55 |
| 25:BD:151:THR:HG22 | 25:BD:152:PRO:HD2 | 1.87 | 0.55 |
| 27:BF:28:VAL:HG13 | 27:BF:28:VAL:O | 2.06 | 0.55 |
| 1:CA:134:G:H2' | 1:CA:135:C:O4' | 2.07 | 0.55 |
| 1:CA:407:U:H2' | 1:CA:408:A:C8 | 2.41 | 0.55 |
| 1:CA:644:U:H2' | 1:CA:645:G:O4' | 2.06 | 0.55 |
| 21:CU:53:VAL:HG13 | 21:CU:54:LYS:N | 2.21 | 0.55 |
| 22:DA:200:U:O4 | 22:DA:248:G:C2 | 2.59 | 0.55 |
| 22:DA:478:A:C6 | 22:DA:480:A:C6 | 2.94 | 0.55 |
| 22:DA:1847:A:C2' | 22:DA:1848:A:OP2 | 2.54 | 0.55 |
| 22:DA:2019:A:H4' | 38:DQ:34:VAL:CG2 | 2.36 | 0.55 |
| 22:DA:2854:G:N2 | 22:DA:2864:G:C2 | 2.75 | 0.55 |
| 39:DR:39:LEU:HA | 39:DR:49:ILE:HG21 | 1.87 | 0.55 |
| 39:DR:66:HIS:CD2 | 39:DR:94:THR:HG23 | 2.41 | 0.55 |
| 45:DX:33:LEU:HD23 | 45:DX:50:ARG:CZ | 2.36 | 0.55 |
| 1:AA:1450:U:H2' | 1:AA:1452:C:C5 | 2.41 | 0.55 |
| 2:AB:151:ILE:O | 2:AB:152:LYS:C | 2.44 | 0.55 |
| 4:AD:130:VAL:HG11 | 4:AD:135:TYR:CD1 | 2.40 | 0.55 |
| 6:AF:9:MET:HE2 | 18:AR:65:LEU:HD22 | 1.87 | 0.55 |
| 22:BA:45:G:H5'' | 22:BA:46:G:H5' | 1.88 | 0.55 |
| 22:BA:58:G:OP1 | 41:BT:78:SER:CB | 2.55 | 0.55 |
| 22:BA:626:A:H2' | 33:BL:78:ARG:NH1 | 2.20 | 0.55 |
| 22:BA:1079:C:C5 | 22:BA:1088:A:N1 | 2.75 | 0.55 |
| 22:BA:1932:A:C2 | 22:BA:1969:A:C2 | 2.95 | 0.55 |
| 22:BA:2153:C:H2' | 22:BA:2154:A:O4' | 2.07 | 0.55 |
| 22:BA:2177:C:O2' | 53:B5:47:LYS:NZ | 2.35 | 0.55 |
| 56:BA:3001:DOL:N5 | 56:BA:3001:DOL:C42 | 2.68 | 0.55 |
| 27:BF:108:VAL:N | 27:BF:109:PRO:CD | 2.69 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BK:70:ARG:HD3 | 32:BK:76:VAL:HG22 | 1.87 | 0.55 |
| 4:CD:9:LEU:CD2 | 4:CD:22:LYS:HD2 | 2.37 | 0.55 |
| 6:CF:80:PHE:CG | 6:CF:80:PHE:O | 2.59 | 0.55 |
| 18:CR:58:ALA:O | 18:CR:61:ARG:N | 2.40 | 0.55 |
| 22:DA:669:G:C2 | 22:DA:801:G:N1 | 2.74 | 0.55 |
| 22:DA:1020:A:C2 | 22:DA:1141:U:C2 | 2.94 | 0.55 |
| 22:DA:1530:G:N2 | 22:DA:1542:U:O2 | 2.38 | 0.55 |
| 22:DA:1856:U:C4 | 22:DA:1857:G:C6 | 2.95 | 0.55 |
| 22:DA:1998:A:OP2 | 25:DD:141:ARG:NH2 | 2.39 | 0.55 |
| 22:DA:2843:G:N2 | 22:DA:2875:C:C2 | 2.74 | 0.55 |
| 30:DI:80:LEU:HD23 | 30:DI:84:ALA:HB2 | 1.88 | 0.55 |
| 41:DT:21:SER:O | 41:DT:22:THR:C | 2.44 | 0.55 |
| 50:D2:35:ARG:O | 50:D2:38:GLY:N | 2.39 | 0.55 |
| 1:AA:1350:A:OP1 | 9:AI:123:ARG:NE | 2.38 | 0.55 |
| 9:AI:58:VAL:O | 9:AI:58:VAL:HG12 | 2.06 | 0.55 |
| 16:AP:38:PHE:CZ | 16:AP:51:ARG:HB2 | 2.42 | 0.55 |
| 20:AT:68:HIS:C | 20:AT:69:LYS:HG3 | 2.25 | 0.55 |
| 22:BA:1911:U:C4 | 22:BA:1918:A:C5 | 2.94 | 0.55 |
| 28:BG:99:LYS:O | 28:BG:100:GLY:C | 2.45 | 0.55 |
| 41:BT:33:LYS:HG3 | 41:BT:80:TRP:CE3 | 2.41 | 0.55 |
| 44:BW:17:GLU:O | 44:BW:19:LYS:NZ | 2.36 | 0.55 |
| 22:DA:699:A:H2' | 22:DA:700:G:O4' | 2.06 | 0.55 |
| 22:DA:1316:U:C2 | 22:DA:1337:G:N2 | 2.75 | 0.55 |
| 22:DA:1438:U:C5 | 22:DA:1552:A:N1 | 2.74 | 0.55 |
| 22:DA:1730:C:O2' | 22:DA:1731:G:C2 | 2.58 | 0.55 |
| 22:DA:1869:G:H3' | 22:DA:1870:C:H5' | 1.88 | 0.55 |
| 22:DA:1935:G:H1' | 22:DA:1964:G:N2 | 2.21 | 0.55 |
| 22:DA:2146:C:H4' | 22:DA:2147:A:OP1 | 2.05 | 0.55 |
| 22:DA:2310:C:C4 | 27:DF:77:PHE:CZ | 2.94 | 0.55 |
| 22:DA:2520:C:HO2' | 22:DA:2565:A:HO2' | 1.52 | 0.55 |
| 25:DD:112:THR:O | 25:DD:195:GLY:HA2 | 2.06 | 0.55 |
| 39:DR:78:ARG:HB3 | 39:DR:83:TYR:CD1 | 2.41 | 0.55 |
| 22:BA:580:U:H2' | 22:BA:581:C:C6 | 2.40 | 0.55 |
| 22:BA:2192:U:C4 | 22:BA:2193:G:C8 | 2.94 | 0.55 |
| 22:BA:2314:A:OP1 | 27:BF:88:LYS:NZ | 2.40 | 0.55 |
| 39:BR:29:THR:O | 39:BR:63:VAL:HB | 2.07 | 0.55 |
| 1:CA:801:U:C2 | 1:CA:802:A:N7 | 2.75 | 0.55 |
| 1:CA:1089:G:N2 | 1:CA:1090:U:H1' | 2.22 | 0.55 |
| 1:CA:1298:U:O2 | 1:CA:1298:U:C2' | 2.54 | 0.55 |
| 1:CA:1345:U:C2 | 1:CA:1377:A:C2 | 2.95 | 0.55 |
| 16:CP:38:PHE:CE2 | 16:CP:51:ARG:HD2 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:121:G:H1' | 22:DA:131:A:C2 | 2.41 | 0.55 |
| 22:DA:484:C:N4 | 22:DA:497:A:C2 | 2.74 | 0.55 |
| 22:DA:902:C:H2' | 22:DA:903:C:C6 | 2.42 | 0.55 |
| 22:DA:1361:G:C5 | 22:DA:1371:G:N2 | 2.74 | 0.55 |
| 22:DA:1570:A:H2' | 22:DA:1571:A:C8 | 2.42 | 0.55 |
| 22:DA:1599:U:P | 41:DT:40:LYS:HD2 | 2.47 | 0.55 |
| 22:DA:1917:U:C2' | 22:DA:1918:A:H5' | 2.37 | 0.55 |
| 22:DA:2162:G:H4' | 22:DA:2163:A:OP1 | 2.06 | 0.55 |
| 34:DM:1:MET:HE3 | 34:DM:43:ALA:HB3 | 1.89 | 0.55 |
| 1:AA:1226:C:OP2 | 13:AM:90:ARG:NH2 | 2.40 | 0.55 |
| 1:AA:1327:C:C2' | 1:AA:1328:C:H5' | 2.37 | 0.55 |
| 4:AD:123:ILE:HD13 | 4:AD:123:ILE:N | 2.20 | 0.55 |
| 9:AI:58:VAL:O | 9:AI:59:GLU:CB | 2.55 | 0.55 |
| 22:BA:587:C:C6 | 22:BA:671:C:H1' | 2.42 | 0.55 |
| 22:BA:2077:A:O2' | 22:BA:2078:C:H5' | 2.07 | 0.55 |
| 22:BA:2683:C:H4' | 25:BD:13:ARG:NH1 | 2.21 | 0.55 |
| 25:BD:12:THR:CG2 | 37:BP:9:GLU:OE2 | 2.55 | 0.55 |
| 29:BH:86:ASP:O | 29:BH:87:GLU:CB | 2.53 | 0.55 |
| 1:CA:624:C:H2' | 1:CA:625:U:O4' | 2.07 | 0.55 |
| 4:CD:34:ILE:O | 4:CD:35:GLU:HB3 | 2.06 | 0.55 |
| 12:CL:82:ILE:HD11 | 12:CL:95:TYR:HB2 | 1.87 | 0.55 |
| 22:DA:35:G:C4 | 22:DA:454:A:C2 | 2.94 | 0.55 |
| 22:DA:150:U:H2' | 22:DA:151:C:C6 | 2.41 | 0.55 |
| 22:DA:1740:G:C2 | 22:DA:1741:C:C2 | 2.95 | 0.55 |
| 22:DA:2103:C:H2' | 22:DA:2104:C:C6 | 2.41 | 0.55 |
| 22:DA:2390:U:OP2 | 51:D3:35:LYS:NZ | 2.39 | 0.55 |
| 22:DA:2412:A:H3' | 22:DA:2413:G:C8 | 2.42 | 0.55 |
| 22:DA:2469:A:H4' | 34:DM:55:ARG:HD3 | 1.87 | 0.55 |
| 26:DE:8:ALA:O | 26:DE:9:GLN:HB2 | 2.06 | 0.55 |
| 38:DQ:50:ARG:O | 38:DQ:54:LYS:NZ | 2.33 | 0.55 |
| 45:DX:68:LEU:HD22 | 45:DX:78:TYR:CE1 | 2.42 | 0.55 |
| 1:AA:316:C:C2 | 1:AA:317:U:C5 | 2.95 | 0.55 |
| 1:AA:1145:A:O2' | 1:AA:1146:A:O5' | 2.23 | 0.55 |
| 5:AE:119:GLY:O | 5:AE:121:HIS:ND1 | 2.39 | 0.55 |
| 9:AI:30:ILE:HD11 | 9:AI:38:TYR:HB3 | 1.87 | 0.55 |
| 22:BA:141:G:H5'' | 22:BA:142:A:C6 | 2.41 | 0.55 |
| 22:BA:253:C:OP2 | 51:B3:5:LYS:HE3 | 2.07 | 0.55 |
| 22:BA:742:A:H2' | 22:BA:743:A:C8 | 2.41 | 0.55 |
| 22:BA:1731:G:C2 | 22:BA:1733:G:C4 | 2.95 | 0.55 |
| 29:BH:98:ASP:O | 29:BH:102:ALA:HB3 | 2.07 | 0.55 |
| 30:BI:18:ALA:C | 30:BI:20:PRO:HD3 | 2.27 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1060:U:C5' | 10:CJ:53:ILE:HG23 | 2.37 | 0.55 |
| 5:CE:80:THR:OG1 | 5:CE:98:PRO:O | 2.25 | 0.55 |
| 15:CO:27:VAL:HG12 | 15:CO:28:GLN:N | 2.21 | 0.55 |
| 17:CQ:69:LYS:O | 17:CQ:69:LYS:HG2 | 2.06 | 0.55 |
| 22:DA:308:G:C8 | 22:DA:501:A:H1' | 2.42 | 0.55 |
| 22:DA:420:C:H2' | 22:DA:421:C:C6 | 2.41 | 0.55 |
| 22:DA:1138:G:O2' | 31:DJ:104:ALA:O | 2.23 | 0.55 |
| 22:DA:1182:G:H2' | 22:DA:1183:U:O4' | 2.07 | 0.55 |
| 22:DA:1352:U:H5 | 22:DA:1377:G:C5 | 2.25 | 0.55 |
| 22:DA:1380:G:OP2 | 58:DA:3751:HOH:O | 2.18 | 0.55 |
| 22:DA:1441:G:H2' | 22:DA:1442:U:C6 | 2.42 | 0.55 |
| 22:DA:1459:G:C2 | 22:DA:1461:C:C2 | 2.95 | 0.55 |
| 22:DA:1623:G:C5 | 22:DA:1624:U:C5 | 2.95 | 0.55 |
| 22:DA:1806:C:O2 | 24:DC:44:ASN:ND2 | 2.40 | 0.55 |
| 22:DA:2107:G:C2 | 22:DA:2183:A:C2 | 2.95 | 0.55 |
| 22:DA:2176:A:H2' | 22:DA:2177:C:C6 | 2.42 | 0.55 |
| 1:AA:263:A:OP2 | 20:AT:74:ARG:NH1 | 2.40 | 0.55 |
| 1:AA:723:U:H5' | 1:AA:724:G:OP1 | 2.05 | 0.55 |
| 10:AJ:6:ILE:HD12 | 10:AJ:76:ILE:HB | 1.89 | 0.55 |
| 12:AL:94:ARG:HB2 | 12:AL:95:TYR:CE2 | 2.42 | 0.55 |
| 15:AO:19:ALA:O | 15:AO:20:ASN:CB | 2.54 | 0.55 |
| 15:AO:19:ALA:O | 15:AO:20:ASN:HB2 | 2.07 | 0.55 |
| 22:BA:996:A:C2 | 22:BA:997:G:C8 | 2.94 | 0.55 |
| 22:BA:1028:A:N6 | 22:BA:1125:G:H2' | 2.22 | 0.55 |
| 22:BA:1083:U:O2 | 22:BA:1085:A:C8 | 2.59 | 0.55 |
| 22:BA:1802:A:N1 | 22:BA:1822:C:H1' | 2.21 | 0.55 |
| 22:BA:2637:U:C2' | 22:BA:2638:G:H5' | 2.37 | 0.55 |
| 29:BH:120:GLY:CA | 29:BH:122:LEU:HA | 2.37 | 0.55 |
| 29:BH:121:VAL:N | 29:BH:122:LEU:CA | 2.69 | 0.55 |
| 29:BH:121:VAL:N | 29:BH:122:LEU:CB | 2.70 | 0.55 |
| 38:BQ:24:TYR:O | 38:BQ:25:TYR:HB2 | 2.07 | 0.55 |
| 39:BR:48:LYS:O | 39:BR:49:ILE:C | 2.45 | 0.55 |
| 40:BS:4:ILE:HG12 | 40:BS:106:VAL:HG22 | 1.89 | 0.55 |
| 1:CA:32:A:H2' | 1:CA:32:A:N3 | 2.21 | 0.55 |
| 1:CA:466:A:C2 | 1:CA:468:A:C8 | 2.94 | 0.55 |
| 1:CA:692:U:H1' | 1:CA:695:A:N7 | 2.21 | 0.55 |
| 1:CA:1171:A:C2 | 1:CA:1172:C:C2 | 2.95 | 0.55 |
| 1:CA:1394:A:N1 | 1:CA:1500:A:O2' | 2.36 | 0.55 |
| 16:CP:51:ARG:C | 16:CP:51:ARG:HD3 | 2.27 | 0.55 |
| 22:DA:126:A:N7 | 22:DA:127:A:N1 | 2.54 | 0.55 |
| 22:DA:144:A:C2 | 22:DA:145:C:C2 | 2.94 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:187:G:N2 | 22:DA:210:C:H1' | 2.22 | 0.55 |
| 22:DA:200:U:C4 | 22:DA:248:G:N2 | 2.75 | 0.55 |
| 22:DA:475:C:N3 | 22:DA:481:G:C6 | 2.75 | 0.55 |
| 22:DA:528:A:H2' | 22:DA:529:A:H5'' | 1.88 | 0.55 |
| 22:DA:1077:A:C2 | 22:DA:1088:A:C2 | 2.95 | 0.55 |
| 22:DA:1293:C:H2' | 22:DA:1294:U:O4' | 2.07 | 0.55 |
| 22:DA:1827:U:H2' | 22:DA:1828:G:O5' | 2.06 | 0.55 |
| 22:DA:1856:U:O4 | 22:DA:1857:G:N1 | 2.40 | 0.55 |
| 22:DA:2395:C:H2' | 22:DA:2396:G:O4' | 2.07 | 0.55 |
| 25:DD:123:LYS:HG2 | 25:DD:165:MET:SD | 2.47 | 0.55 |
| 30:DI:90:SER:HB3 | 30:DI:93:PRO:HG3 | 1.89 | 0.55 |
| 1:AA:1124:G:H3' | 1:AA:1145:A:N6 | 2.21 | 0.55 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.42 | 0.55 |
| 7:AG:15:ASP:OD2 | 7:AG:44:TYR:OH | 2.25 | 0.55 |
| 9:AI:43:THR:O | 9:AI:44:ALA:CB | 2.55 | 0.55 |
| 13:AM:15:ALA:HB1 | 13:AM:34:LEU:HD21 | 1.88 | 0.55 |
| 17:AQ:52:GLU:CD | 17:AQ:52:GLU:N | 2.60 | 0.55 |
| 22:BA:479:A:N3 | 22:BA:481:G:H5'' | 2.22 | 0.55 |
| 22:BA:1084:A:H2' | 22:BA:1085:A:C8 | 2.42 | 0.55 |
| 22:BA:2043:C:OP1 | 22:BA:2777:G:O2' | 2.22 | 0.55 |
| 35:BN:33:ILE:HG13 | 35:BN:114:GLU:HB3 | 1.88 | 0.55 |
| 39:BR:64:VAL:HG23 | 39:BR:65:ALA:N | 2.22 | 0.55 |
| 40:BS:55:ILE:HG23 | 40:BS:66:ILE:HG12 | 1.89 | 0.55 |
| 1:CA:1003:G:C2 | 1:CA:1038:C:C4 | 2.95 | 0.55 |
| 5:CE:50:TYR:O | 5:CE:51:GLY:O | 2.24 | 0.55 |
| 22:DA:277:G:C2' | 22:DA:361:G:O6 | 2.55 | 0.55 |
| 22:DA:374:A:C6 | 22:DA:401:A:C8 | 2.95 | 0.55 |
| 22:DA:1027:A:N6 | 22:DA:1126:A:N3 | 2.55 | 0.55 |
| 22:DA:2091:C:C3' | 22:DA:2092:U:H5'' | 2.35 | 0.55 |
| 22:DA:2120:G:C2 | 22:DA:2121:G:C8 | 2.95 | 0.55 |
| 22:DA:2341:G:C6 | 22:DA:2342:C:C4 | 2.95 | 0.55 |
| 22:DA:2831:G:OP1 | 25:DD:56:LYS:NZ | 2.36 | 0.55 |
| 24:DC:210:ALA:HA | 24:DC:213:TRP:CE2 | 2.41 | 0.55 |
| 29:DH:31:VAL:HB | 29:DH:32:PRO:HD3 | 1.89 | 0.55 |
| 42:DU:41:LEU:HD12 | 42:DU:60:GLU:HG2 | 1.89 | 0.55 |
| 42:DU:72:ILE:HD13 | 42:DU:83:VAL:CG2 | 2.37 | 0.55 |
| 45:DX:31:PRO:HB2 | 45:DX:33:LEU:CD1 | 2.37 | 0.55 |
| 1:AA:254:G:OP1 | 17:AQ:69:LYS:O | 2.25 | 0.55 |
| 1:AA:582:C:C4 | 1:AA:583:A:N7 | 2.74 | 0.55 |
| 1:AA:667:G:H4' | 15:AO:51:HIS:ND1 | 2.22 | 0.55 |
| 6:AF:14:GLN:OE1 | 6:AF:17:GLN:HB2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:AJ:80:THR:O | 10:AJ:82:LYS:N | 2.40 | 0.55 |
| 17:AQ:45:HIS:CD2 | 17:AQ:70:THR:HG23 | 2.42 | 0.55 |
| 22:BA:308:G:C8 | 22:BA:501:A:H1' | 2.41 | 0.55 |
| 22:BA:686:U:H2' | 22:BA:788:A:C2 | 2.42 | 0.55 |
| 22:BA:1288:G:C5 | 22:BA:1327:A:C2 | 2.95 | 0.55 |
| 22:BA:1355:G:C2' | 22:BA:1356:G:H5' | 2.37 | 0.55 |
| 22:BA:1435:G:O2' | 22:BA:1436:G:H5' | 2.07 | 0.55 |
| 22:BA:1587:G:C4 | 22:BA:1588:G:C8 | 2.94 | 0.55 |
| 22:BA:1795:C:C4 | 22:BA:1796:U:C4 | 2.95 | 0.55 |
| 22:BA:1876:A:C2 | 22:BA:1877:A:C4 | 2.95 | 0.55 |
| 24:BC:57:GLY:HA2 | 24:BC:213:TRP:HA | 1.88 | 0.55 |
| 38:BQ:87:SER:HB3 | 39:BR:51:VAL:HA | 1.89 | 0.55 |
| 46:BY:23:ARG:O | 46:BY:24:GLU:C | 2.45 | 0.55 |
| 1:CA:1224:U:C4 | 1:CA:1322:C:O2 | 2.60 | 0.55 |
| 5:CE:98:PRO:O | 5:CE:122:ASN:ND2 | 2.37 | 0.55 |
| 10:CJ:92:LEU:O | 10:CJ:93:ALA:HB2 | 2.07 | 0.55 |
| 17:CQ:69:LYS:C | 17:CQ:70:THR:OG1 | 2.45 | 0.55 |
| 22:DA:24:G:C5 | 22:DA:25:U:C5 | 2.94 | 0.55 |
| 22:DA:202:U:H2' | 22:DA:203:A:C8 | 2.42 | 0.55 |
| 22:DA:289:G:H2' | 22:DA:290:U:O4' | 2.06 | 0.55 |
| 22:DA:630:G:H3' | 22:DA:631:A:C5' | 2.37 | 0.55 |
| 22:DA:647:G:C5 | 22:DA:648:G:N7 | 2.75 | 0.55 |
| 22:DA:1248:G:N7 | 26:DE:46:GLN:NE2 | 2.55 | 0.55 |
| 22:DA:1355:G:C2' | 22:DA:1356:G:H5' | 2.37 | 0.55 |
| 22:DA:1389:G:C2 | 22:DA:1390:U:O2 | 2.60 | 0.55 |
| 22:DA:1769:U:O2' | 22:DA:1958:C:OP1 | 2.25 | 0.55 |
| 22:DA:1826:G:C4 | 22:DA:1827:U:C5 | 2.95 | 0.55 |
| 22:DA:2373:G:C2 | 22:DA:2374:C:C2 | 2.94 | 0.55 |
| 22:DA:2842:G:C2 | 22:DA:2843:G:H1' | 2.42 | 0.55 |
| 22:DA:2888:C:H2' | 22:DA:2889:C:C6 | 2.41 | 0.55 |
| 23:DB:80:U:H2' | 23:DB:81:G:C8 | 2.42 | 0.55 |
| 31:DJ:30:THR:HG22 | 31:DJ:31:GLU:N | 2.21 | 0.55 |
| 31:DJ:36:LEU:O | 31:DJ:121:LYS:NZ | 2.40 | 0.55 |
| 39:DR:81:LYS:O | 39:DR:82:HIS:C | 2.44 | 0.55 |
| 43:DV:9:ARG:NH2 | 43:DV:17:SER:OG | 2.40 | 0.55 |
| 45:DX:12:PRO:HB3 | 45:DX:28:ARG:NH2 | 2.21 | 0.55 |
| 1:AA:405:U:OP1 | 1:AA:406:G:O2' | 2.20 | 0.54 |
| 1:AA:882:C:O2' | 1:AA:883:C:H5' | 2.07 | 0.54 |
| 1:AA:1055:A:C6 | 1:AA:1206:G:C5 | 2.95 | 0.54 |
| 4:AD:65:TYR:O | 4:AD:115:ARG:NH2 | 2.40 | 0.54 |
| 14:AN:51:LEU:CB | 14:AN:52:PRO:HD2 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:760:G:H2' | 22:BA:761:A:O4' | 2.08 | 0.54 |
| 22:BA:1847:A:C8 | 22:BA:1847:A:OP2 | 2.60 | 0.54 |
| 22:BA:1936:A:H2 | 22:BA:1943:U:H3 | 1.53 | 0.54 |
| 22:BA:2017:U:H4' | 48:B0:5:GLN:O | 2.07 | 0.54 |
| 22:BA:2406:A:C2 | 33:BL:69:ARG:NH2 | 2.76 | 0.54 |
| 29:BH:10:ALA:O | 29:BH:12:LEU:N | 2.40 | 0.54 |
| 33:BL:132:ARG:HG3 | 33:BL:142:ILE:HD12 | 1.89 | 0.54 |
| 36:BO:49:VAL:HG13 | 36:BO:50:ALA:N | 2.22 | 0.54 |
| 48:B0:55:ILE:O | 48:B0:56:ALA:HB3 | 2.05 | 0.54 |
| 49:B1:14:SER:HB3 | 49:B1:48:ILE:O | 2.07 | 0.54 |
| 50:B2:18:PHE:HA | 50:B2:43:THR:HG21 | 1.88 | 0.54 |
| 1:CA:636:U:H2' | 1:CA:637:C:C6 | 2.41 | 0.54 |
| 1:CA:728:A:H2' | 1:CA:729:A:C8 | 2.42 | 0.54 |
| 1:CA:1178:G:N2 | 1:CA:1181:G:OP2 | 2.41 | 0.54 |
| 1:CA:1279:G:H5'' | 10:CJ:9:ARG:NH2 | 2.22 | 0.54 |
| 1:CA:1480:A:H2' | 1:CA:1481:U:O4' | 2.08 | 0.54 |
| 9:CI:33:ARG:NE | 9:CI:37:GLN:OE1 | 2.40 | 0.54 |
| 15:CO:53:ARG:O | 15:CO:56:LEU:HB3 | 2.07 | 0.54 |
| 21:CU:12:PHE:O | 21:CU:13:ASP:CB | 2.55 | 0.54 |
| 22:DA:27:G:N2 | 22:DA:512:G:H1' | 2.22 | 0.54 |
| 22:DA:295:G:H2' | 22:DA:295:G:N3 | 2.21 | 0.54 |
| 22:DA:2057:G:OP2 | 58:DA:3485:HOH:O | 2.18 | 0.54 |
| 22:DA:2497:A:N3 | 22:DA:2498:C:N4 | 2.54 | 0.54 |
| 27:DF:128:TYR:CG | 27:DF:170:LEU:CD1 | 2.90 | 0.54 |
| 36:DO:111:ARG:NH2 | 36:DO:117:PHE:O | 2.40 | 0.54 |
| 1:AA:89:U:O2' | 1:AA:90:C:H5' | 2.07 | 0.54 |
| 1:AA:390:U:H2' | 1:AA:391:G:C8 | 2.42 | 0.54 |
| 5:AE:46:VAL:CG2 | 5:AE:118:ALA:HA | 2.37 | 0.54 |
| 6:AF:98:GLU:HG3 | 6:AF:99:ALA:N | 2.22 | 0.54 |
| 9:AI:57:MET:O | 9:AI:59:GLU:N | 2.41 | 0.54 |
| 20:AT:15:GLU:OE1 | 20:AT:19:LYS:NZ | 2.40 | 0.54 |
| 22:BA:273:G:N2 | 22:BA:365:U:C2 | 2.75 | 0.54 |
| 22:BA:1324:G:C4 | 22:BA:1328:A:N6 | 2.75 | 0.54 |
| 22:BA:2660:A:H2' | 22:BA:2661:G:O4' | 2.07 | 0.54 |
| 24:BC:88:SER:HB2 | 24:BC:200:HIS:CD2 | 2.42 | 0.54 |
| 24:BC:146:MET:SD | 24:BC:154:LEU:HD21 | 2.47 | 0.54 |
| 29:BH:90:LEU:CD2 | 29:BH:93:SER:HA | 2.37 | 0.54 |
| 33:BL:77:ILE:HD11 | 33:BL:101:ILE:CG2 | 2.37 | 0.54 |
| 40:BS:38:TYR:CD2 | 48:B0:39:LEU:HD21 | 2.41 | 0.54 |
| 1:CA:71:A:C2 | 1:CA:72:A:C8 | 2.95 | 0.54 |
| 1:CA:1255:G:C6 | 1:CA:1279:G:C8 | 2.95 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:CN:54:ASP:HA | 14:CN:59:ARG:HD3 | 1.89 | 0.54 |
| 20:CT:36:TYR:CD1 | 20:CT:36:TYR:C | 2.81 | 0.54 |
| 22:DA:526:A:N6 | 22:DA:2626:C:H4' | 2.22 | 0.54 |
| 22:DA:537:G:C6 | 22:DA:555:G:C2 | 2.95 | 0.54 |
| 22:DA:732:C:H2' | 22:DA:733:G:O4' | 2.07 | 0.54 |
| 22:DA:834:G:H1' | 22:DA:2358:A:N3 | 2.23 | 0.54 |
| 22:DA:1410:G:N1 | 22:DA:1411:U:O4 | 2.41 | 0.54 |
| 22:DA:1439:A:N7 | 22:DA:1552:A:H2 | 2.04 | 0.54 |
| 22:DA:1585:C:C5 | 22:DA:1586:A:N7 | 2.76 | 0.54 |
| 22:DA:1623:G:C6 | 22:DA:1624:U:C5 | 2.95 | 0.54 |
| 22:DA:1779:U:H5 | 22:DA:1784:A:N7 | 2.05 | 0.54 |
| 36:DO:33:ARG:O | 36:DO:34:HIS:CD2 | 2.60 | 0.54 |
| 1:AA:1000:A:C2 | 1:AA:1041:G:C2 | 2.95 | 0.54 |
| 1:AA:1253:G:C4 | 1:AA:1254:A:C8 | 2.94 | 0.54 |
| 5:AE:101:GLU:CB | 5:AE:122:ASN:HB2 | 2.37 | 0.54 |
| 9:AI:120:LYS:HG3 | 9:AI:123:ARG:HB3 | 1.88 | 0.54 |
| 22:BA:783:A:C8 | 22:BA:784:G:H4' | 2.42 | 0.54 |
| 22:BA:980:A:C6 | 22:BA:981:A:N1 | 2.75 | 0.54 |
| 22:BA:1073:A:OP1 | 22:BA:1073:A:C8 | 2.60 | 0.54 |
| 22:BA:2517:C:C6 | 22:BA:2542:A:C5 | 2.95 | 0.54 |
| 30:BI:16:GLY:HA2 | 30:BI:51:LYS:HB3 | 1.89 | 0.54 |
| 33:BL:94:THR:HG22 | 33:BL:95:LEU:N | 2.22 | 0.54 |
| 44:BW:56:ASP:O | 44:BW:57:HIS:HB2 | 2.07 | 0.54 |
| 1:CA:477:C:H2' | 1:CA:478:A:C8 | 2.43 | 0.54 |
| 1:CA:859:G:H2' | 1:CA:860:A:C8 | 2.42 | 0.54 |
| 2:CB:57:LEU:HD11 | 2:CB:221:VAL:CG2 | 2.37 | 0.54 |
| 5:CE:132:ASN:O | 5:CE:136:VAL:HG12 | 2.08 | 0.54 |
| 8:CH:29:SER:HB2 | 8:CH:59:LEU:HB2 | 1.89 | 0.54 |
| 19:CS:79:THR:OG1 | 19:CS:79:THR:O | 2.24 | 0.54 |
| 22:DA:132:G:N2 | 22:DA:148:U:C2 | 2.75 | 0.54 |
| 22:DA:585:G:C2 | 22:DA:1256:G:C6 | 2.95 | 0.54 |
| 22:DA:909:A:C6 | 22:DA:912:C:C2 | 2.95 | 0.54 |
| 22:DA:1196:C:H1' | 22:DA:1226:A:C4 | 2.42 | 0.54 |
| 22:DA:1356:G:C2 | 22:DA:1357:C:H1' | 2.43 | 0.54 |
| 22:DA:1446:C:H2' | 22:DA:1447:C:O4' | 2.07 | 0.54 |
| 22:DA:1524:G:H2' | 22:DA:1524:G:N3 | 2.23 | 0.54 |
| 29:DH:79:THR:HA | 29:DH:145:ASN:HB2 | 1.89 | 0.54 |
| 34:DM:135:VAL:O | 34:DM:136:MET:CB | 2.54 | 0.54 |
| 1:AA:49:U:O4 | 1:AA:365:U:H5 | 1.89 | 0.54 |
| 1:AA:373:A:C2 | 1:AA:374:A:C8 | 2.95 | 0.54 |
| 1:AA:1093:A:OP2 | 7:AG:4:ARG:NH2 | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1446:A:C2' | 1:AA:1447:A:H5' | 2.37 | 0.54 |
| 4:AD:17:THR:CG2 | 4:AD:18:ASP:N | 2.69 | 0.54 |
| 13:AM:11:ASP:CG | 13:AM:12:HIS:N | 2.61 | 0.54 |
| 22:BA:804:A:H5'' | 22:BA:805:G:OP1 | 2.07 | 0.54 |
| 22:BA:1009:A:P | 31:BJ:39:LYS:HZ1 | 2.30 | 0.54 |
| 22:BA:1022:G:N2 | 22:BA:1142:A:C2 | 2.75 | 0.54 |
| 22:BA:1359:A:C8 | 22:BA:1373:A:C2 | 2.96 | 0.54 |
| 22:BA:1585:C:H2' | 22:BA:1586:A:O4' | 2.07 | 0.54 |
| 22:BA:1731:G:C4 | 22:BA:1733:G:C8 | 2.96 | 0.54 |
| 22:BA:2056:G:H2' | 22:BA:2056:G:N3 | 2.21 | 0.54 |
| 22:BA:2058:A:N6 | 58:BA:3487:HOH:O | 2.40 | 0.54 |
| 29:BH:90:LEU:HA | 29:BH:125:THR:HG23 | 1.90 | 0.54 |
| 30:BI:79:LEU:HD22 | 30:BI:109:ILE:CG2 | 2.37 | 0.54 |
| 39:BR:66:HIS:CE1 | 39:BR:94:THR:CG2 | 2.91 | 0.54 |
| 40:BS:25:ARG:HB2 | 40:BS:74:ILE:CG2 | 2.38 | 0.54 |
| 1:CA:211:G:N3 | 1:CA:211:G:H2' | 2.22 | 0.54 |
| 1:CA:295:C:C4 | 1:CA:296:U:C5 | 2.95 | 0.54 |
| 3:CC:130:PHE:CE1 | 3:CC:157:LEU:HB3 | 2.43 | 0.54 |
| 4:CD:29:ASP:C | 4:CD:31:LYS:H | 2.11 | 0.54 |
| 6:CF:22:ILE:O | 6:CF:26:THR:OG1 | 2.25 | 0.54 |
| 6:CF:69:GLU:O | 6:CF:72:ASP:HB3 | 2.07 | 0.54 |
| 7:CG:92:ARG:NE | 7:CG:93:PRO:CD | 2.71 | 0.54 |
| 12:CL:21:VAL:N | 12:CL:22:PRO:CD | 2.69 | 0.54 |
| 12:CL:90:LEU:HB3 | 12:CL:93:VAL:CG2 | 2.37 | 0.54 |
| 22:DA:247:G:C8 | 22:DA:249:C:C6 | 2.95 | 0.54 |
| 22:DA:513:A:C2 | 22:DA:514:A:C5 | 2.94 | 0.54 |
| 22:DA:677:A:O2' | 22:DA:2071:A:H5' | 2.08 | 0.54 |
| 22:DA:1076:C:H2' | 22:DA:1077:A:O4' | 2.08 | 0.54 |
| 22:DA:1356:G:N2 | 22:DA:1357:C:H1' | 2.22 | 0.54 |
| 22:DA:1805:A:N3 | 22:DA:1813:G:C2 | 2.75 | 0.54 |
| 22:DA:1914:C:H3' | 22:DA:1915:U:C6 | 2.43 | 0.54 |
| 22:DA:2159:G:H2' | 22:DA:2160:C:C6 | 2.42 | 0.54 |
| 22:DA:2345:G:C5 | 22:DA:2381:A:C2 | 2.96 | 0.54 |
| 30:DI:101:ILE:O | 30:DI:102:SER:CB | 2.55 | 0.54 |
| 1:AA:125:U:H2' | 1:AA:126:G:O4' | 2.06 | 0.54 |
| 1:AA:1306:A:C5 | 1:AA:1307:U:C5 | 2.95 | 0.54 |
| 1:AA:1342:C:O2' | 9:AI:126:GLN:HG3 | 2.08 | 0.54 |
| 2:AB:10:LEU:C | 2:AB:10:LEU:HD23 | 2.28 | 0.54 |
| 4:AD:19:LEU:HD22 | 4:AD:64:ILE:HG13 | 1.89 | 0.54 |
| 16:AP:51:ARG:HH11 | 16:AP:51:ARG:CG | 2.20 | 0.54 |
| 22:BA:1006:C:P | 58:BA:3781:HOH:O | 2.66 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BE:149:ILE:HD11 | 26:BE:172:ALA:CA | 2.37 | 0.54 |
| 27:BF:127:ASN:OD1 | 27:BF:157:THR:HA | 2.08 | 0.54 |
| 38:BQ:105:ALA:O | 38:BQ:108:ALA:HB3 | 2.07 | 0.54 |
| 1:CA:212:G:C2 | 1:CA:213:G:C8 | 2.96 | 0.54 |
| 1:CA:769:G:H4' | 1:CA:1513:A:H4' | 1.90 | 0.54 |
| 1:CA:1167:A:N7 | 1:CA:1169:A:C6 | 2.76 | 0.54 |
| 1:CA:1259:C:H3' | 1:CA:1260:G:H5'' | 1.90 | 0.54 |
| 8:CH:106:THR:OG1 | 8:CH:109:GLY:O | 2.16 | 0.54 |
| 11:CK:88:GLY:N | 11:CK:114:THR:HG22 | 2.21 | 0.54 |
| 14:CN:3:LYS:HD3 | 14:CN:6:MET:HG2 | 1.89 | 0.54 |
| 22:DA:235:U:C4 | 22:DA:236:C:C5 | 2.95 | 0.54 |
| 22:DA:449:A:C5 | 22:DA:450:G:C8 | 2.95 | 0.54 |
| 28:DG:27:LYS:HG3 | 28:DG:27:LYS:O | 2.08 | 0.54 |
| 1:AA:760:G:N7 | 1:AA:761:G:C8 | 2.76 | 0.54 |
| 1:AA:1126:U:O2 | 1:AA:1280:A:H5' | 2.08 | 0.54 |
| 1:AA:1167:A:N7 | 1:AA:1169:A:C6 | 2.76 | 0.54 |
| 2:AB:151:ILE:HG23 | 2:AB:152:LYS:N | 2.22 | 0.54 |
| 5:AE:81:LEU:HB3 | 5:AE:147:MET:CE | 2.37 | 0.54 |
| 13:AM:29:ARG:CZ | 13:AM:63:PHE:HB2 | 2.37 | 0.54 |
| 20:AT:5:LYS:O | 20:AT:7:ALA:N | 2.40 | 0.54 |
| 22:BA:744:U:P | 58:BA:3654:HOH:O | 2.64 | 0.54 |
| 22:BA:1095:A:C6 | 22:BA:1096:A:N6 | 2.76 | 0.54 |
| 22:BA:1178:C:H2' | 22:BA:1179:G:C8 | 2.43 | 0.54 |
| 22:BA:1246:A:H2' | 22:BA:1247:A:O5' | 2.08 | 0.54 |
| 22:BA:1414:C:C4 | 22:BA:1415:U:C5 | 2.95 | 0.54 |
| 22:BA:1584:U:O2 | 22:BA:1584:U:C2' | 2.56 | 0.54 |
| 29:BH:14:SER:OG | 29:BH:17:ASP:CG | 2.46 | 0.54 |
| 29:BH:77:THR:O | 29:BH:77:THR:CG2 | 2.56 | 0.54 |
| 29:BH:103:VAL:HG21 | 29:BH:132:PHE:CE1 | 2.42 | 0.54 |
| 30:BI:130:GLU:HB3 | 30:BI:134:ARG:NH2 | 2.22 | 0.54 |
| 1:CA:106:C:C2' | 1:CA:107:G:H5' | 2.37 | 0.54 |
| 1:CA:1521:C:C2 | 1:CA:1522:U:C6 | 2.95 | 0.54 |
| 3:CC:134:MET:SD | 3:CC:153:VAL:CG1 | 2.96 | 0.54 |
| 22:DA:53:A:C2 | 22:DA:179:C:H4' | 2.42 | 0.54 |
| 22:DA:447:A:N1 | 22:DA:454:A:O2' | 2.36 | 0.54 |
| 22:DA:453:A:H4' | 22:DA:472:A:N6 | 2.23 | 0.54 |
| 22:DA:587:C:N3 | 33:DL:33:ARG:NH2 | 2.55 | 0.54 |
| 22:DA:635:C:O2' | 22:DA:639:U:H5'' | 2.07 | 0.54 |
| 22:DA:980:A:C4 | 22:DA:1136:G:O4' | 2.61 | 0.54 |
| 22:DA:1060:U:H4' | 22:DA:1061:U:H5' | 1.90 | 0.54 |
| 22:DA:2817:U:O2 | 22:DA:2836:U:H1' | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DL:81:ASP:O | 33:DL:82:LEU:HB3 | 2.07 | 0.54 |
| 47:DZ:24:LEU:HD11 | 47:DZ:54:MET:HE2 | 1.89 | 0.54 |
| 1:AA:71:A:H3' | 1:AA:71:A:OP2 | 2.07 | 0.54 |
| 1:AA:129:A:H1' | 1:AA:130:A:C8 | 2.43 | 0.54 |
| 1:AA:1093:A:N3 | 1:AA:1109:C:O2' | 2.24 | 0.54 |
| 4:AD:109:ALA:N | 4:AD:113:GLU:OE2 | 2.37 | 0.54 |
| 8:AH:20:ALA:O | 8:AH:21:ASN:C | 2.46 | 0.54 |
| 21:AU:40:LYS:N | 21:AU:41:PRO:CD | 2.71 | 0.54 |
| 22:BA:1027:A:C6 | 22:BA:1126:A:N3 | 2.76 | 0.54 |
| 22:BA:1075:C:H2' | 22:BA:1076:C:C6 | 2.43 | 0.54 |
| 22:BA:1867:G:O2' | 22:BA:1868:C:H5' | 2.07 | 0.54 |
| 22:BA:1939:U:OP1 | 22:BA:2604:U:O2' | 2.26 | 0.54 |
| 53:B5:19:LYS:HG3 | 53:B5:23:ILE:CG1 | 2.38 | 0.54 |
| 1:CA:502:A:H2' | 1:CA:503:C:O4' | 2.08 | 0.54 |
| 1:CA:844:G:H2' | 1:CA:844:G:N3 | 2.23 | 0.54 |
| 1:CA:949:A:C2 | 1:CA:1233:G:C4 | 2.96 | 0.54 |
| 1:CA:1027:C:N4 | 1:CA:1034:G:C6 | 2.76 | 0.54 |
| 1:CA:1089:G:C4 | 1:CA:1090:U:C6 | 2.95 | 0.54 |
| 1:CA:1381:U:H2' | 1:CA:1382:C:O5' | 2.08 | 0.54 |
| 19:CS:15:LEU:HD13 | 19:CS:33:THR:HG21 | 1.90 | 0.54 |
| 22:DA:230:G:C2 | 22:DA:231:A:C8 | 2.96 | 0.54 |
| 22:DA:2146:C:C4' | 22:DA:2147:A:OP1 | 2.55 | 0.54 |
| 22:DA:2803:G:N2 | 22:DA:2804:U:C2 | 2.76 | 0.54 |
| 41:DT:69:ARG:HB2 | 41:DT:74:ILE:HG22 | 1.89 | 0.54 |
| 1:AA:126:G:OP1 | 1:AA:605:U:O2' | 2.17 | 0.54 |
| 1:AA:891:U:C2' | 1:AA:892:A:H5' | 2.37 | 0.54 |
| 1:AA:1053:G:O5' | 1:AA:1054:C:H3' | 2.08 | 0.54 |
| 22:BA:1084:A:HO2' | 22:BA:1105:U:HO2' | 1.54 | 0.54 |
| 22:BA:1508:A:O2' | 22:BA:1509:A:O4' | 2.24 | 0.54 |
| 24:BC:252:THR:O | 24:BC:254:GLY:N | 2.40 | 0.54 |
| 29:BH:90:LEU:O | 1:CA:358:U:H4' | 2.08 | 0.54 |
| 41:BT:88:LYS:O | 41:BT:89:GLU:HG2 | 2.08 | 0.54 |
| 1:CA:280:C:N3 | 17:CQ:40:ARG:HA | 2.23 | 0.54 |
| 1:CA:474:G:H2' | 1:CA:475:C:O4' | 2.08 | 0.54 |
| 1:CA:555:U:H2' | 1:CA:556:C:C6 | 2.43 | 0.54 |
| 1:CA:597:G:H2' | 1:CA:598:U:H5' | 1.90 | 0.54 |
| 1:CA:1151:A:C2 | 1:CA:1152:A:C6 | 2.96 | 0.54 |
| 1:CA:1347:G:O2' | 1:CA:1348:U:OP2 | 2.24 | 0.54 |
| 1:CA:1505:G:H4' | 1:CA:1506:U:H5'' | 1.89 | 0.54 |
| 5:CE:65:GLU:OE1 | 5:CE:69:ARG:NH2 | 2.41 | 0.54 |
| 6:CF:8:PHE:CE2 | 6:CF:60:VAL:HB | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:658:U:C2 | 22:DA:659:G:C8 | 2.96 | 0.54 |
| 22:DA:2835:A:C2 | 22:DA:2879:A:N7 | 2.76 | 0.54 |
| 22:DA:2873:A:H4' | 58:DA:3804:HOH:O | 2.08 | 0.54 |
| 42:DU:98:SER:O | 42:DU:99:ASN:HB3 | 2.08 | 0.54 |
| 1:AA:8:A:C6 | 4:AD:206:LYS:HB3 | 2.43 | 0.54 |
| 1:AA:596:A:C6 | 1:AA:645:G:C2 | 2.96 | 0.54 |
| 1:AA:946:A:C2 | 1:AA:1236:A:C2 | 2.96 | 0.54 |
| 2:AB:22:TYR:N | 2:AB:22:TYR:CD1 | 2.75 | 0.54 |
| 2:AB:28:LYS:N | 2:AB:29:PRO:CD | 2.70 | 0.54 |
| 10:AJ:35:GLN:HG2 | 10:AJ:77:VAL:HB | 1.90 | 0.54 |
| 22:BA:481:G:H1' | 22:BA:507:A:N1 | 2.22 | 0.54 |
| 22:BA:852:U:H2' | 22:BA:853:C:C6 | 2.43 | 0.54 |
| 22:BA:1061:U:O2' | 22:BA:1062:G:C5' | 2.55 | 0.54 |
| 33:BL:57:LEU:CD2 | 51:B3:54:ASP:HB3 | 2.38 | 0.54 |
| 48:B0:15:MET:O | 48:B0:18:SER:HB3 | 2.07 | 0.54 |
| 1:CA:798:U:H2' | 1:CA:799:G:O5' | 2.08 | 0.54 |
| 1:CA:1258:G:H2' | 1:CA:1259:C:C6 | 2.43 | 0.54 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:C8 | 2.42 | 0.54 |
| 3:CC:111:LEU:CD1 | 3:CC:146:ALA:HB2 | 2.38 | 0.54 |
| 21:CU:37:PHE:HA | 21:CU:40:LYS:HE3 | 1.90 | 0.54 |
| 22:DA:1826:G:O2' | 22:DA:1971:U:OP2 | 2.26 | 0.54 |
| 22:DA:2484:G:OP1 | 34:DM:44:ARG:NH2 | 2.41 | 0.54 |
| 22:DA:2531:A:C5' | 28:DG:157:TYR:CZ | 2.91 | 0.54 |
| 42:DU:67:VAL:HA | 42:DU:70:VAL:CG2 | 2.38 | 0.54 |
| 1:AA:202:G:C2 | 1:AA:216:U:O2 | 2.61 | 0.54 |
| 1:AA:343:U:H2' | 1:AA:345:C:C5 | 2.43 | 0.54 |
| 1:AA:702:A:H3' | 1:AA:703:G:C5' | 2.37 | 0.54 |
| 1:AA:821:G:H4' | 58:AA:1740:HOH:O | 2.06 | 0.54 |
| 1:AA:1167:A:N7 | 1:AA:1169:A:C5 | 2.76 | 0.54 |
| 3:AC:60:PRO:O | 3:AC:61:ALA:C | 2.46 | 0.54 |
| 22:BA:962:G:H21 | 22:BA:2250:G:H1 | 1.55 | 0.54 |
| 22:BA:1131:G:C5 | 31:BJ:77:HIS:CD2 | 2.96 | 0.54 |
| 22:BA:2243:U:H2' | 22:BA:2244:U:C6 | 2.43 | 0.54 |
| 26:BE:108:ILE:HD11 | 26:BE:180:LEU:HD13 | 1.89 | 0.54 |
| 32:BK:121:GLU:O | 32:BK:122:VAL:O | 2.26 | 0.54 |
| 37:BP:31:TRP:CZ2 | 37:BP:40:LEU:CD1 | 2.90 | 0.54 |
| 39:BR:49:ILE:HB | 39:BR:51:VAL:O | 2.07 | 0.54 |
| 1:CA:1262:C:C4 | 1:CA:1263:C:C4 | 2.96 | 0.54 |
| 1:CA:1298:U:O2 | 1:CA:1298:U:H2' | 2.07 | 0.54 |
| 6:CF:18:VAL:HG12 | 6:CF:19:PRO:N | 2.22 | 0.54 |
| 9:CI:81:HIS:O | 9:CI:85:ARG:HB2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:71:A:H5' | 22:DA:73:A:C4 | 2.43 | 0.54 |
| 22:DA:852:U:H2' | 22:DA:853:C:O4' | 2.08 | 0.54 |
| 22:DA:1127:A:H2' | 22:DA:1128:G:H5'' | 1.90 | 0.54 |
| 22:DA:1440:U:H2' | 22:DA:1441:G:O4' | 2.08 | 0.54 |
| 22:DA:1453:A:C2 | 35:DN:77:ALA:CB | 2.91 | 0.54 |
| 22:DA:1645:G:H5'' | 22:DA:1646:C:O5' | 2.08 | 0.54 |
| 22:DA:2772:C:H5' | 25:DD:173:GLN:NE2 | 2.23 | 0.54 |
| 23:DB:71:C:C2 | 23:DB:106:G:N2 | 2.76 | 0.54 |
| 24:DC:43:ARG:CZ | 24:DC:49:ILE:HG12 | 2.38 | 0.54 |
| 24:DC:76:ALA:HB2 | 24:DC:96:TYR:CD2 | 2.41 | 0.54 |
| 26:DE:130:LYS:HB2 | 26:DE:133:LEU:CB | 2.38 | 0.54 |
| 30:DI:101:ILE:O | 30:DI:102:SER:HB3 | 2.07 | 0.54 |
| 31:DJ:71:ASP:O | 31:DJ:73:VAL:HG23 | 2.08 | 0.54 |
| 31:DJ:109:LEU:HD23 | 31:DJ:110:PRO:HD2 | 1.90 | 0.54 |
| 32:DK:17:ARG:HG2 | 32:DK:47:ILE:CG2 | 2.38 | 0.54 |
| 40:DS:28:LYS:O | 40:DS:29:VAL:C | 2.47 | 0.54 |
| 42:DU:13:VAL:HG21 | 42:DU:39:ILE:HD12 | 1.90 | 0.54 |
| 45:DX:71:LEU:HA | 45:DX:74:ARG:HG2 | 1.89 | 0.54 |
| 1:AA:11:G:C6 | 1:AA:12:U:C4 | 2.96 | 0.53 |
| 1:AA:110:C:N4 | 1:AA:111:G:C6 | 2.77 | 0.53 |
| 1:AA:1108:G:H5' | 3:AC:176:HIS:ND1 | 2.22 | 0.53 |
| 10:AJ:6:ILE:CD1 | 10:AJ:76:ILE:HB | 2.38 | 0.53 |
| 10:AJ:65:TYR:CB | 14:AN:96:LEU:HD11 | 2.39 | 0.53 |
| 11:AK:128:ARG:HH11 | 11:AK:128:ARG:CG | 2.21 | 0.53 |
| 12:AL:24:LEU:HB2 | 12:AL:59:ASN:ND2 | 2.23 | 0.53 |
| 13:AM:64:VAL:O | 13:AM:69:LEU:HB2 | 2.08 | 0.53 |
| 27:BF:171:ALA:O | 27:BF:174:ASP:N | 2.39 | 0.53 |
| 39:BR:14:VAL:HG13 | 39:BR:98:ILE:HG13 | 1.88 | 0.53 |
| 53:B5:19:LYS:HG3 | 53:B5:23:ILE:HG12 | 1.90 | 0.53 |
| 1:CA:3:A:HO2' | 1:CA:612:C:HO2' | 1.56 | 0.53 |
| 1:CA:803:G:C6 | 1:CA:804:U:N3 | 2.76 | 0.53 |
| 1:CA:1134:G:C6 | 1:CA:1141:C:N4 | 2.76 | 0.53 |
| 1:CA:1150:A:N6 | 1:CA:1151:A:H62 | 2.06 | 0.53 |
| 2:CB:15:HIS:C | 2:CB:15:HIS:ND1 | 2.61 | 0.53 |
| 4:CD:146:ARG:O | 4:CD:150:LYS:HB2 | 2.08 | 0.53 |
| 8:CH:89:LYS:HA | 8:CH:92:LEU:CD1 | 2.38 | 0.53 |
| 22:DA:134:G:C2 | 22:DA:146:A:C2 | 2.96 | 0.53 |
| 22:DA:197:A:H2' | 22:DA:197:A:N3 | 2.23 | 0.53 |
| 22:DA:485:C:C4 | 22:DA:496:G:C6 | 2.96 | 0.53 |
| 22:DA:1027:A:C6 | 22:DA:1126:A:C4 | 2.96 | 0.53 |
| 22:DA:1310:G:C2' | 22:DA:1311:G:H5' | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1774:C:O2 | 24:DC:11:PRO:HB2 | 2.08 | 0.53 |
| 26:DE:128:ALA:O | 26:DE:130:LYS:N | 2.40 | 0.53 |
| 31:DJ:39:LYS:HZ3 | 31:DJ:39:LYS:HB2 | 1.73 | 0.53 |
| 36:DO:100:HIS:CG | 36:DO:101:GLY:N | 2.76 | 0.53 |
| 42:DU:34:VAL:HG22 | 42:DU:67:VAL:HG23 | 1.89 | 0.53 |
| 1:AA:49:U:C2 | 1:AA:361:G:N2 | 2.76 | 0.53 |
| 1:AA:90:C:C2 | 1:AA:91:U:C5 | 2.97 | 0.53 |
| 2:AB:41:ILE:HG21 | 2:AB:202:GLY:HA2 | 1.89 | 0.53 |
| 11:AK:52:PHE:CB | 11:AK:56:ARG:HB3 | 2.38 | 0.53 |
| 22:BA:65:U:H2' | 22:BA:66:C:H6 | 1.73 | 0.53 |
| 22:BA:839:U:H2' | 22:BA:840:C:C6 | 2.43 | 0.53 |
| 22:BA:2306:C:OP2 | 22:BA:2307:G:O2' | 2.17 | 0.53 |
| 22:BA:2343:U:HO2' | 22:BA:2373:G:HO2' | 1.54 | 0.53 |
| 24:BC:197:ASN:CG | 24:BC:197:ASN:O | 2.45 | 0.53 |
| 26:BE:23:PHE:HB2 | 26:BE:111:GLU:HG3 | 1.90 | 0.53 |
| 41:BT:2:ILE:HA | 41:BT:3:ARG:HB2 | 1.90 | 0.53 |
| 49:B1:17:THR:HG22 | 49:B1:42:VAL:CG1 | 2.38 | 0.53 |
| 53:B5:52:PRO:O | 53:B5:53:ARG:CB | 2.57 | 0.53 |
| 1:CA:484:G:N7 | 1:CA:486:U:H1' | 2.23 | 0.53 |
| 1:CA:604:G:C5 | 1:CA:605:U:C5 | 2.96 | 0.53 |
| 1:CA:1288:A:N6 | 1:CA:1289:A:N6 | 2.56 | 0.53 |
| 6:CF:98:GLU:O | 6:CF:99:ALA:CB | 2.57 | 0.53 |
| 9:CI:55:VAL:O | 9:CI:55:VAL:CG2 | 2.56 | 0.53 |
| 22:DA:197:A:H62 | 22:DA:2430:A:H2' | 1.73 | 0.53 |
| 22:DA:445:C:O2' | 22:DA:449:A:N3 | 2.41 | 0.53 |
| 22:DA:548:G:H4' | 22:DA:549:G:C2 | 2.43 | 0.53 |
| 22:DA:696:G:C2 | 22:DA:767:U:O2 | 2.62 | 0.53 |
| 22:DA:770:G:H1' | 22:DA:1379:U:C4 | 2.44 | 0.53 |
| 22:DA:937:C:C2 | 22:DA:938:G:C8 | 2.97 | 0.53 |
| 22:DA:1027:A:N7 | 22:DA:1126:A:C2 | 2.76 | 0.53 |
| 22:DA:1874:C:C4 | 22:DA:1875:G:C6 | 2.96 | 0.53 |
| 22:DA:2104:C:H2' | 22:DA:2105:U:O4' | 2.09 | 0.53 |
| 22:DA:2742:G:H5'' | 52:D4:1:MET:HE1 | 1.90 | 0.53 |
| 24:DC:62:TYR:CE1 | 24:DC:63:ARG:O | 2.61 | 0.53 |
| 25:DD:86:GLU:HG3 | 25:DD:87:GLY:N | 2.22 | 0.53 |
| 33:DL:85:VAL:O | 33:DL:86:GLU:HG3 | 2.09 | 0.53 |
| 42:DU:34:VAL:HG23 | 42:DU:65:ILE:O | 2.08 | 0.53 |
| 1:AA:19:A:N3 | 1:AA:917:G:C2 | 2.77 | 0.53 |
| 1:AA:32:A:H2' | 1:AA:32:A:N3 | 2.23 | 0.53 |
| 1:AA:469:C:C5 | 1:AA:470:C:C4 | 2.97 | 0.53 |
| 1:AA:1181:G:C2 | 1:AA:1182:G:N2 | 2.76 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 5:AE:104:GLY:HA3 | 5:AE:122:ASN:HA | 1.90 | 0.53 |
| 14:AN:41:ARG:O | 14:AN:42:TRP:C | 2.46 | 0.53 |
| 17:AQ:81:LYS:O | 17:AQ:82:ALA:C | 2.46 | 0.53 |
| 22:BA:440:C:C2' | 22:BA:441:U:H5' | 2.39 | 0.53 |
| 22:BA:1474:U:C2' | 22:BA:1475:G:H5' | 2.36 | 0.53 |
| 22:BA:1735:A:C2 | 22:BA:1736:U:H1' | 2.44 | 0.53 |
| 22:BA:2884:U:O2 | 22:BA:2884:U:O4' | 2.26 | 0.53 |
| 24:BC:8:PRO:HB3 | 24:BC:14:ARG:HB2 | 1.90 | 0.53 |
| 43:BV:14:LYS:HD3 | 43:BV:18:ARG:NH1 | 2.23 | 0.53 |
| 1:CA:106:C:H2' | 1:CA:107:G:H5' | 1.90 | 0.53 |
| 1:CA:216:U:H2' | 1:CA:217:C:C6 | 2.43 | 0.53 |
| 1:CA:392:C:C2 | 1:CA:393:A:C8 | 2.96 | 0.53 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C6 | 2.43 | 0.53 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:H6 | 1.73 | 0.53 |
| 6:CF:93:LYS:O | 6:CF:93:LYS:HG2 | 2.08 | 0.53 |
| 8:CH:106:THR:HG21 | 8:CH:121:LEU:HD13 | 1.91 | 0.53 |
| 10:CJ:83:THR:O | 10:CJ:87:LEU:HD12 | 2.08 | 0.53 |
| 17:CQ:61:ILE:HG23 | 17:CQ:73:TRP:CE3 | 2.43 | 0.53 |
| 22:DA:484:C:OP1 | 42:DU:48:PRO:HG3 | 2.08 | 0.53 |
| 22:DA:1420:A:C2 | 22:DA:2211:A:C4 | 2.96 | 0.53 |
| 22:DA:2746:U:H1' | 28:DG:139:GLN:HG3 | 1.91 | 0.53 |
| 30:DI:8:TYR:HA | 30:DI:59:ILE:HB | 1.90 | 0.53 |
| 51:D3:31:HIS:ND1 | 51:D3:32:ILE:HG13 | 2.22 | 0.53 |
| 1:AA:474:G:C2 | 1:AA:475:C:C6 | 2.96 | 0.53 |
| 1:AA:702:A:N6 | 22:BA:1846:G:HO2' | 2.07 | 0.53 |
| 2:AB:67:ILE:HG21 | 2:AB:69:PHE:CE2 | 2.43 | 0.53 |
| 2:AB:120:GLN:O | 2:AB:120:GLN:HG2 | 2.08 | 0.53 |
| 5:AE:46:VAL:HG21 | 5:AE:118:ALA:HB2 | 1.91 | 0.53 |
| 10:AJ:53:ILE:CG2 | 10:AJ:61:ALA:HB1 | 2.39 | 0.53 |
| 19:AS:29:LYS:HB3 | 19:AS:30:PRO:HD2 | 1.91 | 0.53 |
| 21:AU:37:PHE:HB3 | 21:AU:41:PRO:CG | 2.38 | 0.53 |
| 22:BA:276:U:H2' | 22:BA:276:U:O2 | 2.08 | 0.53 |
| 22:BA:2452:C:C2 | 56:BA:3001:DOL:H131 | 2.44 | 0.53 |
| 22:BA:2820:A:C6 | 25:BD:197:THR:HG22 | 2.44 | 0.53 |
| 30:BI:101:ILE:O | 30:BI:102:SER:HB2 | 2.07 | 0.53 |
| 36:BO:49:VAL:O | 36:BO:50:ALA:HB2 | 2.09 | 0.53 |
| 42:BU:39:ILE:HG22 | 42:BU:40:ASN:N | 2.23 | 0.53 |
| 43:BV:6:ALA:HB1 | 43:BV:40:ILE:HG23 | 1.90 | 0.53 |
| 49:B1:51:GLU:OE2 | 49:B1:53:LYS:HG2 | 2.07 | 0.53 |
| 1:CA:1082:A:C6 | 1:CA:1083:U:N3 | 2.76 | 0.53 |
| 1:CA:1491:G:H3' | 1:CA:1492:A:C8 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:183:C:C5 | 22:DA:184:C:C5 | 2.96 | 0.53 |
| 22:DA:600:G:C5 | 22:DA:601:C:C4 | 2.97 | 0.53 |
| 22:DA:1097:U:C4 | 22:DA:1098:A:H1' | 2.44 | 0.53 |
| 22:DA:1364:G:C4 | 22:DA:1368:G:C2 | 2.96 | 0.53 |
| 22:DA:1512:C:C4 | 22:DA:1513:U:C4 | 2.97 | 0.53 |
| 22:DA:2491:U:O4 | 22:DA:2518:A:N6 | 2.41 | 0.53 |
| 22:DA:2571:U:N3 | 22:DA:2574:G:C8 | 2.76 | 0.53 |
| 22:DA:2805:C:H2' | 22:DA:2806:C:C6 | 2.42 | 0.53 |
| 22:DA:2811:G:H2' | 22:DA:2812:G:O4' | 2.09 | 0.53 |
| 29:DH:32:PRO:O | 29:DH:33:GLN:HB2 | 2.08 | 0.53 |
| 30:DI:79:LEU:HD13 | 30:DI:109:ILE:CG2 | 2.37 | 0.53 |
| 34:DM:124:LEU:CD2 | 34:DM:124:LEU:N | 2.70 | 0.53 |
| 1:AA:340:U:H2' | 1:AA:341:C:H6 | 1.74 | 0.53 |
| 1:AA:655:A:C2 | 1:AA:656:G:C4 | 2.97 | 0.53 |
| 1:AA:1349:A:C2 | 1:AA:1374:A:C4 | 2.96 | 0.53 |
| 2:AB:126:PHE:CD2 | 2:AB:126:PHE:N | 2.76 | 0.53 |
| 10:AJ:91:ASP:OD2 | 10:AJ:91:ASP:N | 2.41 | 0.53 |
| 19:AS:14:HIS:O | 19:AS:18:LYS:HB2 | 2.08 | 0.53 |
| 22:BA:997:G:O2' | 22:BA:998:C:H5' | 2.09 | 0.53 |
| 22:BA:1817:G:H2' | 22:BA:1818:U:H5' | 1.91 | 0.53 |
| 29:BH:147:VAL:CG1 | 29:BH:149:GLU:HG3 | 2.36 | 0.53 |
| 33:BL:82:LEU:HD23 | 33:BL:82:LEU:C | 2.29 | 0.53 |
| 53:B5:66:PRO:HG3 | 53:B5:194:ILE:CB | 2.39 | 0.53 |
| 1:CA:667:G:C2 | 1:CA:740:U:O2 | 2.62 | 0.53 |
| 1:CA:1169:A:C2 | 1:CA:1170:A:C4 | 2.96 | 0.53 |
| 1:CA:1296:C:H4' | 1:CA:1302:C:C4 | 2.43 | 0.53 |
| 2:CB:139:ARG:HD2 | 2:CB:139:ARG:C | 2.29 | 0.53 |
| 4:CD:29:ASP:C | 4:CD:31:LYS:N | 2.61 | 0.53 |
| 20:CT:83:ILE:O | 20:CT:87:ALA:HB3 | 2.08 | 0.53 |
| 22:DA:288:U:H2' | 22:DA:289:G:O4' | 2.09 | 0.53 |
| 22:DA:584:C:N4 | 22:DA:585:G:C6 | 2.77 | 0.53 |
| 22:DA:792:A:H1' | 22:DA:2072:C:O2' | 2.08 | 0.53 |
| 22:DA:1926:U:H1' | 22:DA:1929:G:C6 | 2.44 | 0.53 |
| 22:DA:2506:U:C5 | 56:DA:3001:DOL:O41 | 2.61 | 0.53 |
| 25:DD:208:LYS:O | 25:DD:209:ALA:HB2 | 2.06 | 0.53 |
| 1:AA:74:A:H1' | 1:AA:97:G:N2 | 2.24 | 0.53 |
| 1:AA:764:C:H5'' | 15:AO:50:HIS:CD2 | 2.43 | 0.53 |
| 1:AA:1287:A:H2' | 1:AA:1288:A:C8 | 2.43 | 0.53 |
| 2:AB:72:THR:O | 2:AB:73:LYS:HB3 | 2.09 | 0.53 |
| 2:AB:147:SER:O | 2:AB:148:LEU:CB | 2.56 | 0.53 |
| 22:BA:63:A:C2 | 22:BA:64:A:C5 | 2.96 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:BA:1720:U:H2' | 22:BA:1721:G:O4' | 2.08 | 0.53 |
| 22:BA:1923:U:C2' | 22:BA:1924:C:C5' | 2.87 | 0.53 |
| 22:BA:2443:C:O2' | 22:BA:2444:G:H5' | 2.07 | 0.53 |
| 22:BA:2517:C:C6 | 22:BA:2542:A:N7 | 2.77 | 0.53 |
| 30:BI:44:ALA:O | 30:BI:45:LYS:HG3 | 2.09 | 0.53 |
| 53:B5:51:ASP:N | 53:B5:52:PRO:HD3 | 2.23 | 0.53 |
| 1:CA:457:G:C5 | 1:CA:458:U:C4 | 2.97 | 0.53 |
| 1:CA:978:A:O2' | 1:CA:1322:C:C5 | 2.61 | 0.53 |
| 1:CA:1040:U:H2' | 1:CA:1041:G:C8 | 2.43 | 0.53 |
| 1:CA:1072:G:C5 | 1:CA:1073:U:C4 | 2.97 | 0.53 |
| 3:CC:155:GLY:O | 3:CC:157:LEU:N | 2.39 | 0.53 |
| 4:CD:9:LEU:HD12 | 4:CD:32:CYS:SG | 2.49 | 0.53 |
| 5:CE:96:MET:HE3 | 5:CE:111:MET:CE | 2.38 | 0.53 |
| 11:CK:25:ALA:HB3 | 11:CK:87:LYS:O | 2.09 | 0.53 |
| 21:CU:10:GLU:HB2 | 21:CU:11:PRO:HD3 | 1.89 | 0.53 |
| 22:DA:1343:G:N2 | 22:DA:1405:U:C2 | 2.76 | 0.53 |
| 22:DA:2214:C:H2' | 22:DA:2215:C:O5' | 2.09 | 0.53 |
| 22:DA:2300:C:C4 | 22:DA:2317:A:C2 | 2.96 | 0.53 |
| 22:DA:2504:U:C4 | 56:DA:3001:DOL:H161 | 2.43 | 0.53 |
| 22:DA:2810:A:C8 | 22:DA:2811:G:C8 | 2.96 | 0.53 |
| 26:DE:27:LEU:HG | 26:DE:104:ALA:HB2 | 1.91 | 0.53 |
| 28:DG:86:LYS:HB3 | 28:DG:165:ALA:HB2 | 1.89 | 0.53 |
| 29:DH:103:VAL:HA | 29:DH:106:ALA:HB3 | 1.89 | 0.53 |
| 35:DN:20:MET:HG3 | 35:DN:21:PHE:CD1 | 2.43 | 0.53 |
| 38:DQ:72:ASN:HB3 | 38:DQ:110:VAL:HG11 | 1.91 | 0.53 |
| 1:AA:1320:C:N3 | 19:AS:36:ARG:NH1 | 2.57 | 0.53 |
| 2:AB:33:GLY:HA3 | 2:AB:40:ILE:N | 2.24 | 0.53 |
| 2:AB:83:ALA:O | 2:AB:86:SER:OG | 2.26 | 0.53 |
| 2:AB:91:PHE:CD2 | 2:AB:150:GLY:HA3 | 2.44 | 0.53 |
| 2:AB:154:MET:O | 2:AB:155:GLY:C | 2.47 | 0.53 |
| 9:AI:36:GLU:OE2 | 9:AI:36:GLU:N | 2.41 | 0.53 |
| 22:BA:657:U:H2' | 22:BA:658:U:C6 | 2.43 | 0.53 |
| 22:BA:1142:A:C2 | 22:BA:1144:A:C1' | 2.92 | 0.53 |
| 22:BA:2191:A:N1 | 22:BA:2192:U:O4 | 2.42 | 0.53 |
| 22:BA:2327:A:H2' | 22:BA:2328:A:C8 | 2.44 | 0.53 |
| 56:BA:3001:DOL:N44 | 56:BA:3001:DOL:O40 | 2.41 | 0.53 |
| 30:BI:81:LYS:HA | 30:BI:86:ILE:O | 2.09 | 0.53 |
| 34:BM:51:ARG:O | 34:BM:55:ARG:HG3 | 2.09 | 0.53 |
| 1:CA:552:U:C2 | 1:CA:553:A:C8 | 2.96 | 0.53 |
| 1:CA:597:G:N7 | 1:CA:598:U:C5 | 2.76 | 0.53 |
| 1:CA:632:U:H3' | 1:CA:633:G:H5' | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:649:A:H2' | 1:CA:650:G:O4' | 2.08 | 0.53 |
| 1:CA:731:G:H5' | 1:CA:766:A:H4' | 1.91 | 0.53 |
| 5:CE:150:PRO:HA | 8:CH:99:LEU:CD2 | 2.38 | 0.53 |
| 20:CT:32:ILE:HG12 | 20:CT:54:MET:HE3 | 1.90 | 0.53 |
| 22:DA:315:G:H2' | 22:DA:316:C:O4' | 2.09 | 0.53 |
| 22:DA:696:G:N1 | 22:DA:767:U:C2 | 2.76 | 0.53 |
| 22:DA:1101:U:C5 | 22:DA:1102:C:C5 | 2.96 | 0.53 |
| 22:DA:1226:A:OP1 | 38:DQ:16:LYS:NZ | 2.41 | 0.53 |
| 22:DA:1555:G:N2 | 22:DA:1556:C:H1' | 2.24 | 0.53 |
| 22:DA:1581:G:N7 | 22:DA:1582:C:N4 | 2.57 | 0.53 |
| 22:DA:2512:C:H2' | 22:DA:2513:A:O4' | 2.08 | 0.53 |
| 25:DD:133:THR:HG23 | 25:DD:134:HIS:N | 2.24 | 0.53 |
| 29:DH:2:GLN:O | 29:DH:3:VAL:HG22 | 2.09 | 0.53 |
| 30:DI:59:ILE:HG22 | 30:DI:60:THR:N | 2.24 | 0.53 |
| 30:DI:80:LEU:HD23 | 30:DI:84:ALA:CB | 2.38 | 0.53 |
| 33:DL:68:SER:O | 33:DL:69:ARG:HB2 | 2.09 | 0.53 |
| 37:DP:40:LEU:HD23 | 37:DP:41:GLN:N | 2.24 | 0.53 |
| 51:D3:32:ILE:HG22 | 51:D3:32:ILE:O | 2.09 | 0.53 |
| 1:AA:76:G:H2' | 1:AA:76:G:N3 | 2.23 | 0.53 |
| 1:AA:323:U:OP1 | 20:AT:25:ARG:NH2 | 2.42 | 0.53 |
| 3:AC:87:LEU:O | 3:AC:88:ARG:C | 2.46 | 0.53 |
| 13:AM:29:ARG:O | 13:AM:33:ILE:HG12 | 2.08 | 0.53 |
| 22:BA:528:A:C8 | 22:BA:528:A:H3' | 2.43 | 0.53 |
| 22:BA:536:G:C6 | 22:BA:537:G:C4 | 2.96 | 0.53 |
| 22:BA:1246:A:C2' | 22:BA:1247:A:O5' | 2.56 | 0.53 |
| 22:BA:2619:C:OP1 | 25:BD:157:LYS:HE2 | 2.09 | 0.53 |
| 28:BG:127:THR:HG22 | 28:BG:128:GLN:N | 2.24 | 0.53 |
| 34:BM:57:VAL:HG12 | 34:BM:112:LEU:HD23 | 1.90 | 0.53 |
| 1:CA:223:A:H2' | 1:CA:224:U:C6 | 2.44 | 0.53 |
| 1:CA:666:G:C6 | 1:CA:741:G:C6 | 2.97 | 0.53 |
| 1:CA:922:G:H4' | 5:CE:25:VAL:HA | 1.91 | 0.53 |
| 4:CD:3:ARG:HD2 | 4:CD:115:ARG:NE | 2.24 | 0.53 |
| 11:CK:84:VAL:HG11 | 11:CK:97:ILE:HG22 | 1.91 | 0.53 |
| 22:DA:232:G:N1 | 22:DA:420:C:OP1 | 2.41 | 0.53 |
| 22:DA:319:G:C4 | 22:DA:333:G:N2 | 2.77 | 0.53 |
| 22:DA:441:U:O2' | 26:DE:41:GLN:OE1 | 2.26 | 0.53 |
| 22:DA:451:U:H2' | 22:DA:453:A:N7 | 2.24 | 0.53 |
| 22:DA:1428:C:C5 | 22:DA:1569:A:H5'' | 2.44 | 0.53 |
| 29:DH:37:VAL:CG2 | 29:DH:38:PRO:HD2 | 2.39 | 0.53 |
| 33:DL:56:PRO:O | 33:DL:60:ARG:HB2 | 2.09 | 0.53 |
| 36:DO:104:GLN:O | 36:DO:107:ALA:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:258:G:C4 | 1:AA:259:G:C8 | 2.97 | 0.53 |
| 1:AA:452:A:H2' | 1:AA:453:G:C5' | 2.39 | 0.53 |
| 1:AA:568:G:C2 | 1:AA:569:C:C5 | 2.97 | 0.53 |
| 1:AA:933:G:OP2 | 7:AG:3:ARG:HB3 | 2.09 | 0.53 |
| 1:AA:1109:C:OP2 | 3:AC:176:HIS:ND1 | 2.34 | 0.53 |
| 1:AA:1135:U:C2' | 1:AA:1136:C:O5' | 2.57 | 0.53 |
| 1:AA:1353:G:C2 | 1:AA:1354:U:C6 | 2.97 | 0.53 |
| 1:AA:1523:G:OP1 | 11:AK:128:ARG:NH2 | 2.42 | 0.53 |
| 3:AC:12:LEU:O | 3:AC:13:GLY:C | 2.47 | 0.53 |
| 22:BA:1384:A:H1' | 22:BA:1405:U:C1' | 2.38 | 0.53 |
| 22:BA:1627:G:C2 | 22:BA:1628:G:C8 | 2.97 | 0.53 |
| 22:BA:1926:U:O2 | 22:BA:1926:U:H2' | 2.09 | 0.53 |
| 22:BA:2024:G:OP2 | 22:BA:2034:U:H4' | 2.09 | 0.53 |
| 22:BA:2309:A:C6 | 22:BA:2310:C:C4 | 2.97 | 0.53 |
| 34:BM:12:MET:CE | 34:BM:71:LYS:HG3 | 2.39 | 0.53 |
| 40:BS:1:MET:N | 40:BS:109:ASP:OD1 | 2.41 | 0.53 |
| 1:CA:203:G:N2 | 1:CA:215:C:N3 | 2.57 | 0.53 |
| 1:CA:866:C:C4 | 1:CA:867:G:H1' | 2.44 | 0.53 |
| 1:CA:878:A:C5 | 1:CA:879:C:C5 | 2.96 | 0.53 |
| 1:CA:885:G:O2' | 1:CA:914:A:N1 | 2.33 | 0.53 |
| 2:CB:67:ILE:HG22 | 2:CB:68:LEU:N | 2.24 | 0.53 |
| 4:CD:57:GLU:OE2 | 4:CD:196:ASN:N | 2.41 | 0.53 |
| 14:CN:51:LEU:O | 14:CN:53:ARG:N | 2.42 | 0.53 |
| 22:DA:197:A:C2 | 22:DA:198:C:H1' | 2.44 | 0.53 |
| 22:DA:483:A:C2 | 42:DU:58:ILE:HD11 | 2.43 | 0.53 |
| 22:DA:728:G:C2 | 22:DA:730:A:C4 | 2.97 | 0.53 |
| 22:DA:1519:G:C6 | 22:DA:1520:U:C2 | 2.97 | 0.53 |
| 30:DI:33:VAL:HG13 | 30:DI:67:PHE:CZ | 2.43 | 0.53 |
| 1:AA:71:A:O2' | 1:AA:72:A:OP2 | 2.27 | 0.53 |
| 1:AA:259:G:N2 | 1:AA:260:G:H1' | 2.23 | 0.53 |
| 1:AA:1142:G:H2' | 1:AA:1143:G:O4' | 2.09 | 0.53 |
| 9:AI:30:ILE:HD11 | 9:AI:38:TYR:CB | 2.39 | 0.53 |
| 9:AI:40:GLY:O | 9:AI:41:ARG:HB2 | 2.07 | 0.53 |
| 9:AI:50:GLN:C | 9:AI:52:LEU:H | 2.11 | 0.53 |
| 10:AJ:52:LEU:HB2 | 14:AN:81:ARG:NE | 2.24 | 0.53 |
| 21:AU:18:ARG:N | 21:AU:18:ARG:HD2 | 2.24 | 0.53 |
| 22:BA:102:U:C2 | 46:BY:2:LYS:HE3 | 2.44 | 0.53 |
| 22:BA:287:G:H2' | 22:BA:288:U:C6 | 2.45 | 0.53 |
| 22:BA:1411:U:H2' | 22:BA:1412:U:O4' | 2.09 | 0.53 |
| 22:BA:1805:A:H1' | 24:BC:50:THR:O | 2.08 | 0.53 |
| 53:B5:204:GLY:O | 53:B5:205:ALA:HB3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:690:G:H2' | 1:CA:691:G:O4' | 2.09 | 0.53 |
| 2:CB:85:LEU:O | 2:CB:85:LEU:CG | 2.57 | 0.53 |
| 2:CB:167:ASP:O | 2:CB:168:HIS:HB3 | 2.09 | 0.53 |
| 3:CC:57:ILE:HG13 | 3:CC:66:VAL:HG22 | 1.90 | 0.53 |
| 8:CH:35:ALA:O | 8:CH:39:VAL:HG23 | 2.09 | 0.53 |
| 9:CI:30:ILE:HA | 9:CI:65:ILE:HG13 | 1.91 | 0.53 |
| 12:CL:25:GLU:C | 12:CL:27:CYS:N | 2.60 | 0.53 |
| 13:CM:114:LYS:HB2 | 13:CM:115:PRO:HD3 | 1.91 | 0.53 |
| 22:DA:37:C:H2' | 22:DA:38:A:O4' | 2.09 | 0.53 |
| 22:DA:95:A:O2' | 46:DY:40:SER:N | 2.42 | 0.53 |
| 22:DA:301:G:N3 | 22:DA:302:C:C2 | 2.77 | 0.53 |
| 22:DA:658:U:N3 | 22:DA:659:G:N7 | 2.57 | 0.53 |
| 22:DA:979:A:C8 | 22:DA:982:C:N4 | 2.77 | 0.53 |
| 22:DA:1627:G:N2 | 22:DA:1628:G:C8 | 2.77 | 0.53 |
| 22:DA:2223:G:H2' | 22:DA:2224:G:H5' | 1.91 | 0.53 |
| 24:DC:147:LYS:HB2 | 24:DC:150:LYS:HB2 | 1.91 | 0.53 |
| 32:DK:31:ARG:CB | 32:DK:32:TYR:CD2 | 2.92 | 0.53 |
| 1:AA:100:G:N7 | 1:AA:101:A:N7 | 2.57 | 0.52 |
| 1:AA:587:G:C2 | 1:AA:755:G:C5 | 2.97 | 0.52 |
| 1:AA:692:U:O2' | 1:AA:694:A:N7 | 2.24 | 0.52 |
| 1:AA:1157:A:N6 | 1:AA:1180:A:N7 | 2.58 | 0.52 |
| 1:AA:1191:A:OP2 | 3:AC:3:GLN:NE2 | 2.41 | 0.52 |
| 4:AD:37:ALA:HA | 4:AD:42:GLY:HA3 | 1.91 | 0.52 |
| 21:AU:10:GLU:HG3 | 21:AU:11:PRO:HD3 | 1.92 | 0.52 |
| 22:BA:26:G:C6 | 22:BA:27:G:N1 | 2.77 | 0.52 |
| 22:BA:482:A:C5' | 22:BA:483:A:OP1 | 2.56 | 0.52 |
| 22:BA:1206:G:C5 | 22:BA:1207:C:C5 | 2.97 | 0.52 |
| 27:BF:2:ALA:O | 27:BF:4:LEU:N | 2.42 | 0.52 |
| 30:BI:116:ASP:O | 30:BI:117:MET:HB2 | 2.09 | 0.52 |
| 34:BM:77:PRO:HG2 | 34:BM:80:VAL:HG21 | 1.91 | 0.52 |
| 40:BS:28:LYS:O | 40:BS:29:VAL:C | 2.47 | 0.52 |
| 1:CA:60:A:N3 | 1:CA:61:G:H1' | 2.24 | 0.52 |
| 1:CA:259:G:N2 | 1:CA:268:U:C2 | 2.77 | 0.52 |
| 1:CA:1211:U:O2' | 1:CA:1212:U:P | 2.66 | 0.52 |
| 1:CA:1363:A:O2' | 1:CA:1365:G:N7 | 2.37 | 0.52 |
| 2:CB:81:LYS:HG3 | 2:CB:91:PHE:CZ | 2.44 | 0.52 |
| 2:CB:125:THR:O | 2:CB:126:PHE:HB3 | 2.09 | 0.52 |
| 4:CD:202:GLU:OE1 | 5:CE:105:ILE:HG23 | 2.09 | 0.52 |
| 8:CH:66:PHE:CE2 | 8:CH:67:GLN:OE1 | 2.62 | 0.52 |
| 10:CJ:73:LEU:CD2 | 10:CJ:75:ASP:HB2 | 2.38 | 0.52 |
| 20:CT:21:ASN:HB3 | 20:CT:25:ARG:NH2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:CT:33:LYS:O | 20:CT:36:TYR:CE2 | 2.62 | 0.52 |
| 22:DA:134:G:C6 | 22:DA:135:U:N3 | 2.78 | 0.52 |
| 22:DA:406:G:H2' | 22:DA:407:G:O4' | 2.08 | 0.52 |
| 22:DA:630:G:C3' | 22:DA:631:A:H5'' | 2.39 | 0.52 |
| 22:DA:945:A:C5 | 22:DA:2448:A:C2 | 2.97 | 0.52 |
| 22:DA:1352:U:C5 | 22:DA:1377:G:C5 | 2.97 | 0.52 |
| 22:DA:1776:G:N2 | 22:DA:1789:A:H1' | 2.25 | 0.52 |
| 22:DA:2325:G:C6 | 22:DA:2326:C:N4 | 2.77 | 0.52 |
| 22:DA:2550:G:C6 | 22:DA:2551:C:C4 | 2.97 | 0.52 |
| 22:DA:2851:A:O2' | 35:DN:64:ARG:NH2 | 2.41 | 0.52 |
| 25:DD:186:LEU:CD1 | 37:DP:8:LEU:HD12 | 2.39 | 0.52 |
| 29:DH:40:THR:O | 29:DH:41:LYS:C | 2.48 | 0.52 |
| 1:AA:255:G:C6 | 1:AA:256:U:C4 | 2.98 | 0.52 |
| 1:AA:374:A:H5'' | 1:AA:452:A:C2 | 2.44 | 0.52 |
| 1:AA:596:A:N6 | 1:AA:645:G:C6 | 2.77 | 0.52 |
| 1:AA:1305:G:HO2' | 1:AA:1306:A:H8 | 1.55 | 0.52 |
| 2:AB:20:THR:HA | 2:AB:38:VAL:HA | 1.91 | 0.52 |
| 14:AN:72:GLY:O | 14:AN:80:SER:HA | 2.09 | 0.52 |
| 17:AQ:16:LYS:O | 17:AQ:17:MET:HE3 | 2.08 | 0.52 |
| 21:AU:11:PRO:O | 21:AU:12:PHE:CG | 2.62 | 0.52 |
| 22:BA:492:A:H2' | 22:BA:493:G:O4' | 2.08 | 0.52 |
| 22:BA:720:U:H2' | 22:BA:721:A:C8 | 2.45 | 0.52 |
| 22:BA:981:A:H5'' | 58:BA:3595:HOH:O | 2.09 | 0.52 |
| 22:BA:1650:A:N6 | 58:BA:3800:HOH:O | 2.41 | 0.52 |
| 26:BE:91:ASP:C | 26:BE:91:ASP:OD1 | 2.47 | 0.52 |
| 39:BR:9:GLY:C | 39:BR:10:LYS:HG2 | 2.29 | 0.52 |
| 44:BW:56:ASP:N | 44:BW:56:ASP:OD1 | 2.40 | 0.52 |
| 49:B1:47:VAL:HG13 | 49:B1:48:ILE:N | 2.24 | 0.52 |
| 53:B5:52:PRO:O | 53:B5:53:ARG:HB2 | 2.10 | 0.52 |
| 1:CA:183:C:O2' | 1:CA:184:G:C5' | 2.57 | 0.52 |
| 1:CA:1105:A:N3 | 1:CA:1106:G:C8 | 2.77 | 0.52 |
| 1:CA:1126:U:O4 | 10:CJ:73:LEU:HD12 | 2.10 | 0.52 |
| 2:CB:35:ARG:O | 2:CB:37:LYS:N | 2.42 | 0.52 |
| 6:CF:66:ALA:HB1 | 6:CF:67:PRO:HD2 | 1.91 | 0.52 |
| 11:CK:81:ASN:HA | 11:CK:106:ARG:O | 2.09 | 0.52 |
| 20:CT:74:ARG:O | 20:CT:78:ASN:ND2 | 2.41 | 0.52 |
| 22:DA:85:G:OP2 | 42:DU:7:ARG:HB2 | 2.10 | 0.52 |
| 22:DA:329:G:O4' | 22:DA:477:A:H1' | 2.10 | 0.52 |
| 22:DA:547:A:H3' | 22:DA:548:G:H5' | 1.91 | 0.52 |
| 22:DA:1577:C:H2' | 22:DA:1578:U:O4' | 2.09 | 0.52 |
| 22:DA:1645:G:H4' | 22:DA:1646:C:C6 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2519:U:C6 | 22:DA:2542:A:N6 | 2.77 | 0.52 |
| 23:DB:76:G:O2' | 43:DV:78:GLN:OE1 | 2.19 | 0.52 |
| 27:DF:111:ILE:HB | 27:DF:114:PHE:HB2 | 1.90 | 0.52 |
| 29:DH:31:VAL:CB | 29:DH:32:PRO:CD | 2.86 | 0.52 |
| 34:DM:119:LEU:O | 34:DM:119:LEU:HD13 | 2.09 | 0.52 |
| 46:DY:45:GLN:O | 46:DY:47:ARG:N | 2.43 | 0.52 |
| 1:AA:6:G:H3' | 1:AA:6:G:N3 | 2.24 | 0.52 |
| 1:AA:198:G:C5 | 1:AA:220:G:C2 | 2.97 | 0.52 |
| 1:AA:1118:U:C1' | 1:AA:1179:A:C4 | 2.92 | 0.52 |
| 3:AC:145:GLY:O | 3:AC:146:ALA:C | 2.48 | 0.52 |
| 4:AD:2:ALA:O | 4:AD:68:LEU:HD21 | 2.10 | 0.52 |
| 5:AE:15:LEU:HB3 | 5:AE:37:THR:CG2 | 2.39 | 0.52 |
| 8:AH:111:MET:HE2 | 8:AH:116:ALA:N | 2.24 | 0.52 |
| 22:BA:441:U:H2' | 22:BA:442:G:C8 | 2.45 | 0.52 |
| 22:BA:1026:G:C8 | 22:BA:1134:A:C4 | 2.97 | 0.52 |
| 22:BA:1061:U:H3' | 22:BA:1062:G:H5' | 1.91 | 0.52 |
| 23:BB:2:G:C2 | 23:BB:119:A:C2 | 2.98 | 0.52 |
| 53:B5:40:GLU:HA | 53:B5:181:PHE:HA | 1.91 | 0.52 |
| 53:B5:67:HIS:CD2 | 53:B5:188:ASP:HA | 2.45 | 0.52 |
| 1:CA:332:G:OP2 | 20:CT:5:LYS:HB3 | 2.09 | 0.52 |
| 1:CA:1478:U:H2' | 1:CA:1479:C:C6 | 2.44 | 0.52 |
| 3:CC:117:ALA:HB1 | 3:CC:187:SER:CB | 2.39 | 0.52 |
| 7:CG:68:ASN:ND2 | 7:CG:130:ASN:OD1 | 2.42 | 0.52 |
| 22:DA:404:A:H1' | 22:DA:405:U:OP2 | 2.10 | 0.52 |
| 22:DA:634:C:H2' | 22:DA:635:C:C6 | 2.45 | 0.52 |
| 22:DA:681:G:C2 | 22:DA:682:G:C8 | 2.98 | 0.52 |
| 22:DA:747:U:O2 | 22:DA:2014:A:H1' | 2.09 | 0.52 |
| 22:DA:1355:G:C6 | 22:DA:1377:G:C2 | 2.96 | 0.52 |
| 22:DA:2093:G:O2' | 22:DA:2094:A:H5' | 2.08 | 0.52 |
| 22:DA:2267:A:H5'' | 22:DA:2268:A:H5' | 1.90 | 0.52 |
| 22:DA:2505:G:N2 | 54:D6:4:PRO:HB3 | 2.23 | 0.52 |
| 22:DA:2575:C:H2' | 22:DA:2578:G:O6 | 2.10 | 0.52 |
| 22:DA:2611:C:H1' | 54:D6:8:MHT:H2 | 1.91 | 0.52 |
| 26:DE:59:PRO:HB2 | 26:DE:70:SER:OG | 2.09 | 0.52 |
| 29:DH:72:ILE:HG22 | 29:DH:72:ILE:O | 2.09 | 0.52 |
| 40:DS:61:ASN:O | 40:DS:62:ASP:HB3 | 2.09 | 0.52 |
| 48:D0:28:LEU:HD23 | 48:D0:37:LYS:HB3 | 1.92 | 0.52 |
| 1:AA:1014:A:H2' | 1:AA:1015:G:O4' | 2.10 | 0.52 |
| 1:AA:1195:C:H5'' | 1:AA:1196:A:OP2 | 2.09 | 0.52 |
| 2:AB:53:ALA:O | 2:AB:57:LEU:HB2 | 2.10 | 0.52 |
| 22:BA:15:G:C5 | 22:BA:16:C:C5 | 2.97 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:136:G:H2' | 22:BA:137:U:C6 | 2.44 | 0.52 |
| 22:BA:244:A:OP2 | 51:B3:8:ARG:NH2 | 2.40 | 0.52 |
| 22:BA:1153:C:P | 58:BA:3362:HOH:O | 2.67 | 0.52 |
| 22:BA:1379:U:OP1 | 22:BA:1379:U:C5 | 2.62 | 0.52 |
| 22:BA:1565:C:OP1 | 24:BC:18:LYS:NZ | 2.41 | 0.52 |
| 22:BA:1594:U:H2' | 22:BA:1595:C:C6 | 2.45 | 0.52 |
| 22:BA:1916:A:N1 | 22:BA:1917:U:C2 | 2.77 | 0.52 |
| 22:BA:2441:U:OP2 | 22:BA:2586:U:O2' | 2.28 | 0.52 |
| 26:BE:145:ASP:HB3 | 26:BE:184:ASP:OD2 | 2.09 | 0.52 |
| 29:BH:77:THR:HA | 29:BH:143:ILE:O | 2.10 | 0.52 |
| 30:BI:97:LYS:HG3 | 30:BI:139:VAL:HG22 | 1.91 | 0.52 |
| 31:BJ:65:THR:O | 31:BJ:68:LYS:HG3 | 2.09 | 0.52 |
| 37:BP:26:VAL:HG13 | 37:BP:47:VAL:HG23 | 1.89 | 0.52 |
| 1:CA:406:G:C2 | 1:CA:407:U:C6 | 2.98 | 0.52 |
| 1:CA:747:A:C6 | 1:CA:748:G:C6 | 2.97 | 0.52 |
| 1:CA:1133:G:H2' | 1:CA:1133:G:N3 | 2.25 | 0.52 |
| 1:CA:1235:U:H2' | 1:CA:1236:A:O4' | 2.08 | 0.52 |
| 1:CA:1252:A:H2' | 1:CA:1253:G:O4' | 2.09 | 0.52 |
| 1:CA:1296:C:C5' | 1:CA:1297:G:OP2 | 2.57 | 0.52 |
| 2:CB:162:PHE:HA | 2:CB:184:PHE:O | 2.09 | 0.52 |
| 6:CF:4:TYR:CD2 | 6:CF:71:ILE:HG12 | 2.44 | 0.52 |
| 13:CM:6:GLY:O | 13:CM:8:ASN:N | 2.42 | 0.52 |
| 18:CR:22:ASP:OD2 | 18:CR:24:LYS:NZ | 2.42 | 0.52 |
| 19:CS:6:LYS:CB | 19:CS:7:LYS:HE2 | 2.40 | 0.52 |
| 22:DA:749:A:C5 | 22:DA:750:A:C8 | 2.97 | 0.52 |
| 22:DA:1638:C:H4' | 22:DA:2710:C:O2 | 2.09 | 0.52 |
| 22:DA:1874:C:H3' | 22:DA:1875:G:C8 | 2.44 | 0.52 |
| 22:DA:2225:A:H1' | 22:DA:2226:C:OP2 | 2.09 | 0.52 |
| 24:DC:141:VAL:CG1 | 24:DC:190:ALA:HB1 | 2.39 | 0.52 |
| 30:DI:28:LEU:C | 30:DI:28:LEU:HD12 | 2.30 | 0.52 |
| 36:DO:7:ARG:HD2 | 36:DO:97:PHE:CE1 | 2.44 | 0.52 |
| 1:AA:118:U:O4 | 1:AA:288:A:H2' | 2.10 | 0.52 |
| 1:AA:260:G:H2' | 1:AA:261:U:C6 | 2.45 | 0.52 |
| 1:AA:624:C:H4' | 16:AP:11:ALA:HB2 | 1.91 | 0.52 |
| 1:AA:1060:U:OP1 | 14:AN:85:ARG:NH2 | 2.39 | 0.52 |
| 1:AA:1277:C:HO2' | 1:AA:1279:G:H8 | 1.54 | 0.52 |
| 3:AC:193:TYR:N | 3:AC:193:TYR:CD2 | 2.76 | 0.52 |
| 22:BA:1124:G:N3 | 52:B4:38:GLY:O | 2.43 | 0.52 |
| 22:BA:1575:C:H2' | 22:BA:1576:U:O4' | 2.10 | 0.52 |
| 22:BA:1593:A:H2' | 22:BA:1594:U:O4' | 2.09 | 0.52 |
| 22:BA:1680:U:H2' | 22:BA:1681:G:O4' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2243:U:O2' | 22:BA:2244:U:H5' | 2.10 | 0.52 |
| 22:BA:2318:G:C6 | 22:BA:2319:G:C6 | 2.97 | 0.52 |
| 22:BA:2512:C:H4' | 25:BD:127:PHE:CE1 | 2.45 | 0.52 |
| 24:BC:21:ASN:O | 24:BC:24:LEU:HB2 | 2.10 | 0.52 |
| 29:BH:51:ARG:NH1 | 29:BH:55:GLU:OE1 | 2.43 | 0.52 |
| 35:BN:66:ALA:O | 35:BN:69:ARG:O | 2.27 | 0.52 |
| 1:CA:72:A:C6 | 1:CA:73:C:C4 | 2.98 | 0.52 |
| 1:CA:179:A:C5 | 1:CA:180:U:C4 | 2.97 | 0.52 |
| 1:CA:186:C:O2' | 1:CA:187:G:H5' | 2.10 | 0.52 |
| 1:CA:802:A:N3 | 1:CA:802:A:H2' | 2.25 | 0.52 |
| 3:CC:77:ILE:HD11 | 3:CC:103:ILE:HG12 | 1.92 | 0.52 |
| 3:CC:173:VAL:O | 3:CC:175:LEU:N | 2.42 | 0.52 |
| 10:CJ:84:VAL:O | 10:CJ:88:MET:HB2 | 2.10 | 0.52 |
| 22:DA:459:U:C5 | 22:DA:469:G:N2 | 2.77 | 0.52 |
| 22:DA:593:U:C2 | 22:DA:594:U:C5 | 2.98 | 0.52 |
| 22:DA:931:U:H4' | 22:DA:932:U:OP2 | 2.08 | 0.52 |
| 22:DA:1055:G:O2' | 22:DA:1085:A:N1 | 2.31 | 0.52 |
| 22:DA:1253:A:OP2 | 58:DA:3283:HOH:O | 2.19 | 0.52 |
| 22:DA:1370:C:H2' | 22:DA:1371:G:C8 | 2.45 | 0.52 |
| 22:DA:1838:C:H4' | 22:DA:1839:G:C8 | 2.45 | 0.52 |
| 37:DP:106:LYS:HA | 37:DP:109:ARG:HD2 | 1.90 | 0.52 |
| 51:D3:24:HIS:CE1 | 51:D3:48:ALA:HB3 | 2.45 | 0.52 |
| 1:AA:1160:G:O2' | 1:AA:1161:C:P | 2.68 | 0.52 |
| 3:AC:130:PHE:CZ | 3:AC:131:ARG:HD3 | 2.45 | 0.52 |
| 4:AD:26:ARG:HD2 | 4:AD:31:LYS:HD2 | 1.92 | 0.52 |
| 22:BA:528:A:N1 | 22:BA:2043:C:H5' | 2.24 | 0.52 |
| 22:BA:947:A:HO2' | 22:BA:984:A:H2 | 1.51 | 0.52 |
| 22:BA:996:A:N6 | 22:BA:1160:G:C6 | 2.77 | 0.52 |
| 22:BA:2307:G:H4' | 22:BA:2308:G:O5' | 2.10 | 0.52 |
| 27:BF:42:GLU:O | 27:BF:42:GLU:CG | 2.57 | 0.52 |
| 1:CA:31:G:C5 | 1:CA:306:A:H1' | 2.44 | 0.52 |
| 1:CA:321:A:C8 | 1:CA:328:C:C2 | 2.97 | 0.52 |
| 1:CA:505:G:C5 | 1:CA:535:A:C2 | 2.98 | 0.52 |
| 1:CA:1052:U:H5'' | 1:CA:1053:G:OP2 | 2.08 | 0.52 |
| 1:CA:1511:G:C5 | 1:CA:1512:U:C5 | 2.97 | 0.52 |
| 4:CD:173:VAL:HG13 | 4:CD:174:ASP:N | 2.25 | 0.52 |
| 6:CF:6:ILE:HG22 | 6:CF:7:VAL:N | 2.24 | 0.52 |
| 10:CJ:57:VAL:HG13 | 10:CJ:58:ASN:N | 2.25 | 0.52 |
| 11:CK:72:ASP:OD1 | 11:CK:73:ALA:N | 2.42 | 0.52 |
| 14:CN:10:GLU:O | 14:CN:13:ARG:N | 2.43 | 0.52 |
| 17:CQ:16:LYS:C | 17:CQ:17:MET:SD | 2.88 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:247:G:OP2 | 22:DA:249:C:N4 | 2.43 | 0.52 |
| 22:DA:1082:U:H5' | 30:DI:119:GLY:HA2 | 1.92 | 0.52 |
| 22:DA:1139:G:O2' | 22:DA:1140:C:H5' | 2.09 | 0.52 |
| 22:DA:1281:G:C2' | 22:DA:1282:U:H5' | 2.39 | 0.52 |
| 22:DA:1438:U:C4 | 22:DA:1552:A:C2 | 2.98 | 0.52 |
| 22:DA:1439:A:C8 | 22:DA:1440:U:C6 | 2.98 | 0.52 |
| 22:DA:1645:G:OP1 | 22:DA:1646:C:H5' | 2.09 | 0.52 |
| 22:DA:2314:A:C2 | 22:DA:2315:G:C4 | 2.97 | 0.52 |
| 22:DA:2563:U:H1' | 22:DA:2566:A:N6 | 2.25 | 0.52 |
| 24:DC:34:LEU:O | 24:DC:35:GLU:CB | 2.57 | 0.52 |
| 29:DH:34:GLY:O | 29:DH:35:LYS:HB2 | 2.08 | 0.52 |
| 29:DH:34:GLY:O | 29:DH:35:LYS:HD2 | 2.10 | 0.52 |
| 42:DU:83:VAL:CG1 | 42:DU:84:GLY:N | 2.73 | 0.52 |
| 45:DX:27:ARG:NE | 45:DX:28:ARG:O | 2.40 | 0.52 |
| 1:AA:208:U:C5 | 1:AA:210:C:N3 | 2.78 | 0.52 |
| 1:AA:1311:A:H2' | 1:AA:1312:G:O5' | 2.10 | 0.52 |
| 13:AM:11:ASP:O | 13:AM:12:HIS:HB2 | 2.09 | 0.52 |
| 22:BA:2669:G:C2' | 22:BA:2670:A:H5' | 2.40 | 0.52 |
| 36:BO:51:ALA:O | 36:BO:74:VAL:HG13 | 2.10 | 0.52 |
| 45:BX:17:ASN:OD1 | 45:BX:27:ARG:HD2 | 2.09 | 0.52 |
| 53:B5:122:GLY:HA3 | 53:B5:146:VAL:CB | 2.40 | 0.52 |
| 1:CA:513:C:H2' | 1:CA:514:C:C6 | 2.45 | 0.52 |
| 1:CA:734:G:C4 | 1:CA:735:C:C5 | 2.98 | 0.52 |
| 1:CA:838:G:H2' | 1:CA:839:C:O4' | 2.09 | 0.52 |
| 2:CB:186:ILE:HG13 | 2:CB:200:ILE:O | 2.10 | 0.52 |
| 5:CE:15:LEU:C | 5:CE:15:LEU:HD12 | 2.30 | 0.52 |
| 6:CF:43:GLY:HA2 | 6:CF:58:HIS:NE2 | 2.24 | 0.52 |
| 7:CG:116:MET:HA | 7:CG:119:ARG:HD3 | 1.91 | 0.52 |
| 16:CP:23:ASP:OD2 | 16:CP:25:ARG:CG | 2.58 | 0.52 |
| 22:DA:1352:U:C5 | 22:DA:1377:G:C6 | 2.98 | 0.52 |
| 22:DA:1355:G:C2 | 22:DA:1356:G:C8 | 2.98 | 0.52 |
| 22:DA:1363:C:H2' | 22:DA:1364:G:H8 | 1.75 | 0.52 |
| 22:DA:2093:G:C6 | 22:DA:2225:A:C8 | 2.98 | 0.52 |
| 22:DA:2677:G:C4 | 22:DA:2731:G:N2 | 2.77 | 0.52 |
| 24:DC:141:VAL:HG11 | 24:DC:190:ALA:HB1 | 1.90 | 0.52 |
| 26:DE:8:ALA:HB2 | 26:DE:122:GLU:HG3 | 1.92 | 0.52 |
| 27:DF:122:PHE:CE1 | 27:DF:166:GLY:HA3 | 2.45 | 0.52 |
| 30:DI:62:TYR:HB2 | 30:DI:66:SER:O | 2.08 | 0.52 |
| 1:AA:202:G:O2' | 1:AA:468:A:C8 | 2.62 | 0.52 |
| 1:AA:1118:U:O2 | 1:AA:1179:A:C6 | 2.63 | 0.52 |
| 4:AD:88:GLU:HG2 | 4:AD:188:ARG:HD3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:AM:11:ASP:OD1 | 13:AM:45:ILE:HB | 2.09 | 0.52 |
| 15:AO:35:GLN:HB3 | 15:AO:59:MET:CE | 2.40 | 0.52 |
| 19:AS:5:LEU:HD23 | 19:AS:9:PRO:HA | 1.92 | 0.52 |
| 22:BA:1317:G:C2 | 22:BA:1336:A:C2 | 2.98 | 0.52 |
| 22:BA:2291:U:H2' | 22:BA:2292:U:C5 | 2.45 | 0.52 |
| 23:BB:2:G:N1 | 23:BB:119:A:C2 | 2.78 | 0.52 |
| 29:BH:2:GLN:O | 29:BH:3:VAL:HG22 | 2.10 | 0.52 |
| 29:BH:94:ILE:HD12 | 29:BH:98:ASP:HB3 | 1.92 | 0.52 |
| 41:BT:19:LYS:NZ | 41:BT:84:TYR:OH | 2.42 | 0.52 |
| 17:CQ:50:ASN:O | 17:CQ:51:ASN:C | 2.48 | 0.52 |
| 22:DA:30:G:C6 | 22:DA:31:C:N3 | 2.78 | 0.52 |
| 22:DA:61:C:OP1 | 46:DY:44:LYS:HD3 | 2.10 | 0.52 |
| 22:DA:67:U:H2' | 22:DA:68:G:O4' | 2.10 | 0.52 |
| 22:DA:142:A:C6 | 22:DA:143:C:N4 | 2.77 | 0.52 |
| 22:DA:158:U:H2' | 22:DA:159:G:H5' | 1.92 | 0.52 |
| 22:DA:250:G:H2' | 22:DA:251:A:C8 | 2.44 | 0.52 |
| 22:DA:996:A:C2 | 22:DA:997:G:C8 | 2.98 | 0.52 |
| 22:DA:1722:A:C6 | 22:DA:1739:A:C8 | 2.98 | 0.52 |
| 22:DA:1893:C:C5 | 22:DA:1894:C:C5 | 2.98 | 0.52 |
| 22:DA:2024:G:N2 | 22:DA:2040:G:H1' | 2.25 | 0.52 |
| 22:DA:2073:C:H5'' | 24:DC:228:VAL:HB | 1.91 | 0.52 |
| 22:DA:2690:U:C5 | 22:DA:2873:A:N1 | 2.78 | 0.52 |
| 28:DG:126:PRO:C | 28:DG:127:THR:OG1 | 2.48 | 0.52 |
| 29:DH:25:TYR:CZ | 29:DH:30:LEU:HD21 | 2.45 | 0.52 |
| 33:DL:2:ARG:HD3 | 33:DL:2:ARG:N | 2.25 | 0.52 |
| 42:DU:88:GLU:O | 42:DU:89:ASP:CB | 2.58 | 0.52 |
| 1:AA:92:U:H2' | 1:AA:93:U:C6 | 2.45 | 0.52 |
| 1:AA:502:A:H2' | 1:AA:503:C:O4' | 2.09 | 0.52 |
| 1:AA:926:G:N2 | 1:AA:1505:G:H2' | 2.25 | 0.52 |
| 1:AA:1296:C:H4' | 1:AA:1302:C:C4 | 2.44 | 0.52 |
| 2:AB:27:MET:HG2 | 2:AB:189:THR:HA | 1.92 | 0.52 |
| 2:AB:219:ALA:O | 2:AB:220:THR:CB | 2.57 | 0.52 |
| 7:AG:71:PRO:HD2 | 7:AG:96:ARG:O | 2.10 | 0.52 |
| 10:AJ:57:VAL:HG22 | 10:AJ:58:ASN:N | 2.25 | 0.52 |
| 14:AN:10:GLU:OE2 | 14:AN:61:ARG:HB3 | 2.10 | 0.52 |
| 19:AS:50:ALA:HB1 | 19:AS:57:HIS:HB3 | 1.90 | 0.52 |
| 22:BA:65:U:H2' | 22:BA:66:C:C6 | 2.44 | 0.52 |
| 22:BA:1224:U:C4 | 22:BA:1225:G:C6 | 2.98 | 0.52 |
| 22:BA:1779:U:C5 | 22:BA:1784:A:N7 | 2.78 | 0.52 |
| 22:BA:1916:A:OP2 | 22:BA:1917:U:OP2 | 2.28 | 0.52 |
| 22:BA:1993:U:H4' | 25:BD:133:THR:HG21 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2154:A:H2' | 22:BA:2155:U:C5 | 2.45 | 0.52 |
| 22:BA:2339:C:H2' | 22:BA:2340:A:C8 | 2.44 | 0.52 |
| 26:BE:164:LEU:HB3 | 26:BE:167:VAL:HB | 1.92 | 0.52 |
| 27:BF:36:LEU:HD21 | 27:BF:99:PHE:CE1 | 2.45 | 0.52 |
| 48:B0:48:TYR:CE2 | 48:B0:53:LYS:HB2 | 2.44 | 0.52 |
| 53:B5:83:LYS:HB3 | 53:B5:87:ALA:HB3 | 1.92 | 0.52 |
| 1:CA:197:A:C6 | 1:CA:221:C:H4' | 2.45 | 0.52 |
| 1:CA:328:C:O2 | 1:CA:328:C:C2' | 2.58 | 0.52 |
| 1:CA:632:U:O2 | 1:CA:632:U:C2' | 2.58 | 0.52 |
| 1:CA:1001:C:H2' | 1:CA:1002:G:N7 | 2.25 | 0.52 |
| 4:CD:65:TYR:CG | 4:CD:94:LEU:HD22 | 2.45 | 0.52 |
| 5:CE:104:GLY:O | 5:CE:105:ILE:CG2 | 2.57 | 0.52 |
| 5:CE:125:ALA:O | 5:CE:126:LYS:HB3 | 2.09 | 0.52 |
| 11:CK:51:GLY:O | 11:CK:52:PHE:O | 2.28 | 0.52 |
| 22:DA:207:A:H2' | 22:DA:207:A:N3 | 2.24 | 0.52 |
| 22:DA:249:C:P | 22:DA:2394:C:O2' | 2.68 | 0.52 |
| 22:DA:927:A:O2' | 47:DZ:39:GLU:OE1 | 2.28 | 0.52 |
| 22:DA:1289:C:O2' | 22:DA:1330:C:H4' | 2.10 | 0.52 |
| 22:DA:1318:U:H2' | 22:DA:1319:C:C6 | 2.45 | 0.52 |
| 22:DA:1338:G:H5'' | 41:DT:17:SER:HB2 | 1.92 | 0.52 |
| 22:DA:1566:A:C2 | 24:DC:213:TRP:CG | 2.98 | 0.52 |
| 22:DA:1731:G:C6 | 22:DA:1733:G:N7 | 2.77 | 0.52 |
| 22:DA:2199:A:N7 | 22:DA:2225:A:N6 | 2.58 | 0.52 |
| 22:DA:2214:C:C2' | 22:DA:2215:C:O5' | 2.57 | 0.52 |
| 22:DA:2621:G:OP1 | 25:DD:124:ARG:NH2 | 2.43 | 0.52 |
| 25:DD:151:THR:HB | 25:DD:152:PRO:HD2 | 1.92 | 0.52 |
| 30:DI:97:LYS:N | 30:DI:97:LYS:HD2 | 2.25 | 0.52 |
| 42:DU:10:GLU:OE2 | 42:DU:73:PHE:CD2 | 2.62 | 0.52 |
| 1:AA:1452:C:O4' | 1:AA:1453:G:C2 | 2.63 | 0.52 |
| 1:AA:1463:U:H2' | 1:AA:1464:U:C6 | 2.45 | 0.52 |
| 2:AB:126:PHE:N | 2:AB:126:PHE:HD2 | 2.06 | 0.52 |
| 2:AB:147:SER:O | 2:AB:148:LEU:HB2 | 2.08 | 0.52 |
| 8:AH:25:VAL:HG12 | 8:AH:61:LEU:HB2 | 1.92 | 0.52 |
| 10:AJ:53:ILE:HG22 | 10:AJ:61:ALA:HB1 | 1.92 | 0.52 |
| 11:AK:36:ASP:OD2 | 11:AK:38:GLN:N | 2.42 | 0.52 |
| 16:AP:20:VAL:HG21 | 16:AP:32:PHE:CG | 2.45 | 0.52 |
| 17:AQ:16:LYS:O | 17:AQ:16:LYS:CG | 2.57 | 0.52 |
| 22:BA:141:G:N1 | 41:BT:1:MET:HE1 | 2.25 | 0.52 |
| 22:BA:271:G:H4' | 22:BA:272:A:OP1 | 2.10 | 0.52 |
| 22:BA:280:U:H2' | 22:BA:281:C:O4' | 2.09 | 0.52 |
| 22:BA:819:A:N3 | 22:BA:1189:A:C2 | 2.77 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1007:C:OP1 | 31:BJ:39:LYS:HD2 | 2.10 | 0.52 |
| 22:BA:2393:U:C2' | 22:BA:2394:C:O5' | 2.58 | 0.52 |
| 32:BK:107:LEU:O | 32:BK:109:SER:N | 2.43 | 0.52 |
| 35:BN:69:ARG:O | 35:BN:70:THR:HG23 | 2.10 | 0.52 |
| 53:B5:65:LEU:HD21 | 53:B5:191:ARG:CB | 2.39 | 0.52 |
| 1:CA:109:A:C6 | 1:CA:327:A:C5 | 2.98 | 0.52 |
| 1:CA:455:G:C6 | 1:CA:456:A:C6 | 2.98 | 0.52 |
| 1:CA:518:C:H5'' | 1:CA:519:C:C6 | 2.45 | 0.52 |
| 1:CA:892:A:O2' | 1:CA:1415:G:H4' | 2.09 | 0.52 |
| 1:CA:892:A:C5 | 1:CA:893:C:C5 | 2.98 | 0.52 |
| 1:CA:1053:G:O5' | 1:CA:1054:C:H3' | 2.09 | 0.52 |
| 1:CA:1098:C:H2' | 1:CA:1099:G:O4' | 2.10 | 0.52 |
| 1:CA:1458:G:O2' | 20:CT:23:SER:HB3 | 2.09 | 0.52 |
| 1:CA:1467:C:H2' | 1:CA:1468:A:C8 | 2.45 | 0.52 |
| 13:CM:29:ARG:NH1 | 13:CM:59:GLU:O | 2.43 | 0.52 |
| 14:CN:31:ILE:O | 14:CN:33:ASP:N | 2.43 | 0.52 |
| 22:DA:294:A:C6 | 22:DA:345:A:C4 | 2.97 | 0.52 |
| 22:DA:815:C:H2' | 22:DA:816:C:C6 | 2.45 | 0.52 |
| 22:DA:1204:A:C2 | 22:DA:1240:U:N3 | 2.77 | 0.52 |
| 22:DA:2230:G:H5' | 45:DX:30:LEU:HD13 | 1.92 | 0.52 |
| 22:DA:2297:A:N3 | 22:DA:2297:A:H2' | 2.25 | 0.52 |
| 22:DA:2870:C:H5'' | 35:DN:65:LEU:HD21 | 1.92 | 0.52 |
| 29:DH:23:ALA:O | 29:DH:27:ARG:N | 2.38 | 0.52 |
| 33:DL:102:GLY:N | 58:DL:301:HOH:O | 2.43 | 0.52 |
| 37:DP:39:ARG:HA | 37:DP:39:ARG:HE | 1.74 | 0.52 |
| 41:DT:77:ARG:O | 41:DT:78:SER:CB | 2.57 | 0.52 |
| 47:DZ:10:THR:HG23 | 47:DZ:54:MET:C | 2.30 | 0.52 |
| 50:D2:10:LEU:O | 50:D2:14:ARG:HG3 | 2.10 | 0.52 |
| 1:AA:47:C:O2 | 1:AA:49:U:C5 | 2.62 | 0.51 |
| 1:AA:102:G:C2 | 1:AA:103:U:C5 | 2.98 | 0.51 |
| 1:AA:760:G:C5 | 1:AA:761:G:C8 | 2.98 | 0.51 |
| 1:AA:862:C:C2' | 1:AA:863:U:H5' | 2.40 | 0.51 |
| 1:AA:878:A:OP2 | 8:AH:80:ARG:NH1 | 2.43 | 0.51 |
| 1:AA:1171:A:C2 | 1:AA:1172:C:C2 | 2.98 | 0.51 |
| 1:AA:1367:C:OP2 | 9:AI:114:LYS:NZ | 2.41 | 0.51 |
| 2:AB:169:GLU:O | 2:AB:170:HIS:C | 2.47 | 0.51 |
| 2:AB:206:ALA:O | 2:AB:210:VAL:HG22 | 2.10 | 0.51 |
| 4:AD:125:VAL:O | 4:AD:126:ASN:C | 2.47 | 0.51 |
| 5:AE:13:GLU:CB | 5:AE:39:VAL:HG12 | 2.41 | 0.51 |
| 6:AF:47:LEU:HD13 | 6:AF:51:ILE:HG23 | 1.91 | 0.51 |
| 22:BA:195:A:C6 | 22:BA:198:C:C5 | 2.97 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:225:C:H2' | 22:BA:226:A:O4' | 2.10 | 0.51 |
| 22:BA:1098:A:C8 | 22:BA:1099:G:N7 | 2.78 | 0.51 |
| 27:BF:85:ILE:O | 27:BF:85:ILE:HG12 | 2.10 | 0.51 |
| 27:BF:103:LEU:O | 27:BF:108:VAL:HB | 2.10 | 0.51 |
| 30:BI:24:VAL:CG2 | 30:BI:28:LEU:HD23 | 2.40 | 0.51 |
| 31:BJ:17:VAL:HG22 | 31:BJ:55:ILE:HB | 1.92 | 0.51 |
| 1:CA:519:C:H2' | 1:CA:520:A:O4' | 2.10 | 0.51 |
| 3:CC:117:ALA:HB1 | 3:CC:187:SER:HB2 | 1.90 | 0.51 |
| 4:CD:26:ARG:CG | 4:CD:27:ALA:N | 2.73 | 0.51 |
| 12:CL:38:TYR:CB | 12:CL:52:VAL:HG13 | 2.40 | 0.51 |
| 17:CQ:50:ASN:O | 17:CQ:52:GLU:N | 2.43 | 0.51 |
| 18:CR:25:ASP:OD1 | 18:CR:25:ASP:N | 2.43 | 0.51 |
| 22:DA:425:G:N2 | 22:DA:426:C:N3 | 2.58 | 0.51 |
| 22:DA:522:A:C6 | 22:DA:523:C:N3 | 2.78 | 0.51 |
| 22:DA:740:C:H5' | 22:DA:1784:A:C3' | 2.39 | 0.51 |
| 22:DA:973:A:O4' | 22:DA:1188:U:C6 | 2.63 | 0.51 |
| 22:DA:1544:A:C6 | 22:DA:1545:A:N1 | 2.78 | 0.51 |
| 22:DA:1678:A:C5 | 22:DA:1679:A:C8 | 2.98 | 0.51 |
| 22:DA:1809:A:C6 | 22:DA:1810:A:C6 | 2.98 | 0.51 |
| 22:DA:1853:A:N3 | 22:DA:2233:U:O2' | 2.37 | 0.51 |
| 22:DA:2209:G:C2 | 22:DA:2216:G:N3 | 2.78 | 0.51 |
| 22:DA:2221:G:C5 | 22:DA:2222:C:C5 | 2.98 | 0.51 |
| 25:DD:140:HIS:CE1 | 58:DD:303:HOH:O | 2.63 | 0.51 |
| 26:DE:47:LYS:O | 26:DE:83:VAL:HB | 2.10 | 0.51 |
| 30:DI:80:LEU:HA | 30:DI:84:ALA:HB2 | 1.92 | 0.51 |
| 32:DK:71:ARG:HB3 | 32:DK:72:PRO:HD2 | 1.92 | 0.51 |
| 49:D1:5:ILE:HG22 | 49:D1:28:ARG:NH1 | 2.25 | 0.51 |
| 51:D3:4:ILE:HG21 | 51:D3:63:PRO:HG3 | 1.92 | 0.51 |
| 1:AA:601:G:H2' | 1:AA:602:A:C8 | 2.44 | 0.51 |
| 1:AA:1315:U:C4 | 1:AA:1316:G:C6 | 2.98 | 0.51 |
| 2:AB:164:ILE:HD12 | 2:AB:210:VAL:CG1 | 2.41 | 0.51 |
| 9:AI:50:GLN:O | 9:AI:52:LEU:N | 2.42 | 0.51 |
| 14:AN:49:GLN:HA | 14:AN:49:GLN:OE1 | 2.09 | 0.51 |
| 17:AQ:80:GLU:C | 17:AQ:81:LYS:HD3 | 2.30 | 0.51 |
| 22:BA:307:G:N2 | 22:BA:309:A:H3' | 2.25 | 0.51 |
| 22:BA:563:A:C2 | 22:BA:564:C:C2 | 2.99 | 0.51 |
| 22:BA:861:A:C2 | 22:BA:917:A:C4 | 2.99 | 0.51 |
| 22:BA:1056:G:C2 | 22:BA:1102:C:C5 | 2.98 | 0.51 |
| 22:BA:1730:C:O2' | 22:BA:1731:G:C4 | 2.55 | 0.51 |
| 22:BA:1737:G:C6 | 22:BA:1738:G:N1 | 2.78 | 0.51 |
| 22:BA:2140:G:N3 | 22:BA:2140:G:H2' | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BF:21:ASN:O | 27:BF:21:ASN:CG | 2.48 | 0.51 |
| 49:B1:23:THR:OG1 | 49:B1:24:THR:N | 2.44 | 0.51 |
| 1:CA:137:U:H1' | 1:CA:227:G:N2 | 2.25 | 0.51 |
| 1:CA:151:A:H2' | 1:CA:152:A:O4' | 2.10 | 0.51 |
| 3:CC:172:ARG:HG3 | 3:CC:174:PRO:HD3 | 1.92 | 0.51 |
| 15:CO:67:LEU:O | 15:CO:70:LEU:N | 2.44 | 0.51 |
| 22:DA:169:G:C2 | 22:DA:170:U:C6 | 2.98 | 0.51 |
| 22:DA:176:A:N7 | 22:DA:177:G:C6 | 2.79 | 0.51 |
| 22:DA:195:A:C6 | 22:DA:198:C:C5 | 2.99 | 0.51 |
| 22:DA:270:A:C2 | 22:DA:369:U:H4' | 2.46 | 0.51 |
| 22:DA:398:C:OP1 | 45:DX:53:ALA:CB | 2.59 | 0.51 |
| 22:DA:856:G:H2' | 22:DA:857:G:C8 | 2.44 | 0.51 |
| 22:DA:914:G:H5' | 22:DA:915:C:OP2 | 2.10 | 0.51 |
| 22:DA:1049:C:H2' | 22:DA:1050:A:H5' | 1.92 | 0.51 |
| 22:DA:2174:C:H2' | 22:DA:2175:C:O4' | 2.09 | 0.51 |
| 42:DU:13:VAL:HG21 | 42:DU:39:ILE:CG2 | 2.40 | 0.51 |
| 1:AA:1236:A:H4' | 1:AA:1304:G:H4' | 1.92 | 0.51 |
| 1:AA:1255:G:O2' | 1:AA:1258:G:N3 | 2.40 | 0.51 |
| 10:AJ:10:LEU:CD1 | 10:AJ:98:VAL:HG12 | 2.40 | 0.51 |
| 12:AL:23:ALA:O | 12:AL:24:LEU:O | 2.27 | 0.51 |
| 22:BA:547:A:H3' | 22:BA:548:G:C5' | 2.40 | 0.51 |
| 22:BA:1050:A:H2' | 22:BA:1051:G:O4' | 2.10 | 0.51 |
| 22:BA:1075:C:H2' | 22:BA:1076:C:C2 | 2.46 | 0.51 |
| 22:BA:1171:G:N3 | 22:BA:1179:G:N1 | 2.57 | 0.51 |
| 22:BA:1432:G:O2' | 22:BA:1433:A:H5' | 2.10 | 0.51 |
| 22:BA:2882:A:OP1 | 35:BN:96:ARG:HD3 | 2.10 | 0.51 |
| 29:BH:99:ILE:O | 29:BH:103:VAL:CG2 | 2.58 | 0.51 |
| 1:CA:74:A:C2 | 1:CA:75:G:C5 | 2.98 | 0.51 |
| 1:CA:620:C:N1 | 4:CD:132:ILE:HD13 | 2.25 | 0.51 |
| 1:CA:1072:G:C5 | 1:CA:1073:U:C5 | 2.99 | 0.51 |
| 1:CA:1240:U:C5 | 7:CG:109:ARG:NH1 | 2.78 | 0.51 |
| 2:CB:187:VAL:HG23 | 2:CB:188:ASP:O | 2.09 | 0.51 |
| 8:CH:75:ILE:HD13 | 8:CH:129:VAL:HG22 | 1.92 | 0.51 |
| 17:CQ:8:LEU:HD13 | 17:CQ:73:TRP:CZ3 | 2.46 | 0.51 |
| 19:CS:31:LEU:O | 19:CS:33:THR:N | 2.42 | 0.51 |
| 22:DA:333:G:C5 | 22:DA:334:C:C5 | 2.99 | 0.51 |
| 22:DA:370:G:O2' | 22:DA:423:A:H3' | 2.09 | 0.51 |
| 22:DA:491:G:C6 | 22:DA:492:A:C5 | 2.98 | 0.51 |
| 22:DA:617:G:H2' | 22:DA:618:G:O4' | 2.10 | 0.51 |
| 22:DA:963:U:H2' | 22:DA:964:C:C6 | 2.45 | 0.51 |
| 22:DA:1286:A:N6 | 22:DA:1329:U:C2 | 2.79 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1607:C:H4' | 22:DA:1608:A:O5' | 2.10 | 0.51 |
| 22:DA:2145:C:H5'' | 22:DA:2146:C:P | 2.51 | 0.51 |
| 22:DA:2284:A:O2' | 22:DA:2288:A:N1 | 2.33 | 0.51 |
| 29:DH:121:VAL:O | 29:DH:122:LEU:HB2 | 2.11 | 0.51 |
| 30:DI:76:ALA:HA | 30:DI:79:LEU:HB2 | 1.91 | 0.51 |
| 31:DJ:142:ILE:OXT | 31:DJ:142:ILE:HG23 | 2.10 | 0.51 |
| 37:DP:54:GLY:O | 37:DP:77:HIS:NE2 | 2.44 | 0.51 |
| 37:DP:113:ARG:O | 37:DP:114:LEU:C | 2.48 | 0.51 |
| 50:D2:18:PHE:O | 50:D2:21:ARG:N | 2.44 | 0.51 |
| 51:D3:31:HIS:CE1 | 51:D3:32:ILE:CD1 | 2.94 | 0.51 |
| 1:AA:340:U:H2' | 1:AA:341:C:C6 | 2.45 | 0.51 |
| 1:AA:374:A:C6 | 1:AA:375:U:C4 | 2.99 | 0.51 |
| 4:AD:26:ARG:HD2 | 4:AD:31:LYS:HE3 | 1.93 | 0.51 |
| 7:AG:13:LEU:HD22 | 7:AG:13:LEU:N | 2.26 | 0.51 |
| 14:AN:4:GLN:O | 14:AN:7:LYS:N | 2.44 | 0.51 |
| 21:AU:12:PHE:N | 21:AU:12:PHE:CD2 | 2.76 | 0.51 |
| 22:BA:244:A:C2 | 22:BA:255:A:C4 | 2.98 | 0.51 |
| 22:BA:2009:A:OP1 | 40:BS:41:LYS:HE2 | 2.11 | 0.51 |
| 22:BA:2298:A:C4 | 22:BA:2321:U:C5 | 2.98 | 0.51 |
| 23:BB:78:A:C2 | 23:BB:99:A:C4 | 2.98 | 0.51 |
| 24:BC:238:ARG:O | 24:BC:239:ASN:ND2 | 2.43 | 0.51 |
| 25:BD:38:LYS:O | 25:BD:46:ARG:HA | 2.10 | 0.51 |
| 26:BE:77:ILE:O | 26:BE:77:ILE:CG1 | 2.58 | 0.51 |
| 33:BL:95:LEU:HD22 | 33:BL:100:ILE:CD1 | 2.40 | 0.51 |
| 44:BW:23:VAL:HA | 44:BW:38:VAL:HG12 | 1.92 | 0.51 |
| 53:B5:50:ILE:HG22 | 53:B5:51:ASP:N | 2.26 | 0.51 |
| 1:CA:686:U:O2' | 1:CA:687:A:OP2 | 2.22 | 0.51 |
| 1:CA:743:A:C6 | 1:CA:744:C:C4 | 2.98 | 0.51 |
| 1:CA:963:G:C2' | 1:CA:964:A:H5' | 2.40 | 0.51 |
| 1:CA:972:C:H4' | 10:CJ:59:LYS:HG2 | 1.91 | 0.51 |
| 3:CC:145:GLY:O | 3:CC:146:ALA:O | 2.28 | 0.51 |
| 4:CD:74:ASN:HA | 4:CD:77:LYS:HB2 | 1.92 | 0.51 |
| 12:CL:57:LEU:O | 12:CL:58:THR:C | 2.49 | 0.51 |
| 15:CO:35:GLN:NE2 | 15:CO:39:LEU:HD21 | 2.25 | 0.51 |
| 22:DA:491:G:C6 | 22:DA:492:A:C6 | 2.98 | 0.51 |
| 22:DA:621:A:C5 | 22:DA:622:G:H1' | 2.45 | 0.51 |
| 22:DA:749:A:C6 | 22:DA:1618:A:C2 | 2.99 | 0.51 |
| 22:DA:1324:G:O4' | 22:DA:1616:A:N6 | 2.43 | 0.51 |
| 22:DA:1620:G:C6 | 22:DA:1621:U:C4 | 2.99 | 0.51 |
| 33:DL:59:ARG:HB3 | 33:DL:59:ARG:CZ | 2.40 | 0.51 |
| 35:DN:12:ARG:HG2 | 35:DN:16:HIS:HB3 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:261:U:P | 20:AT:71:LYS:HE2 | 2.51 | 0.51 |
| 1:AA:560:A:C6 | 5:AE:128:TYR:CE1 | 2.98 | 0.51 |
| 1:AA:992:U:O2 | 1:AA:1043:G:N7 | 2.44 | 0.51 |
| 8:AH:79:SER:HA | 8:AH:85:ILE:HG12 | 1.92 | 0.51 |
| 11:AK:88:GLY:H | 11:AK:114:THR:HG22 | 1.76 | 0.51 |
| 13:AM:15:ALA:O | 13:AM:18:ALA:N | 2.44 | 0.51 |
| 20:AT:44:LYS:NZ | 20:AT:86:LEU:O | 2.38 | 0.51 |
| 22:BA:283:G:N7 | 22:BA:284:U:C5 | 2.78 | 0.51 |
| 22:BA:304:U:H2' | 22:BA:305:C:C6 | 2.46 | 0.51 |
| 22:BA:929:U:H1' | 47:BZ:26:GLY:O | 2.11 | 0.51 |
| 22:BA:2223:G:OP1 | 24:BC:171:TYR:OH | 2.23 | 0.51 |
| 22:BA:2492:U:C2 | 22:BA:2493:U:C5 | 2.99 | 0.51 |
| 23:BB:63:C:C2 | 23:BB:64:G:C8 | 2.99 | 0.51 |
| 24:BC:28:LYS:HD3 | 24:BC:28:LYS:N | 2.26 | 0.51 |
| 29:BH:85:GLY:HA2 | 29:BH:91:PHE:CE2 | 2.46 | 0.51 |
| 29:BH:94:ILE:CG2 | 29:BH:99:ILE:CG1 | 2.88 | 0.51 |
| 29:BH:110:VAL:HG22 | 29:BH:114:GLU:HB2 | 1.90 | 0.51 |
| 35:BN:2:ARG:HA | 35:BN:5:LYS:HD2 | 1.92 | 0.51 |
| 43:BV:61:LEU:HD13 | 43:BV:61:LEU:N | 2.25 | 0.51 |
| 1:CA:16:A:C2' | 1:CA:17:U:H5' | 2.41 | 0.51 |
| 1:CA:213:G:C8 | 1:CA:214:C:C5 | 2.99 | 0.51 |
| 1:CA:756:C:H2' | 1:CA:757:U:C5' | 2.40 | 0.51 |
| 1:CA:927:G:O2' | 1:CA:1503:A:N7 | 2.36 | 0.51 |
| 1:CA:1380:U:C5 | 7:CG:3:ARG:HA | 2.45 | 0.51 |
| 2:CB:10:LEU:CD2 | 2:CB:12:ALA:O | 2.58 | 0.51 |
| 2:CB:15:HIS:O | 2:CB:16:PHE:C | 2.48 | 0.51 |
| 3:CC:64:ILE:HG12 | 3:CC:66:VAL:HG23 | 1.92 | 0.51 |
| 5:CE:137:VAL:O | 5:CE:138:ARG:CB | 2.58 | 0.51 |
| 8:CH:10:MET:HE1 | 8:CH:36:ILE:HB | 1.92 | 0.51 |
| 9:CI:13:LYS:O | 9:CI:14:SER:HB3 | 2.10 | 0.51 |
| 9:CI:32:GLN:NE2 | 9:CI:64:TYR:OH | 2.43 | 0.51 |
| 9:CI:88:MET:O | 9:CI:88:MET:HG2 | 2.09 | 0.51 |
| 9:CI:120:LYS:CG | 9:CI:123:ARG:HB3 | 2.40 | 0.51 |
| 22:DA:32:C:H5'' | 22:DA:33:C:OP2 | 2.10 | 0.51 |
| 22:DA:228:C:H4' | 22:DA:229:C:H5'' | 1.91 | 0.51 |
| 22:DA:410:G:C2 | 22:DA:2407:A:C5 | 2.98 | 0.51 |
| 22:DA:415:A:C2 | 22:DA:2409:G:C6 | 2.98 | 0.51 |
| 22:DA:504:A:C2 | 22:DA:1234:U:H4' | 2.46 | 0.51 |
| 22:DA:547:A:H3' | 22:DA:548:G:C5' | 2.40 | 0.51 |
| 22:DA:1435:G:C2' | 22:DA:1436:G:H5' | 2.41 | 0.51 |
| 22:DA:1651:G:C2 | 22:DA:2007:U:O2 | 2.64 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1817:G:C2' | 22:DA:1818:U:H5' | 2.41 | 0.51 |
| 22:DA:1917:U:H2' | 22:DA:1918:A:H5' | 1.92 | 0.51 |
| 22:DA:2019:A:H4' | 38:DQ:34:VAL:HG22 | 1.92 | 0.51 |
| 27:DF:128:TYR:CG | 27:DF:170:LEU:HD13 | 2.46 | 0.51 |
| 29:DH:26:ALA:HA | 29:DH:30:LEU:HB2 | 1.92 | 0.51 |
| 29:DH:53:GLU:O | 29:DH:54:LEU:C | 2.49 | 0.51 |
| 30:DI:51:LYS:N | 30:DI:51:LYS:HD3 | 2.24 | 0.51 |
| 46:DY:18:LEU:O | 46:DY:22:LEU:CB | 2.58 | 0.51 |
| 1:AA:651:C:C2' | 1:AA:652:U:O5' | 2.59 | 0.51 |
| 1:AA:1349:A:C6 | 1:AA:1374:A:C8 | 2.99 | 0.51 |
| 1:AA:1429:A:C2 | 1:AA:1430:A:N9 | 2.78 | 0.51 |
| 2:AB:14:VAL:HG23 | 2:AB:208:ARG:NH2 | 2.25 | 0.51 |
| 2:AB:59:LYS:O | 2:AB:63:ARG:HG3 | 2.11 | 0.51 |
| 5:AE:136:VAL:O | 5:AE:138:ARG:N | 2.43 | 0.51 |
| 10:AJ:51:VAL:HB | 14:AN:81:ARG:HB2 | 1.91 | 0.51 |
| 22:BA:1176:U:H2' | 22:BA:1177:G:C4 | 2.46 | 0.51 |
| 22:BA:1366:A:C5 | 22:BA:1367:A:C8 | 2.98 | 0.51 |
| 22:BA:1838:C:C5 | 22:BA:1899:A:C6 | 2.99 | 0.51 |
| 22:BA:2831:G:OP1 | 25:BD:56:LYS:NZ | 2.36 | 0.51 |
| 27:BF:106:ILE:C | 27:BF:109:PRO:HD2 | 2.31 | 0.51 |
| 29:BH:100:ALA:CB | 29:BH:112:LYS:HA | 2.41 | 0.51 |
| 29:BH:117:LEU:CD2 | 29:BH:121:VAL:N | 2.70 | 0.51 |
| 29:BH:132:PHE:O | 29:BH:139:PHE:HB3 | 2.11 | 0.51 |
| 43:BV:14:LYS:CD | 43:BV:18:ARG:NH1 | 2.73 | 0.51 |
| 1:CA:101:A:C4 | 1:CA:102:G:C8 | 2.98 | 0.51 |
| 1:CA:437:U:C4 | 1:CA:438:U:C5 | 2.99 | 0.51 |
| 1:CA:736:C:H2' | 1:CA:737:C:C6 | 2.45 | 0.51 |
| 1:CA:1014:A:O4' | 19:CS:34:TRP:CZ3 | 2.63 | 0.51 |
| 1:CA:1285:A:H4' | 1:CA:1286:U:C5 | 2.46 | 0.51 |
| 2:CB:133:GLU:O | 2:CB:137:ARG:HB3 | 2.10 | 0.51 |
| 4:CD:147:GLU:O | 4:CD:150:LYS:HB3 | 2.11 | 0.51 |
| 10:CJ:91:ASP:O | 10:CJ:92:LEU:HB2 | 2.11 | 0.51 |
| 12:CL:38:TYR:N | 12:CL:52:VAL:O | 2.43 | 0.51 |
| 20:CT:28:MET:HE3 | 20:CT:58:VAL:HG22 | 1.92 | 0.51 |
| 22:DA:38:A:H5' | 26:DE:45:ALA:HB3 | 1.92 | 0.51 |
| 22:DA:531:C:C5 | 22:DA:2035:G:C2 | 2.98 | 0.51 |
| 22:DA:777:G:N7 | 22:DA:793:A:C2 | 2.78 | 0.51 |
| 22:DA:1319:C:H2' | 22:DA:1320:C:H5' | 1.91 | 0.51 |
| 22:DA:2111:U:C4 | 22:DA:2147:A:C2 | 2.99 | 0.51 |
| 22:DA:2341:G:C5 | 22:DA:2342:C:C4 | 2.99 | 0.51 |
| 22:DA:2829:A:H2' | 22:DA:2830:C:H5' | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:DI:6:GLN:O | 30:DI:7:ALA:HB3 | 2.10 | 0.51 |
| 32:DK:31:ARG:HB3 | 32:DK:32:TYR:CE2 | 2.46 | 0.51 |
| 41:DT:59:ASN:O | 41:DT:84:TYR:N | 2.44 | 0.51 |
| 42:DU:44:LYS:HE3 | 42:DU:46:GLN:HB2 | 1.92 | 0.51 |
| 44:DW:56:ASP:O | 44:DW:57:HIS:HB2 | 2.10 | 0.51 |
| 1:AA:139:A:C2' | 1:AA:140:U:H5' | 2.40 | 0.51 |
| 1:AA:201:G:C2 | 1:AA:217:C:O2 | 2.64 | 0.51 |
| 1:AA:702:A:H3' | 1:AA:703:G:H5' | 1.91 | 0.51 |
| 1:AA:921:U:H2' | 1:AA:922:G:O4' | 2.11 | 0.51 |
| 1:AA:1040:U:H2' | 1:AA:1041:G:C8 | 2.46 | 0.51 |
| 4:AD:151:LYS:HB3 | 4:AD:178:MET:HE3 | 1.93 | 0.51 |
| 5:AE:16:ILE:CG2 | 5:AE:110:ALA:HA | 2.40 | 0.51 |
| 6:AF:98:GLU:O | 6:AF:99:ALA:O | 2.28 | 0.51 |
| 9:AI:52:LEU:HD13 | 9:AI:57:MET:HG3 | 1.93 | 0.51 |
| 21:AU:11:PRO:O | 21:AU:12:PHE:CB | 2.58 | 0.51 |
| 22:BA:142:A:N7 | 22:BA:143:C:C4 | 2.79 | 0.51 |
| 22:BA:478:A:C6 | 22:BA:480:A:C6 | 2.99 | 0.51 |
| 22:BA:2243:U:H2' | 22:BA:2244:U:H6 | 1.76 | 0.51 |
| 25:BD:150:GLN:O | 25:BD:153:GLY:N | 2.44 | 0.51 |
| 39:BR:39:LEU:CA | 39:BR:49:ILE:HG23 | 2.41 | 0.51 |
| 1:CA:57:G:C5 | 1:CA:58:C:C4 | 2.98 | 0.51 |
| 1:CA:130:A:N1 | 1:CA:233:C:O2' | 2.43 | 0.51 |
| 1:CA:1238:A:N3 | 1:CA:1241:G:O2' | 2.38 | 0.51 |
| 1:CA:1255:G:N1 | 1:CA:1279:G:C8 | 2.79 | 0.51 |
| 1:CA:1347:G:O2' | 1:CA:1348:U:P | 2.68 | 0.51 |
| 3:CC:36:ASP:C | 3:CC:38:LYS:H | 2.14 | 0.51 |
| 3:CC:75:ILE:O | 3:CC:75:ILE:HG13 | 2.10 | 0.51 |
| 7:CG:5:ARG:HA | 7:CG:5:ARG:HE | 1.75 | 0.51 |
| 8:CH:64:LYS:HB3 | 8:CH:71:VAL:HG21 | 1.93 | 0.51 |
| 14:CN:91:GLY:O | 14:CN:93:ILE:N | 2.43 | 0.51 |
| 16:CP:28:ARG:HG3 | 16:CP:29:ASN:OD1 | 2.10 | 0.51 |
| 20:CT:55:GLN:N | 20:CT:56:PRO:HD2 | 2.26 | 0.51 |
| 22:DA:200:U:C4 | 22:DA:248:G:C2 | 2.98 | 0.51 |
| 22:DA:201:C:C4 | 22:DA:202:U:C5 | 2.98 | 0.51 |
| 22:DA:488:G:N2 | 22:DA:493:G:C6 | 2.79 | 0.51 |
| 22:DA:2335:A:C6 | 22:DA:2337:G:H1' | 2.45 | 0.51 |
| 22:DA:2531:A:H5' | 28:DG:157:TYR:CE2 | 2.45 | 0.51 |
| 26:DE:77:ILE:O | 26:DE:77:ILE:CG1 | 2.59 | 0.51 |
| 30:DI:57:VAL:CG2 | 30:DI:69:PHE:HB2 | 2.40 | 0.51 |
| 31:DJ:104:ALA:O | 31:DJ:108:MET:HG3 | 2.10 | 0.51 |
| 39:DR:80:ARG:C | 39:DR:82:HIS:H | 2.14 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:DZ:13:ALA:HB2 | 47:DZ:24:LEU:CD1 | 2.41 | 0.51 |
| 1:AA:475:C:H2' | 1:AA:476:U:O4' | 2.10 | 0.51 |
| 5:AE:74:VAL:HG23 | 5:AE:76:LEU:CD1 | 2.41 | 0.51 |
| 21:AU:34:ARG:O | 21:AU:36:GLU:N | 2.42 | 0.51 |
| 22:BA:13:A:N3 | 22:BA:15:G:C6 | 2.79 | 0.51 |
| 22:BA:277:G:O2' | 22:BA:361:G:C6 | 2.57 | 0.51 |
| 22:BA:1386:C:H2' | 22:BA:1387:A:C8 | 2.45 | 0.51 |
| 22:BA:1791:A:O2' | 24:BC:206:GLY:HA2 | 2.11 | 0.51 |
| 24:BC:25:HIS:CE1 | 24:BC:26:LYS:O | 2.64 | 0.51 |
| 24:BC:125:LYS:HB2 | 24:BC:126:PRO:HD2 | 1.93 | 0.51 |
| 25:BD:4:LEU:HD21 | 25:BD:100:LEU:HB3 | 1.92 | 0.51 |
| 1:CA:298:A:H2' | 1:CA:299:G:O4' | 2.10 | 0.51 |
| 1:CA:1474:U:H2' | 1:CA:1475:G:H5'' | 1.93 | 0.51 |
| 4:CD:32:CYS:O | 4:CD:33:LYS:HB3 | 2.09 | 0.51 |
| 7:CG:4:ARG:HG3 | 7:CG:5:ARG:N | 2.26 | 0.51 |
| 20:CT:60:ARG:O | 20:CT:64:LYS:HB2 | 2.11 | 0.51 |
| 21:CU:12:PHE:N | 21:CU:12:PHE:CD1 | 2.79 | 0.51 |
| 22:DA:195:A:C4 | 22:DA:198:C:N4 | 2.78 | 0.51 |
| 22:DA:471:A:OP1 | 26:DE:79:ARG:NH1 | 2.44 | 0.51 |
| 22:DA:563:A:C6 | 22:DA:2018:G:C4 | 2.99 | 0.51 |
| 22:DA:915:C:C4 | 22:DA:916:G:C5 | 2.99 | 0.51 |
| 22:DA:1029:A:N1 | 22:DA:2465:C:O2' | 2.36 | 0.51 |
| 22:DA:1054:A:H2' | 22:DA:1055:G:C8 | 2.46 | 0.51 |
| 22:DA:1096:A:C5 | 22:DA:1097:U:C5 | 2.99 | 0.51 |
| 22:DA:1246:A:O2' | 26:DE:40:ARG:NH2 | 2.44 | 0.51 |
| 22:DA:1584:U:O2 | 22:DA:1584:U:H3' | 2.10 | 0.51 |
| 22:DA:1731:G:C6 | 22:DA:1733:G:C5 | 2.99 | 0.51 |
| 22:DA:1916:A:H2' | 22:DA:1917:U:O4' | 2.09 | 0.51 |
| 22:DA:2127:G:N3 | 22:DA:2162:G:C8 | 2.79 | 0.51 |
| 22:DA:2645:G:H3' | 22:DA:2646:C:C5' | 2.41 | 0.51 |
| 23:DB:62:C:H2' | 23:DB:63:C:C6 | 2.45 | 0.51 |
| 29:DH:5:LEU:HA | 29:DH:36:ALA:HA | 1.93 | 0.51 |
| 36:DO:49:VAL:HG21 | 36:DO:82:ALA:HA | 1.93 | 0.51 |
| 44:DW:45:PHE:HB3 | 44:DW:80:ILE:HD12 | 1.92 | 0.51 |
| 1:AA:109:A:C6 | 1:AA:326:G:C6 | 2.99 | 0.51 |
| 1:AA:704:A:C6 | 1:AA:705:G:C4 | 2.99 | 0.51 |
| 1:AA:901:A:N7 | 1:AA:902:G:H1' | 2.26 | 0.51 |
| 1:AA:1138:G:C2 | 1:AA:1140:C:C5 | 2.99 | 0.51 |
| 5:AE:97:GLN:HB3 | 5:AE:124:LEU:HD12 | 1.92 | 0.51 |
| 8:AH:47:GLU:N | 8:AH:64:LYS:HG3 | 2.26 | 0.51 |
| 22:BA:958:U:OP2 | 34:BM:14:LYS:NZ | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:962:G:N2 | 22:BA:2250:G:H1 | 2.08 | 0.51 |
| 22:BA:1485:U:H2' | 22:BA:1486:U:C6 | 2.45 | 0.51 |
| 22:BA:1917:U:O2 | 22:BA:1917:U:H2' | 2.09 | 0.51 |
| 22:BA:2514:U:H2' | 22:BA:2515:C:C6 | 2.46 | 0.51 |
| 22:BA:2579:C:H2' | 22:BA:2580:U:O4' | 2.11 | 0.51 |
| 29:BH:83:LYS:HA | 29:BH:148:ALA:HA | 1.93 | 0.51 |
| 33:BL:77:ILE:HG23 | 33:BL:100:ILE:HD11 | 1.93 | 0.51 |
| 49:B1:17:THR:HG21 | 49:B1:43:VAL:HG13 | 1.92 | 0.51 |
| 1:CA:97:G:C5 | 1:CA:98:A:H1' | 2.46 | 0.51 |
| 1:CA:355:C:H2' | 1:CA:356:A:O4' | 2.11 | 0.51 |
| 1:CA:1202:U:H2' | 1:CA:1203:C:O4' | 2.11 | 0.51 |
| 2:CB:53:ALA:O | 2:CB:57:LEU:HB2 | 2.11 | 0.51 |
| 3:CC:40:ARG:HG2 | 3:CC:55:ILE:HD11 | 1.93 | 0.51 |
| 8:CH:21:ASN:O | 8:CH:23:ALA:N | 2.44 | 0.51 |
| 9:CI:21:ILE:HG12 | 9:CI:62:ASP:O | 2.10 | 0.51 |
| 13:CM:14:HIS:HB2 | 13:CM:17:ILE:CD1 | 2.41 | 0.51 |
| 22:DA:321:U:OP2 | 26:DE:130:LYS:HA | 2.11 | 0.51 |
| 22:DA:912:C:N4 | 22:DA:913:U:O4 | 2.44 | 0.51 |
| 22:DA:971:G:H2' | 22:DA:972:A:O4' | 2.09 | 0.51 |
| 22:DA:1831:G:C6 | 22:DA:1832:C:C4 | 2.99 | 0.51 |
| 22:DA:2331:G:C5 | 22:DA:2332:C:C5 | 2.99 | 0.51 |
| 22:DA:2845:U:H5'' | 37:DP:52:ASN:O | 2.11 | 0.51 |
| 24:DC:92:ALA:HB3 | 24:DC:104:ILE:CD1 | 2.41 | 0.51 |
| 24:DC:141:VAL:HG13 | 24:DC:191:THR:O | 2.11 | 0.51 |
| 25:DD:52:THR:OG1 | 25:DD:53:GLY:N | 2.44 | 0.51 |
| 26:DE:149:ILE:HG23 | 26:DE:188:MET:HA | 1.92 | 0.51 |
| 33:DL:68:SER:O | 33:DL:69:ARG:CB | 2.57 | 0.51 |
| 35:DN:28:LEU:HG | 35:DN:28:LEU:O | 2.11 | 0.51 |
| 41:DT:69:ARG:NH1 | 58:DT:102:HOH:O | 2.43 | 0.51 |
| 1:AA:208:U:C6 | 1:AA:210:C:C4 | 2.99 | 0.51 |
| 1:AA:706:A:C5 | 1:AA:707:U:C5 | 2.98 | 0.51 |
| 1:AA:1037:C:H2' | 1:AA:1038:C:C6 | 2.46 | 0.51 |
| 1:AA:1356:G:N2 | 1:AA:1357:A:C2 | 2.79 | 0.51 |
| 2:AB:72:THR:O | 2:AB:73:LYS:CB | 2.59 | 0.51 |
| 5:AE:74:VAL:HG23 | 5:AE:76:LEU:HD12 | 1.93 | 0.51 |
| 9:AI:120:LYS:HG3 | 9:AI:123:ARG:CB | 2.41 | 0.51 |
| 14:AN:52:PRO:O | 14:AN:53:ARG:HB3 | 2.11 | 0.51 |
| 22:BA:869:G:H2' | 22:BA:870:U:O4' | 2.11 | 0.51 |
| 22:BA:1138:G:H5'' | 22:BA:1139:G:OP2 | 2.11 | 0.51 |
| 22:BA:1161:C:H1' | 39:BR:8:GLY:O | 2.11 | 0.51 |
| 22:BA:1458:U:H5' | 22:BA:1459:G:C2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1846:G:N2 | 22:BA:1895:C:C2 | 2.79 | 0.51 |
| 22:BA:2230:G:H1' | 45:BX:32:ASN:OD1 | 2.11 | 0.51 |
| 29:BH:117:LEU:CD2 | 29:BH:121:VAL:CA | 2.89 | 0.51 |
| 43:BV:8:VAL:HG23 | 43:BV:9:ARG:N | 2.25 | 0.51 |
| 1:CA:39:G:C6 | 1:CA:40:C:C4 | 2.99 | 0.51 |
| 1:CA:374:A:OP1 | 1:CA:452:A:N1 | 2.43 | 0.51 |
| 1:CA:608:A:H2' | 1:CA:609:A:O4' | 2.12 | 0.51 |
| 1:CA:1048:G:OP2 | 58:CA:1849:HOH:O | 2.20 | 0.51 |
| 2:CB:94:HIS:CD2 | 2:CB:146:ASN:HB2 | 2.45 | 0.51 |
| 2:CB:131:LYS:O | 2:CB:135:LEU:N | 2.44 | 0.51 |
| 8:CH:126:ILE:N | 8:CH:126:ILE:HD12 | 2.26 | 0.51 |
| 11:CK:43:GLY:HA3 | 11:CK:74:VAL:HG12 | 1.93 | 0.51 |
| 12:CL:90:LEU:CB | 12:CL:93:VAL:CG2 | 2.88 | 0.51 |
| 17:CQ:47:HIS:HB2 | 17:CQ:67:LEU:HD12 | 1.92 | 0.51 |
| 22:DA:85:G:OP2 | 42:DU:28:VAL:CG1 | 2.59 | 0.51 |
| 22:DA:228:C:N3 | 22:DA:418:C:O4' | 2.44 | 0.51 |
| 22:DA:344:A:C2 | 22:DA:345:A:N7 | 2.79 | 0.51 |
| 22:DA:669:G:N2 | 22:DA:670:A:C2 | 2.79 | 0.51 |
| 22:DA:1559:U:H4' | 22:DA:1560:G:OP2 | 2.10 | 0.51 |
| 22:DA:1596:A:N6 | 22:DA:1597:A:C6 | 2.79 | 0.51 |
| 22:DA:1651:G:N2 | 22:DA:2007:U:O2 | 2.45 | 0.51 |
| 22:DA:1674:G:N2 | 22:DA:1677:A:H61 | 2.08 | 0.51 |
| 22:DA:2127:G:N3 | 22:DA:2162:G:N7 | 2.59 | 0.51 |
| 24:DC:51:THR:CG2 | 24:DC:54:ILE:HD11 | 2.42 | 0.51 |
| 33:DL:93:ASN:O | 33:DL:95:LEU:N | 2.40 | 0.51 |
| 35:DN:29:VAL:HG13 | 35:DN:83:LEU:HD11 | 1.93 | 0.51 |
| 35:DN:54:LEU:HD21 | 35:DN:66:ALA:HB2 | 1.93 | 0.51 |
| 36:DO:36:TYR:N | 36:DO:36:TYR:CD1 | 2.78 | 0.51 |
| 46:DY:27:ASN:HA | 46:DY:30:MET:HB2 | 1.93 | 0.51 |
| 1:AA:1203:C:H4' | 14:AN:67:THR:HG22 | 1.93 | 0.50 |
| 1:AA:1319:A:C8 | 1:AA:1323:G:C5 | 2.99 | 0.50 |
| 1:AA:1366:C:O2' | 10:AJ:62:ARG:NH2 | 2.43 | 0.50 |
| 1:AA:1464:U:OP2 | 37:BP:109:ARG:NH1 | 2.45 | 0.50 |
| 3:AC:11:ARG:NH1 | 3:AC:182:ILE:HB | 2.26 | 0.50 |
| 4:AD:197:GLU:O | 4:AD:199:LEU:N | 2.43 | 0.50 |
| 6:AF:36:ILE:HG23 | 6:AF:36:ILE:O | 2.11 | 0.50 |
| 7:AG:49:THR:O | 7:AG:53:ARG:CB | 2.59 | 0.50 |
| 9:AI:58:VAL:O | 9:AI:59:GLU:CG | 2.59 | 0.50 |
| 10:AJ:65:TYR:HB3 | 14:AN:96:LEU:HD11 | 1.93 | 0.50 |
| 11:AK:31:ILE:HB | 11:AK:46:THR:HG22 | 1.93 | 0.50 |
| 14:AN:20:TYR:CE1 | 14:AN:52:PRO:HG2 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:AT:44:LYS:HG2 | 20:AT:87:ALA:CB | 2.41 | 0.50 |
| 22:BA:998:C:H2' | 22:BA:999:U:O5' | 2.11 | 0.50 |
| 22:BA:1542:U:H2' | 22:BA:1543:G:O4' | 2.11 | 0.50 |
| 22:BA:2846:G:H2' | 22:BA:2847:U:O4' | 2.11 | 0.50 |
| 29:BH:14:SER:OG | 29:BH:17:ASP:OD1 | 2.29 | 0.50 |
| 45:BX:68:LEU:HD13 | 45:BX:78:TYR:CE1 | 2.46 | 0.50 |
| 1:CA:409:U:H2' | 1:CA:410:G:O4' | 2.11 | 0.50 |
| 1:CA:939:G:C6 | 1:CA:940:C:N4 | 2.79 | 0.50 |
| 1:CA:1096:C:H2' | 1:CA:1097:C:C6 | 2.45 | 0.50 |
| 5:CE:10:GLU:OE1 | 5:CE:10:GLU:N | 2.44 | 0.50 |
| 5:CE:36:LEU:HD21 | 5:CE:137:VAL:HG11 | 1.93 | 0.50 |
| 7:CG:99:LEU:HB3 | 7:CG:103:TRP:CZ2 | 2.46 | 0.50 |
| 9:CI:54:LEU:O | 9:CI:55:VAL:HG22 | 2.11 | 0.50 |
| 12:CL:61:PHE:N | 12:CL:61:PHE:CD1 | 2.79 | 0.50 |
| 17:CQ:8:LEU:N | 17:CQ:8:LEU:HD12 | 2.25 | 0.50 |
| 19:CS:50:ALA:HB1 | 19:CS:57:HIS:HB3 | 1.94 | 0.50 |
| 22:DA:77:G:OP1 | 46:DY:52:ARG:HD3 | 2.11 | 0.50 |
| 22:DA:126:A:C2 | 50:D2:18:PHE:CE2 | 3.00 | 0.50 |
| 22:DA:748:G:C8 | 40:DS:89:ALA:HB1 | 2.47 | 0.50 |
| 22:DA:807:U:OP2 | 33:DL:41:ARG:NH1 | 2.44 | 0.50 |
| 22:DA:1231:U:H2' | 22:DA:1232:G:H8 | 1.76 | 0.50 |
| 22:DA:1301:A:N6 | 22:DA:1303:G:C2 | 2.79 | 0.50 |
| 22:DA:1519:G:C2 | 22:DA:1520:U:H1' | 2.47 | 0.50 |
| 22:DA:1567:G:C8 | 24:DC:83:TYR:CE1 | 2.99 | 0.50 |
| 22:DA:1627:G:N2 | 22:DA:1628:G:C5 | 2.79 | 0.50 |
| 22:DA:1805:A:C2 | 22:DA:1813:G:C2 | 2.99 | 0.50 |
| 22:DA:1946:U:H2' | 22:DA:1947:C:C6 | 2.45 | 0.50 |
| 22:DA:2209:G:C6 | 22:DA:2210:U:C4 | 2.99 | 0.50 |
| 22:DA:2718:G:C6 | 22:DA:2719:G:C4 | 2.99 | 0.50 |
| 22:DA:2883:A:OP2 | 48:D0:49:TYR:OH | 2.24 | 0.50 |
| 24:DC:33:LEU:O | 24:DC:64:ILE:HD12 | 2.11 | 0.50 |
| 26:DE:75:SER:O | 26:DE:78:TRP:HB2 | 2.11 | 0.50 |
| 33:DL:50:PHE:CE2 | 33:DL:52:GLY:O | 2.63 | 0.50 |
| 33:DL:77:ILE:O | 33:DL:110:VAL:O | 2.29 | 0.50 |
| 38:DQ:86:ALA:O | 38:DQ:87:SER:CB | 2.58 | 0.50 |
| 1:AA:148:G:H2' | 1:AA:149:A:O5' | 2.12 | 0.50 |
| 1:AA:251:G:C6 | 1:AA:266:G:O6 | 2.64 | 0.50 |
| 1:AA:524:G:C6 | 1:AA:525:C:N4 | 2.79 | 0.50 |
| 1:AA:1107:C:C4 | 1:AA:1108:G:C8 | 3.00 | 0.50 |
| 2:AB:68:LEU:HD22 | 2:AB:70:VAL:HG23 | 1.93 | 0.50 |
| 2:AB:106:THR:O | 2:AB:107:VAL:HG23 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:AI:22:LYS:O | 9:AI:62:ASP:HB2 | 2.10 | 0.50 |
| 11:AK:69:ARG:HD3 | 22:BA:2146:C:N3 | 2.26 | 0.50 |
| 11:AK:126:LYS:CA | 21:AU:34:ARG:HH21 | 2.24 | 0.50 |
| 22:BA:64:A:H2' | 22:BA:65:U:C6 | 2.46 | 0.50 |
| 22:BA:136:G:C2 | 22:BA:144:A:C6 | 2.98 | 0.50 |
| 22:BA:753:A:H2' | 22:BA:754:U:H6 | 1.77 | 0.50 |
| 22:BA:1384:A:H5'' | 22:BA:1385:A:OP2 | 2.11 | 0.50 |
| 22:BA:1483:G:C6 | 22:BA:1484:U:C4 | 2.99 | 0.50 |
| 22:BA:1494:A:O2' | 22:BA:1495:A:O5' | 2.30 | 0.50 |
| 22:BA:2665:A:C2 | 22:BA:2666:C:N1 | 2.79 | 0.50 |
| 31:BJ:31:GLU:OE1 | 31:BJ:34:ARG:HD3 | 2.11 | 0.50 |
| 33:BL:63:LYS:HA | 51:B3:13:ARG:HG3 | 1.93 | 0.50 |
| 52:B4:10:LEU:HD12 | 52:B4:33:HIS:CD2 | 2.47 | 0.50 |
| 1:CA:170:U:O2' | 1:CA:171:A:H5' | 2.11 | 0.50 |
| 1:CA:562:U:H2' | 12:CL:14:ARG:HD3 | 1.91 | 0.50 |
| 1:CA:575:G:C6 | 1:CA:821:G:N7 | 2.80 | 0.50 |
| 1:CA:991:U:N3 | 1:CA:1212:U:O4' | 2.45 | 0.50 |
| 1:CA:1296:C:H5'' | 1:CA:1297:G:OP2 | 2.11 | 0.50 |
| 1:CA:1343:G:O2' | 9:CI:123:ARG:HD2 | 2.11 | 0.50 |
| 1:CA:1461:G:H2' | 1:CA:1462:C:O4' | 2.10 | 0.50 |
| 9:CI:30:ILE:HA | 9:CI:65:ILE:O | 2.10 | 0.50 |
| 17:CQ:81:LYS:CD | 17:CQ:81:LYS:N | 2.74 | 0.50 |
| 20:CT:67:ILE:O | 20:CT:68:HIS:C | 2.49 | 0.50 |
| 22:DA:58:G:C4 | 22:DA:70:G:N2 | 2.79 | 0.50 |
| 22:DA:122:G:H2' | 22:DA:123:G:O4' | 2.11 | 0.50 |
| 22:DA:289:G:N2 | 22:DA:352:A:C2 | 2.80 | 0.50 |
| 22:DA:295:G:N2 | 22:DA:296:U:C6 | 2.80 | 0.50 |
| 22:DA:570:G:C4 | 22:DA:2030:A:N7 | 2.80 | 0.50 |
| 22:DA:577:G:O2' | 22:DA:1254:A:OP1 | 2.30 | 0.50 |
| 22:DA:1500:G:C6 | 22:DA:1501:G:N7 | 2.79 | 0.50 |
| 22:DA:1640:A:H2' | 22:DA:1641:A:C8 | 2.46 | 0.50 |
| 22:DA:1791:A:H2' | 22:DA:1792:G:H5' | 1.93 | 0.50 |
| 24:DC:67:PHE:CE2 | 24:DC:156:ARG:NH2 | 2.79 | 0.50 |
| 25:DD:32:ASN:N | 25:DD:96:ILE:O | 2.44 | 0.50 |
| 33:DL:117:THR:HG22 | 33:DL:118:THR:N | 2.25 | 0.50 |
| 41:DT:12:ARG:O | 41:DT:13:ALA:HB2 | 2.11 | 0.50 |
| 1:AA:545:C:H5' | 4:AD:69:GLU:CG | 2.41 | 0.50 |
| 1:AA:1182:G:H4' | 1:AA:1183:U:H5' | 1.93 | 0.50 |
| 2:AB:51:ASN:O | 2:AB:52:GLU:HB2 | 2.12 | 0.50 |
| 2:AB:64:LYS:HE2 | 2:AB:64:LYS:HA | 1.92 | 0.50 |
| 3:AC:79:LYS:O | 3:AC:82:GLU:HG3 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:152:GLN:O | 4:AD:153:SER:C | 2.49 | 0.50 |
| 6:AF:4:TYR:CD2 | 6:AF:71:ILE:HD13 | 2.46 | 0.50 |
| 10:AJ:67:ILE:O | 10:AJ:67:ILE:HG22 | 2.11 | 0.50 |
| 20:AT:44:LYS:CB | 20:AT:87:ALA:HB1 | 2.41 | 0.50 |
| 22:BA:686:U:O4 | 50:B2:12:ARG:HB2 | 2.11 | 0.50 |
| 22:BA:790:U:O2' | 22:BA:791:C:P | 2.69 | 0.50 |
| 22:BA:945:A:OP2 | 22:BA:945:A:H4' | 2.12 | 0.50 |
| 22:BA:1070:A:H2' | 22:BA:1097:U:OP1 | 2.11 | 0.50 |
| 25:BD:129:THR:HG23 | 25:BD:130:GLN:O | 2.11 | 0.50 |
| 31:BJ:81:ILE:CG2 | 31:BJ:82:GLY:N | 2.72 | 0.50 |
| 32:BK:4:GLU:O | 32:BK:5:GLN:HB2 | 2.11 | 0.50 |
| 40:BS:17:VAL:HG12 | 40:BS:76:VAL:HG21 | 1.93 | 0.50 |
| 42:BU:38:GLY:N | 42:BU:62:GLU:OE2 | 2.35 | 0.50 |
| 1:CA:79:G:N2 | 1:CA:91:U:O2 | 2.45 | 0.50 |
| 1:CA:206:C:C2' | 1:CA:207:C:H5' | 2.40 | 0.50 |
| 1:CA:373:A:C2 | 1:CA:374:A:C8 | 2.98 | 0.50 |
| 1:CA:436:C:C2 | 1:CA:437:U:C5 | 2.99 | 0.50 |
| 1:CA:573:A:C2 | 1:CA:574:A:C2 | 2.99 | 0.50 |
| 1:CA:673:A:H2' | 1:CA:674:G:C8 | 2.46 | 0.50 |
| 1:CA:1309:G:C6 | 1:CA:1329:A:C2 | 2.99 | 0.50 |
| 1:CA:1321:U:C4 | 1:CA:1322:C:C5 | 2.99 | 0.50 |
| 14:CN:61:ARG:O | 14:CN:62:ASN:CB | 2.59 | 0.50 |
| 21:CU:37:PHE:CD1 | 21:CU:40:LYS:HE3 | 2.46 | 0.50 |
| 22:DA:753:A:H2' | 22:DA:754:U:C6 | 2.46 | 0.50 |
| 22:DA:1791:A:O3' | 24:DC:205:LEU:HB2 | 2.11 | 0.50 |
| 22:DA:1992:G:N2 | 22:DA:1996:C:O2' | 2.45 | 0.50 |
| 22:DA:2163:A:H2' | 22:DA:2164:C:H4' | 1.93 | 0.50 |
| 22:DA:2344:U:H4' | 22:DA:2345:G:OP1 | 2.11 | 0.50 |
| 23:DB:39:A:H2' | 23:DB:40:U:C6 | 2.46 | 0.50 |
| 26:DE:108:ILE:HD13 | 26:DE:181:ILE:HG12 | 1.93 | 0.50 |
| 29:DH:44:ILE:O | 29:DH:48:GLU:HB2 | 2.11 | 0.50 |
| 30:DI:10:LYS:HB2 | 30:DI:56:PRO:HB3 | 1.93 | 0.50 |
| 30:DI:22:PRO:HB2 | 30:DI:23:PRO:HD3 | 1.94 | 0.50 |
| 30:DI:58:VAL:CG1 | 30:DI:59:ILE:H | 2.24 | 0.50 |
| 48:D0:55:ILE:O | 48:D0:56:ALA:HB3 | 2.11 | 0.50 |
| 1:AA:275:G:O3' | 17:AQ:17:MET:HE2 | 2.11 | 0.50 |
| 1:AA:728:A:C6 | 1:AA:729:A:C6 | 3.00 | 0.50 |
| 1:AA:1201:A:H1' | 1:AA:1202:U:OP2 | 2.11 | 0.50 |
| 4:AD:78:GLU:HG3 | 4:AD:93:LEU:HD21 | 1.93 | 0.50 |
| 8:AH:83:LEU:C | 8:AH:83:LEU:HD22 | 2.32 | 0.50 |
| 11:AK:34:ILE:HG13 | 11:AK:70:CYS:SG | 2.51 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:417:C:H2' | 22:BA:418:C:C6 | 2.46 | 0.50 |
| 22:BA:454:A:H4' | 22:BA:455:C:OP2 | 2.11 | 0.50 |
| 22:BA:1670:C:C5 | 22:BA:1671:U:C4 | 2.99 | 0.50 |
| 22:BA:1916:A:N9 | 22:BA:1917:U:H1' | 2.26 | 0.50 |
| 22:BA:2526:G:C2' | 52:B4:1:MET:H1 | 2.24 | 0.50 |
| 23:BB:110:C:C4 | 23:BB:111:U:C5 | 3.00 | 0.50 |
| 26:BE:149:ILE:HD12 | 26:BE:150:THR:N | 2.26 | 0.50 |
| 29:BH:66:ASN:OD1 | 29:BH:138:VAL:HG21 | 2.11 | 0.50 |
| 35:BN:28:LEU:O | 35:BN:32:GLU:N | 2.44 | 0.50 |
| 37:BP:53:ARG:HH11 | 37:BP:53:ARG:HG2 | 1.77 | 0.50 |
| 37:BP:53:ARG:HH11 | 37:BP:53:ARG:HG3 | 1.76 | 0.50 |
| 43:BV:1:MET:SD | 43:BV:1:MET:C | 2.90 | 0.50 |
| 48:B0:55:ILE:HG22 | 48:B0:57:LYS:H | 1.76 | 0.50 |
| 1:CA:642:A:H2' | 1:CA:643:C:C6 | 2.46 | 0.50 |
| 1:CA:728:A:C8 | 15:CO:54:ARG:CZ | 2.94 | 0.50 |
| 1:CA:1359:C:OP2 | 14:CN:75:ARG:NH1 | 2.45 | 0.50 |
| 4:CD:34:ILE:O | 4:CD:34:ILE:HG23 | 2.10 | 0.50 |
| 5:CE:20:ARG:NH2 | 5:CE:31:PHE:CZ | 2.79 | 0.50 |
| 14:CN:80:SER:O | 14:CN:81:ARG:C | 2.50 | 0.50 |
| 20:CT:48:GLN:OE1 | 20:CT:52:ASN:ND2 | 2.42 | 0.50 |
| 22:DA:12:U:O2 | 22:DA:12:U:C2' | 2.59 | 0.50 |
| 22:DA:219:A:N6 | 22:DA:220:G:C6 | 2.80 | 0.50 |
| 22:DA:508:A:H3' | 22:DA:509:C:H5' | 1.93 | 0.50 |
| 22:DA:694:U:C3' | 22:DA:695:G:H5'' | 2.41 | 0.50 |
| 22:DA:747:U:O4' | 40:DS:92:ARG:NH1 | 2.44 | 0.50 |
| 22:DA:1317:G:H2' | 22:DA:1318:U:O4' | 2.11 | 0.50 |
| 22:DA:1343:G:C4 | 22:DA:1597:A:C6 | 3.00 | 0.50 |
| 22:DA:1544:A:N6 | 22:DA:1545:A:N1 | 2.58 | 0.50 |
| 22:DA:2060:A:O4' | 22:DA:2502:G:H1' | 2.11 | 0.50 |
| 22:DA:2109:U:H4' | 22:DA:2110:G:OP1 | 2.10 | 0.50 |
| 22:DA:2297:A:N1 | 22:DA:2321:U:C5 | 2.80 | 0.50 |
| 24:DC:267:ILE:O | 24:DC:267:ILE:HG22 | 2.12 | 0.50 |
| 40:DS:63:GLY:O | 40:DS:64:ALA:HB3 | 2.11 | 0.50 |
| 44:DW:45:PHE:CD2 | 44:DW:80:ILE:HD11 | 2.46 | 0.50 |
| 1:AA:1143:G:C4 | 1:AA:1144:G:C8 | 2.99 | 0.50 |
| 2:AB:21:ARG:HA | 2:AB:21:ARG:NH1 | 2.26 | 0.50 |
| 3:AC:64:ILE:CG2 | 3:AC:99:ALA:HB2 | 2.41 | 0.50 |
| 5:AE:60:ILE:HD13 | 5:AE:61:GLN:N | 2.27 | 0.50 |
| 21:AU:11:PRO:C | 21:AU:12:PHE:CD2 | 2.84 | 0.50 |
| 22:BA:624:C:O2' | 22:BA:657:U:H5'' | 2.11 | 0.50 |
| 22:BA:769:U:C2 | 22:BA:770:G:C8 | 2.99 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:796:C:H2' | 22:BA:797:G:C8 | 2.46 | 0.50 |
| 22:BA:1668:A:H4' | 22:BA:1669:A:O5' | 2.12 | 0.50 |
| 22:BA:2297:A:N1 | 22:BA:2321:U:C5 | 2.80 | 0.50 |
| 22:BA:2458:G:C2 | 22:BA:2490:G:N2 | 2.79 | 0.50 |
| 22:BA:2469:A:O2' | 34:BM:55:ARG:NH1 | 2.45 | 0.50 |
| 22:BA:2609:U:H2' | 54:B6:7:004:CB | 2.42 | 0.50 |
| 27:BF:92:ARG:HA | 27:BF:96:MET:HE2 | 1.93 | 0.50 |
| 30:BI:122:ILE:HG23 | 30:BI:125:MET:SD | 2.52 | 0.50 |
| 45:BX:2:SER:O | 45:BX:4:VAL:N | 2.44 | 0.50 |
| 45:BX:43:GLU:OE2 | 45:BX:45:ARG:NH2 | 2.44 | 0.50 |
| 1:CA:374:A:C2 | 1:CA:375:U:C6 | 2.99 | 0.50 |
| 1:CA:484:G:C5 | 1:CA:486:U:H1' | 2.46 | 0.50 |
| 1:CA:695:A:H2' | 1:CA:696:A:C8 | 2.47 | 0.50 |
| 1:CA:756:C:O2' | 1:CA:757:U:H5' | 2.11 | 0.50 |
| 1:CA:951:G:C6 | 1:CA:952:U:C4 | 3.00 | 0.50 |
| 1:CA:1244:G:H2' | 1:CA:1245:C:C6 | 2.47 | 0.50 |
| 1:CA:1530:G:H2' | 1:CA:1531:A:C8 | 2.47 | 0.50 |
| 2:CB:207:ILE:HD13 | 2:CB:207:ILE:N | 2.26 | 0.50 |
| 4:CD:105:MET:SD | 4:CD:143:VAL:CG1 | 3.00 | 0.50 |
| 4:CD:198:HIS:CE1 | 4:CD:199:LEU:CD2 | 2.95 | 0.50 |
| 5:CE:16:ILE:HD11 | 5:CE:38:VAL:HG23 | 1.92 | 0.50 |
| 5:CE:111:MET:HG3 | 5:CE:140:THR:HG21 | 1.93 | 0.50 |
| 12:CL:65:SER:OG | 12:CL:97:THR:HG23 | 2.12 | 0.50 |
| 12:CL:68:GLY:O | 12:CL:99:ARG:NH1 | 2.45 | 0.50 |
| 17:CQ:19:LYS:CD | 17:CQ:49:GLU:HA | 2.41 | 0.50 |
| 20:CT:80:THR:O | 20:CT:83:ILE:HG13 | 2.11 | 0.50 |
| 22:DA:20:C:H2' | 22:DA:21:A:C8 | 2.47 | 0.50 |
| 22:DA:21:A:N1 | 22:DA:520:G:C6 | 2.80 | 0.50 |
| 22:DA:532:A:H4' | 22:DA:533:G:C8 | 2.46 | 0.50 |
| 22:DA:668:A:C2 | 22:DA:670:A:C6 | 3.00 | 0.50 |
| 22:DA:769:U:C4 | 22:DA:770:G:N7 | 2.79 | 0.50 |
| 22:DA:1364:G:C6 | 22:DA:1368:G:C6 | 2.99 | 0.50 |
| 22:DA:1566:A:N3 | 24:DC:213:TRP:CG | 2.80 | 0.50 |
| 24:DC:57:GLY:O | 24:DC:58:HIS:O | 2.29 | 0.50 |
| 24:DC:68:LYS:HG2 | 24:DC:151:GLY:HA2 | 1.94 | 0.50 |
| 25:DD:101:PHE:HA | 25:DD:104:VAL:HG13 | 1.94 | 0.50 |
| 25:DD:125:TRP:O | 25:DD:126:ASN:HB2 | 2.11 | 0.50 |
| 27:DF:108:VAL:HG11 | 27:DF:176:PRO:CG | 2.42 | 0.50 |
| 47:DZ:40:ASP:OD2 | 47:DZ:45:ARG:NH1 | 2.44 | 0.50 |
| 1:AA:1151:A:C4 | 1:AA:1152:A:N7 | 2.80 | 0.50 |
| 7:AG:137:LYS:O | 7:AG:141:VAL:HG23 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:BA:271:G:C4' | 22:BA:272:A:OP1 | 2.59 | 0.50 |
| 22:BA:641:U:C5 | 22:BA:642:U:O4 | 2.64 | 0.50 |
| 22:BA:947:A:O2' | 22:BA:984:A:H2 | 1.94 | 0.50 |
| 22:BA:1014:A:C5 | 22:BA:1015:U:C5 | 2.99 | 0.50 |
| 22:BA:1071:G:O2' | 22:BA:1072:C:O4' | 2.30 | 0.50 |
| 22:BA:1402:U:H2' | 22:BA:1403:A:O5' | 2.12 | 0.50 |
| 22:BA:1721:G:O2' | 22:BA:1739:A:N6 | 2.44 | 0.50 |
| 22:BA:1731:G:C5 | 22:BA:1733:G:N7 | 2.80 | 0.50 |
| 22:BA:1735:A:N3 | 22:BA:1735:A:H2' | 2.26 | 0.50 |
| 22:BA:1866:A:C2 | 22:BA:1876:A:C5 | 3.00 | 0.50 |
| 22:BA:2217:G:O2' | 22:BA:2218:G:H5' | 2.11 | 0.50 |
| 22:BA:2506:U:C2 | 56:BA:3001:DOL:H472 | 2.46 | 0.50 |
| 29:BH:80:ILE:O | 29:BH:147:VAL:N | 2.44 | 0.50 |
| 39:BR:67:GLY:C | 39:BR:93:PHE:CE2 | 2.84 | 0.50 |
| 41:BT:67:VAL:HG22 | 41:BT:76:ARG:HG2 | 1.92 | 0.50 |
| 51:B3:42:ARG:HG3 | 51:B3:45:ARG:NH2 | 2.27 | 0.50 |
| 1:CA:135:C:O2 | 16:CP:1:MET:HB2 | 2.12 | 0.50 |
| 1:CA:425:G:H2' | 1:CA:426:U:O4' | 2.11 | 0.50 |
| 1:CA:427:U:OP1 | 4:CD:13:ARG:NH2 | 2.45 | 0.50 |
| 1:CA:811:C:C5 | 1:CA:812:G:C6 | 3.00 | 0.50 |
| 1:CA:1345:U:N3 | 1:CA:1377:A:C2 | 2.80 | 0.50 |
| 4:CD:22:LYS:O | 4:CD:23:SER:C | 2.49 | 0.50 |
| 4:CD:116:GLN:HG3 | 4:CD:120:HIS:CE1 | 2.47 | 0.50 |
| 9:CI:57:MET:HB3 | 9:CI:61:LEU:CD2 | 2.42 | 0.50 |
| 13:CM:4:ILE:HA | 13:CM:57:ARG:CZ | 2.41 | 0.50 |
| 22:DA:532:A:N1 | 22:DA:2020:A:H1' | 2.26 | 0.50 |
| 22:DA:777:G:N3 | 22:DA:778:G:C8 | 2.80 | 0.50 |
| 22:DA:825:A:H4' | 22:DA:2428:G:C5 | 2.47 | 0.50 |
| 22:DA:1009:A:O2' | 22:DA:1153:C:H4' | 2.12 | 0.50 |
| 22:DA:1360:G:C6 | 22:DA:1372:U:C2 | 2.99 | 0.50 |
| 22:DA:1390:U:C2' | 22:DA:1391:U:H5' | 2.41 | 0.50 |
| 22:DA:1754:A:C6 | 22:DA:1755:A:C6 | 2.99 | 0.50 |
| 22:DA:2454:G:H1' | 58:DA:3531:HOH:O | 2.12 | 0.50 |
| 22:DA:2707:U:H2' | 22:DA:2708:G:C8 | 2.46 | 0.50 |
| 28:DG:87:LEU:HD12 | 28:DG:87:LEU:N | 2.26 | 0.50 |
| 29:DH:5:LEU:HD11 | 29:DH:13:GLY:HA2 | 1.93 | 0.50 |
| 35:DN:36:THR:HG23 | 35:DN:41:ALA:HB2 | 1.94 | 0.50 |
| 41:DT:10:VAL:HG12 | 41:DT:11:LEU:N | 2.26 | 0.50 |
| 1:AA:224:U:H2' | 1:AA:225:C:C6 | 2.47 | 0.50 |
| 1:AA:453:G:H2' | 1:AA:454:G:C8 | 2.47 | 0.50 |
| 1:AA:685:G:N1 | 1:AA:686:U:O4 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1520:C:C2 | 1:AA:1521:C:C5 | 3.00 | 0.50 |
| 2:AB:42:ASN:O | 2:AB:44:GLU:N | 2.45 | 0.50 |
| 2:AB:140:GLU:O | 2:AB:144:LEU:HG | 2.12 | 0.50 |
| 4:AD:65:TYR:CG | 4:AD:94:LEU:HD22 | 2.47 | 0.50 |
| 4:AD:170:TRP:CD2 | 4:AD:186:PRO:HG3 | 2.47 | 0.50 |
| 5:AE:25:VAL:O | 5:AE:26:LYS:C | 2.50 | 0.50 |
| 11:AK:126:LYS:O | 21:AU:34:ARG:NE | 2.45 | 0.50 |
| 12:AL:44:LYS:HB3 | 12:AL:45:PRO:CD | 2.41 | 0.50 |
| 20:AT:54:MET:HE1 | 20:AT:58:VAL:HG21 | 1.94 | 0.50 |
| 22:BA:102:U:C4 | 46:BY:2:LYS:HD2 | 2.47 | 0.50 |
| 22:BA:125:A:OP2 | 50:B2:19:ARG:NH2 | 2.41 | 0.50 |
| 22:BA:734:A:C4 | 22:BA:735:A:C8 | 3.00 | 0.50 |
| 22:BA:1168:G:H2' | 22:BA:1169:A:O4' | 2.12 | 0.50 |
| 22:BA:1586:A:N7 | 22:BA:1587:G:C8 | 2.80 | 0.50 |
| 22:BA:1958:C:C2' | 22:BA:1959:G:H5' | 2.41 | 0.50 |
| 22:BA:2376:A:N3 | 36:BO:111:ARG:NH1 | 2.60 | 0.50 |
| 47:BZ:24:LEU:HD11 | 47:BZ:54:MET:HE1 | 1.94 | 0.50 |
| 1:CA:453:G:H2' | 1:CA:454:G:C8 | 2.47 | 0.50 |
| 1:CA:782:A:C8 | 1:CA:783:C:C5 | 2.99 | 0.50 |
| 1:CA:1034:G:H5' | 1:CA:1035:A:OP2 | 2.11 | 0.50 |
| 1:CA:1228:C:H5' | 13:CM:113:ARG:HB2 | 1.94 | 0.50 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:C6 | 2.46 | 0.50 |
| 2:CB:120:GLN:HG2 | 2:CB:125:THR:O | 2.12 | 0.50 |
| 5:CE:35:ALA:O | 5:CE:50:TYR:O | 2.29 | 0.50 |
| 5:CE:153:VAL:HG23 | 5:CE:157:ARG:HB2 | 1.92 | 0.50 |
| 11:CK:52:PHE:CE2 | 11:CK:62:ALA:HB1 | 2.47 | 0.50 |
| 14:CN:80:SER:O | 14:CN:83:LYS:N | 2.44 | 0.50 |
| 16:CP:14:ARG:N | 16:CP:15:PRO:HD2 | 2.25 | 0.50 |
| 22:DA:64:A:H2' | 22:DA:65:U:O4' | 2.12 | 0.50 |
| 22:DA:392:U:H2' | 22:DA:393:C:C6 | 2.47 | 0.50 |
| 22:DA:586:A:H1' | 22:DA:672:C:H1' | 1.93 | 0.50 |
| 22:DA:1351:C:C2 | 22:DA:1381:G:C2 | 3.00 | 0.50 |
| 22:DA:1930:G:O2' | 22:DA:1931:U:P | 2.69 | 0.50 |
| 22:DA:2013:A:N6 | 22:DA:2014:A:C6 | 2.80 | 0.50 |
| 22:DA:2250:G:C2 | 34:DM:82:MET:HB2 | 2.47 | 0.50 |
| 22:DA:2308:G:C5' | 22:DA:2309:A:OP2 | 2.60 | 0.50 |
| 22:DA:2379:G:H4' | 36:DO:21:LEU:HD11 | 1.94 | 0.50 |
| 22:DA:2461:A:C2 | 22:DA:2490:G:N2 | 2.80 | 0.50 |
| 22:DA:2546:U:O4' | 22:DA:2565:A:C2 | 2.65 | 0.50 |
| 22:DA:2852:G:H2' | 22:DA:2853:C:O4' | 2.12 | 0.50 |
| 28:DG:19:ILE:O | 28:DG:21:GLY:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:DO:33:ARG:O | 36:DO:34:HIS:CG | 2.64 | 0.50 |
| 42:DU:44:LYS:O | 42:DU:58:ILE:HA | 2.12 | 0.50 |
| 1:AA:202:G:O2' | 1:AA:468:A:H2' | 2.11 | 0.50 |
| 1:AA:520:A:N1 | 1:AA:536:C:H1' | 2.27 | 0.50 |
| 1:AA:568:G:C4 | 1:AA:569:C:C5 | 2.99 | 0.50 |
| 1:AA:872:A:C4 | 1:AA:874:G:C8 | 3.00 | 0.50 |
| 1:AA:876:C:OP1 | 8:AH:76:GLN:NE2 | 2.44 | 0.50 |
| 1:AA:927:G:N1 | 1:AA:1391:U:O2 | 2.45 | 0.50 |
| 1:AA:1010:U:H2' | 1:AA:1011:C:C6 | 2.46 | 0.50 |
| 1:AA:1029:U:O2' | 1:AA:1032:G:O6 | 2.30 | 0.50 |
| 5:AE:46:VAL:HG21 | 5:AE:118:ALA:CB | 2.41 | 0.50 |
| 6:AF:35:LYS:HD3 | 6:AF:35:LYS:N | 2.26 | 0.50 |
| 9:AI:113:ARG:NH2 | 14:AN:101:TRP:CZ2 | 2.79 | 0.50 |
| 13:AM:33:ILE:HG23 | 13:AM:59:GLU:HB3 | 1.94 | 0.50 |
| 16:AP:70:ARG:HD2 | 16:AP:70:ARG:O | 2.12 | 0.50 |
| 22:BA:15:G:C6 | 22:BA:16:C:C4 | 3.00 | 0.50 |
| 22:BA:226:A:C6 | 22:BA:227:A:C6 | 3.00 | 0.50 |
| 22:BA:362:A:C8 | 22:BA:362:A:OP2 | 2.65 | 0.50 |
| 22:BA:510:C:OP1 | 22:BA:512:G:O6 | 2.30 | 0.50 |
| 22:BA:693:A:O2' | 22:BA:694:U:H5' | 2.11 | 0.50 |
| 22:BA:1153:C:OP1 | 38:BQ:92:ARG:NH1 | 2.45 | 0.50 |
| 22:BA:1452:G:H2' | 22:BA:1457:U:O4 | 2.11 | 0.50 |
| 24:BC:141:VAL:HG12 | 24:BC:142:HIS:H | 1.76 | 0.50 |
| 25:BD:99:GLU:HG2 | 25:BD:182:ALA:HB2 | 1.94 | 0.50 |
| 37:BP:22:PRO:HD3 | 37:BP:50:ILE:HD12 | 1.94 | 0.50 |
| 1:CA:687:A:O2' | 1:CA:701:U:O4 | 2.11 | 0.50 |
| 1:CA:756:C:H2' | 1:CA:757:U:H5' | 1.94 | 0.50 |
| 2:CB:167:ASP:HA | 2:CB:170:HIS:HB3 | 1.94 | 0.50 |
| 4:CD:58:LYS:NZ | 4:CD:59:GLN:OE1 | 2.41 | 0.50 |
| 7:CG:148:ASN:O | 7:CG:151:PHE:N | 2.43 | 0.50 |
| 22:DA:477:A:C2' | 22:DA:478:A:O5' | 2.59 | 0.50 |
| 22:DA:526:A:C6 | 22:DA:2626:C:H4' | 2.46 | 0.50 |
| 22:DA:695:G:C5 | 22:DA:768:G:C6 | 2.99 | 0.50 |
| 22:DA:747:U:C5 | 22:DA:2613:U:C5 | 2.99 | 0.50 |
| 22:DA:1310:G:H1' | 22:DA:1611:C:H5'' | 1.93 | 0.50 |
| 22:DA:1383:A:C2 | 22:DA:1384:A:C4 | 2.99 | 0.50 |
| 22:DA:1476:U:H1' | 22:DA:1732:C:C2 | 2.47 | 0.50 |
| 22:DA:1654:A:OP2 | 35:DN:1:MET:N | 2.43 | 0.50 |
| 22:DA:2199:A:N7 | 22:DA:2225:A:C6 | 2.80 | 0.50 |
| 22:DA:2308:G:O6 | 22:DA:2311:A:N7 | 2.45 | 0.50 |
| 22:DA:2544:G:H5' | 22:DA:2645:G:C2 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2824:C:N4 | 22:DA:2825:G:C5 | 2.80 | 0.50 |
| 23:DB:39:A:N6 | 23:DB:44:G:C6 | 2.79 | 0.50 |
| 24:DC:171:TYR:CD2 | 24:DC:185:GLU:HA | 2.47 | 0.50 |
| 27:DF:108:VAL:N | 27:DF:109:PRO:CD | 2.75 | 0.50 |
| 45:DX:51:VAL:HG23 | 45:DX:52:SER:N | 2.27 | 0.50 |
| 1:AA:575:G:H4' | 1:AA:576:C:OP1 | 2.12 | 0.50 |
| 1:AA:601:G:C6 | 1:AA:602:A:C6 | 3.00 | 0.50 |
| 1:AA:614:C:H2' | 1:AA:615:G:O5' | 2.11 | 0.50 |
| 1:AA:803:G:C6 | 1:AA:804:U:N3 | 2.80 | 0.50 |
| 1:AA:1179:A:H2' | 1:AA:1180:A:O4' | 2.12 | 0.50 |
| 1:AA:1287:A:C6 | 1:AA:1288:A:C6 | 2.99 | 0.50 |
| 3:AC:85:GLU:O | 3:AC:87:LEU:N | 2.45 | 0.50 |
| 11:AK:55:SER:O | 11:AK:57:LYS:N | 2.44 | 0.50 |
| 22:BA:1068:G:H2' | 22:BA:1069:A:H5' | 1.94 | 0.50 |
| 22:BA:1695:G:C8 | 24:BC:8:PRO:HG2 | 2.46 | 0.50 |
| 22:BA:1870:C:H4' | 22:BA:1871:A:OP2 | 2.12 | 0.50 |
| 22:BA:2547:A:C2 | 22:BA:2562:U:C2 | 3.00 | 0.50 |
| 22:BA:2714:G:C2' | 22:BA:2715:C:H5' | 2.42 | 0.50 |
| 26:BE:15:SER:N | 26:BE:197:GLU:OE2 | 2.45 | 0.50 |
| 26:BE:29:HIS:CE1 | 26:BE:33:VAL:HG21 | 2.46 | 0.50 |
| 26:BE:48:THR:C | 26:BE:50:ALA:N | 2.63 | 0.50 |
| 32:BK:58:LEU:HD23 | 32:BK:59:LYS:O | 2.12 | 0.50 |
| 35:BN:60:VAL:O | 35:BN:61:ALA:C | 2.50 | 0.50 |
| 46:BY:20:ASN:O | 46:BY:24:GLU:HB2 | 2.11 | 0.50 |
| 1:CA:4:U:O2 | 1:CA:4:U:H2' | 2.11 | 0.50 |
| 1:CA:174:A:C4 | 1:CA:175:C:C6 | 2.99 | 0.50 |
| 1:CA:263:A:P | 20:CT:74:ARG:NH1 | 2.85 | 0.50 |
| 1:CA:717:U:O2' | 1:CA:734:G:O4' | 2.24 | 0.50 |
| 1:CA:756:C:C2' | 1:CA:757:U:H5' | 2.42 | 0.50 |
| 1:CA:840:C:C4 | 1:CA:842:U:H4' | 2.47 | 0.50 |
| 1:CA:1002:G:C6 | 1:CA:1039:G:C2 | 2.99 | 0.50 |
| 2:CB:68:LEU:HD22 | 2:CB:70:VAL:HG23 | 1.93 | 0.50 |
| 2:CB:90:PHE:CZ | 2:CB:154:MET:HA | 2.47 | 0.50 |
| 8:CH:30:SER:O | 8:CH:34:VAL:HG23 | 2.12 | 0.50 |
| 9:CI:116:VAL:HG21 | 10:CJ:62:ARG:HD3 | 1.93 | 0.50 |
| 11:CK:33:THR:HG22 | 11:CK:33:THR:O | 2.11 | 0.50 |
| 11:CK:107:ILE:C | 11:CK:107:ILE:HD13 | 2.32 | 0.50 |
| 19:CS:73:GLU:HB2 | 19:CS:74:PHE:CE1 | 2.47 | 0.50 |
| 21:CU:28:VAL:O | 21:CU:32:VAL:HG23 | 2.11 | 0.50 |
| 22:DA:301:G:C2 | 22:DA:302:C:C2 | 3.00 | 0.50 |
| 22:DA:397:U:OP1 | 45:DX:31:PRO:HA | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:1243:C:H2' | 22:DA:1244:A:O4' | 2.12 | 0.50 |
| 22:DA:1301:A:H2' | 22:DA:1301:A:N3 | 2.27 | 0.50 |
| 22:DA:1454:C:H5' | 35:DN:63:ARG:HD3 | 1.93 | 0.50 |
| 22:DA:1734:G:H2' | 22:DA:1735:A:C8 | 2.47 | 0.50 |
| 22:DA:1855:U:C5 | 22:DA:1856:U:C4 | 3.00 | 0.50 |
| 22:DA:1876:A:C8 | 22:DA:1877:A:N7 | 2.80 | 0.50 |
| 22:DA:2024:G:C4 | 22:DA:2040:G:N2 | 2.80 | 0.50 |
| 22:DA:2461:A:H1' | 22:DA:2492:U:C2 | 2.47 | 0.50 |
| 22:DA:2473:U:O2 | 22:DA:2473:U:H2' | 2.10 | 0.50 |
| 23:DB:42:C:O2' | 27:DF:63:GLN:NE2 | 2.45 | 0.50 |
| 26:DE:108:ILE:HD12 | 26:DE:108:ILE:O | 2.12 | 0.50 |
| 27:DF:121:SER:O | 27:DF:123:ASP:N | 2.44 | 0.50 |
| 28:DG:91:GLY:O | 28:DG:94:TYR:CD1 | 2.65 | 0.50 |
| 32:DK:47:ILE:HB | 32:DK:48:PRO:HD2 | 1.93 | 0.50 |
| 33:DL:94:THR:O | 33:DL:98:ALA:N | 2.45 | 0.50 |
| 38:DQ:76:TYR:CZ | 38:DQ:80:ILE:HG13 | 2.47 | 0.50 |
| 49:D1:10:LYS:O | 49:D1:51:GLU:CG | 2.60 | 0.50 |
| 1:AA:2:A:C6 | 1:AA:3:A:N1 | 2.80 | 0.49 |
| 1:AA:858:G:C2' | 1:AA:859:G:H5' | 2.42 | 0.49 |
| 1:AA:939:G:H2' | 1:AA:940:C:C6 | 2.47 | 0.49 |
| 1:AA:1145:A:HO2' | 1:AA:1146:A:P | 2.34 | 0.49 |
| 3:AC:148:GLY:HA3 | 3:AC:172:ARG:O | 2.12 | 0.49 |
| 3:AC:149:ILE:HG12 | 3:AC:150:LYS:N | 2.27 | 0.49 |
| 4:AD:195:ILE:O | 4:AD:195:ILE:HG13 | 2.11 | 0.49 |
| 6:AF:91:ARG:HG3 | 6:AF:92:THR:N | 2.26 | 0.49 |
| 10:AJ:56:HIS:O | 10:AJ:57:VAL:CG1 | 2.60 | 0.49 |
| 12:AL:88:LYS:O | 12:AL:88:LYS:HG3 | 2.11 | 0.49 |
| 22:BA:26:G:H1' | 22:BA:514:A:N6 | 2.27 | 0.49 |
| 22:BA:641:U:C5 | 22:BA:642:U:C4 | 3.00 | 0.49 |
| 22:BA:819:A:H1' | 22:BA:1189:A:N1 | 2.26 | 0.49 |
| 22:BA:933:A:H5' | 22:BA:934:U:OP2 | 2.12 | 0.49 |
| 22:BA:1712:U:C4 | 22:BA:1713:A:C5 | 3.00 | 0.49 |
| 22:BA:2127:G:H4' | 22:BA:2128:G:OP1 | 2.11 | 0.49 |
| 22:BA:2307:G:N3 | 22:BA:2308:G:O6 | 2.45 | 0.49 |
| 22:BA:2309:A:N6 | 22:BA:2310:C:N4 | 2.60 | 0.49 |
| 22:BA:2552:U:C2 | 22:BA:2554:U:H5' | 2.48 | 0.49 |
| 22:BA:2728:U:HO2' | 22:BA:2729:G:P | 2.30 | 0.49 |
| 22:BA:2869:G:H2' | 22:BA:2870:C:O4' | 2.11 | 0.49 |
| 26:BE:171:ASP:OD1 | 26:BE:173:THR:N | 2.44 | 0.49 |
| 29:BH:43:ASN:O | 29:BH:46:PHE:HB3 | 2.12 | 0.49 |
| 29:BH:86:ASP:O | 29:BH:87:GLU:HB2 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BM:42:THR:HG22 | 34:BM:93:VAL:CG1 | 2.42 | 0.49 |
| 35:BN:73:ASN:HA | 35:BN:76:VAL:HG12 | 1.93 | 0.49 |
| 38:BQ:58:ARG:HA | 38:BQ:61:TRP:CE3 | 2.47 | 0.49 |
| 40:BS:28:LYS:O | 40:BS:31:GLN:N | 2.45 | 0.49 |
| 1:CA:157:U:O2 | 1:CA:165:G:C2 | 2.64 | 0.49 |
| 1:CA:158:G:C5 | 1:CA:164:G:C6 | 2.99 | 0.49 |
| 1:CA:256:U:H2' | 1:CA:257:G:O4' | 2.12 | 0.49 |
| 1:CA:408:A:H2' | 1:CA:409:U:O4' | 2.12 | 0.49 |
| 1:CA:1055:A:C6 | 1:CA:1206:G:C5 | 3.00 | 0.49 |
| 7:CG:101:MET:HA | 7:CG:104:ILE:HD12 | 1.94 | 0.49 |
| 12:CL:90:LEU:HB3 | 12:CL:93:VAL:HG21 | 1.94 | 0.49 |
| 17:CQ:60:GLU:HB3 | 17:CQ:76:VAL:HG23 | 1.94 | 0.49 |
| 22:DA:621:A:C6 | 22:DA:622:G:H1' | 2.47 | 0.49 |
| 22:DA:679:C:H2' | 22:DA:680:C:H6 | 1.77 | 0.49 |
| 22:DA:753:A:C2 | 22:DA:754:U:C2 | 3.00 | 0.49 |
| 22:DA:1340:U:H4' | 22:DA:1341:G:OP2 | 2.12 | 0.49 |
| 22:DA:1456:G:C6 | 22:DA:1457:U:C4 | 2.99 | 0.49 |
| 22:DA:1911:U:H2' | 22:DA:1918:A:C2 | 2.47 | 0.49 |
| 22:DA:2067:G:C6 | 22:DA:2444:G:C2 | 3.00 | 0.49 |
| 22:DA:2156:G:C6 | 22:DA:2157:G:C2 | 3.00 | 0.49 |
| 22:DA:2539:C:H4' | 52:D4:3:VAL:HG11 | 1.94 | 0.49 |
| 29:DH:127:GLU:HG3 | 29:DH:145:ASN:HA | 1.93 | 0.49 |
| 46:DY:31:GLN:HG2 | 46:DY:36:GLN:HB2 | 1.95 | 0.49 |
| 1:AA:978:A:C4 | 1:AA:1319:A:C2 | 3.00 | 0.49 |
| 1:AA:1027:C:C5 | 1:AA:1028:C:N4 | 2.80 | 0.49 |
| 1:AA:1048:G:N3 | 1:AA:1050:G:C8 | 2.80 | 0.49 |
| 2:AB:54:LEU:HD12 | 2:AB:220:THR:HG21 | 1.94 | 0.49 |
| 3:AC:92:ALA:HB2 | 3:AC:99:ALA:HB3 | 1.94 | 0.49 |
| 7:AG:64:VAL:O | 7:AG:65:ALA:C | 2.51 | 0.49 |
| 10:AJ:32:THR:OG1 | 10:AJ:33:GLY:N | 2.39 | 0.49 |
| 12:AL:86:ARG:CZ | 12:AL:88:LYS:HB3 | 2.41 | 0.49 |
| 22:BA:1022:G:C5 | 22:BA:1140:C:C4 | 3.00 | 0.49 |
| 22:BA:2366:A:H2' | 22:BA:2367:G:O4' | 2.12 | 0.49 |
| 26:BE:79:ARG:CG | 26:BE:79:ARG:HH11 | 2.23 | 0.49 |
| 30:BI:75:PRO:O | 30:BI:79:LEU:HD12 | 2.11 | 0.49 |
| 33:BL:62:PRO:HB2 | 51:B3:30:ARG:NH2 | 2.26 | 0.49 |
| 44:BW:52:GLY:HA3 | 44:BW:60:PHE:CE2 | 2.48 | 0.49 |
| 1:CA:71:A:C6 | 1:CA:72:A:N7 | 2.80 | 0.49 |
| 1:CA:104:G:C2 | 1:CA:105:G:C8 | 3.00 | 0.49 |
| 1:CA:106:C:O2 | 1:CA:379:C:C5' | 2.59 | 0.49 |
| 1:CA:580:C:H2' | 1:CA:581:G:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:609:A:N7 | 58:CA:1799:HOH:O | 2.33 | 0.49 |
| 1:CA:609:A:N7 | 1:CA:610:U:C5 | 2.81 | 0.49 |
| 1:CA:1114:C:O2' | 14:CN:100:SER:O | 2.24 | 0.49 |
| 1:CA:1167:A:C8 | 1:CA:1169:A:C5 | 2.99 | 0.49 |
| 1:CA:1363:A:H2' | 1:CA:1363:A:N3 | 2.27 | 0.49 |
| 1:CA:1423:G:H2' | 1:CA:1424:U:O4' | 2.12 | 0.49 |
| 2:CB:123:ASP:O | 2:CB:124:GLY:C | 2.51 | 0.49 |
| 3:CC:42:TYR:CZ | 3:CC:46:GLU:HG3 | 2.47 | 0.49 |
| 3:CC:69:HIS:HA | 3:CC:104:ALA:HB3 | 1.93 | 0.49 |
| 3:CC:83:ASP:O | 3:CC:84:VAL:C | 2.51 | 0.49 |
| 5:CE:83:HIS:NE2 | 8:CH:96:MET:HE3 | 2.27 | 0.49 |
| 6:CF:86:ARG:HH11 | 6:CF:86:ARG:HG2 | 1.77 | 0.49 |
| 11:CK:82:LEU:HD22 | 11:CK:105:PHE:HB3 | 1.94 | 0.49 |
| 14:CN:62:ASN:HB3 | 14:CN:73:PHE:CD1 | 2.48 | 0.49 |
| 22:DA:35:G:O2' | 22:DA:451:U:O4 | 2.30 | 0.49 |
| 22:DA:36:G:H4' | 22:DA:451:U:C2 | 2.48 | 0.49 |
| 22:DA:443:A:N7 | 26:DE:40:ARG:CG | 2.75 | 0.49 |
| 22:DA:600:G:OP1 | 26:DE:24:ASN:ND2 | 2.42 | 0.49 |
| 22:DA:776:G:C8 | 22:DA:793:A:C5 | 3.00 | 0.49 |
| 22:DA:864:G:O6 | 22:DA:865:C:N4 | 2.45 | 0.49 |
| 22:DA:2283:C:C2' | 22:DA:2284:A:H5' | 2.42 | 0.49 |
| 25:DD:150:GLN:C | 25:DD:151:THR:O | 2.50 | 0.49 |
| 35:DN:69:ARG:O | 35:DN:70:THR:HG23 | 2.12 | 0.49 |
| 39:DR:14:VAL:CG2 | 39:DR:98:ILE:HG13 | 2.42 | 0.49 |
| 1:AA:142:G:H2' | 1:AA:142:G:N3 | 2.27 | 0.49 |
| 1:AA:662:U:H2' | 1:AA:663:A:C8 | 2.46 | 0.49 |
| 2:AB:63:ARG:O | 2:AB:64:LYS:CB | 2.56 | 0.49 |
| 2:AB:88:ASP:C | 2:AB:89:GLN:HG3 | 2.31 | 0.49 |
| 4:AD:138:SER:HB2 | 4:AD:139:PRO:HD2 | 1.94 | 0.49 |
| 22:BA:894:U:H2' | 22:BA:895:U:C6 | 2.46 | 0.49 |
| 22:BA:1171:G:C6 | 22:BA:1172:C:N3 | 2.80 | 0.49 |
| 22:BA:1180:U:C2' | 22:BA:1181:U:H5' | 2.42 | 0.49 |
| 22:BA:1277:G:H5' | 35:BN:20:MET:HE1 | 1.95 | 0.49 |
| 22:BA:1909:C:C4 | 22:BA:1921:G:O6 | 2.66 | 0.49 |
| 26:BE:104:ALA:O | 26:BE:108:ILE:HG23 | 2.13 | 0.49 |
| 27:BF:69:LYS:N | 27:BF:69:LYS:HD2 | 2.27 | 0.49 |
| 29:BH:99:ILE:O | 29:BH:99:ILE:HG22 | 2.12 | 0.49 |
| 30:BI:116:ASP:OD2 | 30:BI:117:MET:N | 2.45 | 0.49 |
| 53:B5:73:VAL:CG2 | 53:B5:162:ILE:CB | 2.90 | 0.49 |
| 1:CA:242:G:N2 | 1:CA:285:C:C2 | 2.80 | 0.49 |
| 1:CA:375:U:N3 | 1:CA:376:G:N7 | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:577:G:C2 | 1:CA:578:C:C6 | 3.00 | 0.49 |
| 1:CA:1240:U:OP2 | 7:CG:116:MET:N | 2.44 | 0.49 |
| 1:CA:1244:G:C6 | 1:CA:1245:C:N4 | 2.81 | 0.49 |
| 1:CA:1261:A:C2 | 1:CA:1262:C:C5 | 3.01 | 0.49 |
| 1:CA:1273:C:H2' | 1:CA:1274:A:O4' | 2.12 | 0.49 |
| 5:CE:101:GLU:C | 5:CE:103:THR:N | 2.64 | 0.49 |
| 7:CG:92:ARG:NE | 7:CG:93:PRO:HD2 | 2.27 | 0.49 |
| 17:CQ:70:THR:O | 17:CQ:71:LYS:C | 2.49 | 0.49 |
| 19:CS:40:ILE:HA | 19:CS:44:MET:SD | 2.52 | 0.49 |
| 19:CS:55:ARG:CZ | 19:CS:79:THR:HG22 | 2.42 | 0.49 |
| 22:DA:104:A:H2' | 22:DA:105:C:O4' | 2.12 | 0.49 |
| 22:DA:136:G:N2 | 22:DA:144:A:N7 | 2.61 | 0.49 |
| 22:DA:819:A:C8 | 22:DA:1188:U:O4 | 2.64 | 0.49 |
| 22:DA:1299:G:H5'' | 22:DA:1300:G:H5'' | 1.93 | 0.49 |
| 22:DA:1360:G:O6 | 22:DA:1372:U:C2 | 2.65 | 0.49 |
| 22:DA:1378:A:N3 | 22:DA:1379:U:H2' | 2.27 | 0.49 |
| 22:DA:1562:U:H2' | 22:DA:1563:U:O4' | 2.12 | 0.49 |
| 22:DA:1869:G:C3' | 22:DA:1870:C:H5' | 2.43 | 0.49 |
| 22:DA:2209:G:C5 | 22:DA:2210:U:C4 | 3.00 | 0.49 |
| 22:DA:2392:A:OP2 | 51:D3:31:HIS:CE1 | 2.65 | 0.49 |
| 22:DA:2747:G:C2 | 22:DA:2756:U:C5 | 3.00 | 0.49 |
| 22:DA:2824:C:C4 | 22:DA:2825:G:C5 | 3.01 | 0.49 |
| 24:DC:240:PHE:CE1 | 24:DC:242:LYS:O | 2.65 | 0.49 |
| 25:DD:183:GLU:OE1 | 25:DD:183:GLU:N | 2.45 | 0.49 |
| 26:DE:150:THR:O | 26:DE:172:ALA:HB2 | 2.12 | 0.49 |
| 30:DI:37:GLU:OE1 | 30:DI:65:ARG:NH2 | 2.45 | 0.49 |
| 35:DN:1:MET:CE | 35:DN:1:MET:N | 2.75 | 0.49 |
| 43:DV:80:HIS:CE1 | 43:DV:83:LYS:HB2 | 2.47 | 0.49 |
| 1:AA:8:A:N6 | 4:AD:202:GLU:O | 2.45 | 0.49 |
| 1:AA:1005:A:N6 | 1:AA:1006:G:N2 | 2.61 | 0.49 |
| 1:AA:1005:A:H4' | 1:AA:1037:C:H1' | 1.94 | 0.49 |
| 2:AB:163:VAL:HG22 | 2:AB:185:ALA:HB1 | 1.94 | 0.49 |
| 4:AD:3:ARG:NH2 | 4:AD:115:ARG:HD3 | 2.28 | 0.49 |
| 4:AD:120:HIS:O | 4:AD:122:ALA:N | 2.45 | 0.49 |
| 11:AK:126:LYS:HA | 21:AU:34:ARG:HH21 | 1.77 | 0.49 |
| 18:AR:52:GLN:OE1 | 18:AR:52:GLN:HA | 2.12 | 0.49 |
| 22:BA:84:A:H4' | 22:BA:85:G:O5' | 2.12 | 0.49 |
| 22:BA:839:U:H1' | 22:BA:1191:G:H1' | 1.94 | 0.49 |
| 22:BA:1177:G:C2' | 22:BA:1178:C:O5' | 2.60 | 0.49 |
| 22:BA:2531:A:OP2 | 28:BG:174:ALA:O | 2.30 | 0.49 |
| 22:BA:2688:G:N1 | 22:BA:2720:U:OP2 | 2.37 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BC:17:VAL:HB | 24:BC:204:VAL:HG13 | 1.94 | 0.49 |
| 24:BC:167:ARG:O | 24:BC:168:ASP:CB | 2.58 | 0.49 |
| 38:BQ:79:PHE:CZ | 38:BQ:83:LEU:HD11 | 2.48 | 0.49 |
| 1:CA:237:G:C6 | 1:CA:238:A:C5 | 3.01 | 0.49 |
| 1:CA:238:A:O2' | 1:CA:239:U:H5' | 2.13 | 0.49 |
| 1:CA:527:G:N1 | 1:CA:528:C:C5 | 2.80 | 0.49 |
| 1:CA:861:G:C5 | 1:CA:862:C:C5 | 3.00 | 0.49 |
| 1:CA:1088:G:C4 | 1:CA:1089:G:C8 | 3.00 | 0.49 |
| 2:CB:93:ASN:OD1 | 2:CB:94:HIS:ND1 | 2.46 | 0.49 |
| 5:CE:147:MET:HG2 | 5:CE:147:MET:O | 2.12 | 0.49 |
| 5:CE:154:ALA:C | 5:CE:156:LYS:N | 2.66 | 0.49 |
| 7:CG:51:ALA:CB | 7:CG:58:GLU:HA | 2.43 | 0.49 |
| 7:CG:126:ASP:N | 7:CG:126:ASP:OD1 | 2.45 | 0.49 |
| 8:CH:2:SER:C | 8:CH:4:GLN:H | 2.14 | 0.49 |
| 9:CI:101:ALA:HB1 | 9:CI:103:PHE:CZ | 2.47 | 0.49 |
| 12:CL:74:LEU:HD11 | 12:CL:80:ILE:HG21 | 1.94 | 0.49 |
| 19:CS:66:MET:O | 19:CS:68:GLY:N | 2.46 | 0.49 |
| 22:DA:241:A:N1 | 22:DA:255:A:H5'' | 2.27 | 0.49 |
| 22:DA:307:G:N2 | 22:DA:310:A:C8 | 2.81 | 0.49 |
| 22:DA:528:A:N1 | 22:DA:2042:A:H2' | 2.27 | 0.49 |
| 22:DA:861:A:H2' | 22:DA:862:G:O4' | 2.12 | 0.49 |
| 22:DA:937:C:H2' | 22:DA:938:G:C8 | 2.47 | 0.49 |
| 22:DA:1087:G:N1 | 22:DA:1089:A:C2 | 2.80 | 0.49 |
| 22:DA:1230:A:H2' | 22:DA:1231:U:C6 | 2.47 | 0.49 |
| 22:DA:1330:C:O2' | 22:DA:1331:G:H5' | 2.11 | 0.49 |
| 22:DA:1663:G:C6 | 22:DA:1992:G:C8 | 2.99 | 0.49 |
| 22:DA:1695:G:H3' | 22:DA:1695:G:N3 | 2.27 | 0.49 |
| 22:DA:2056:G:H2' | 22:DA:2056:G:N3 | 2.27 | 0.49 |
| 22:DA:2121:G:C2 | 22:DA:2122:U:C2 | 3.01 | 0.49 |
| 22:DA:2808:G:N2 | 22:DA:2891:U:C6 | 2.81 | 0.49 |
| 27:DF:147:ASP:O | 27:DF:148:ARG:HB2 | 2.13 | 0.49 |
| 29:DH:81:ALA:C | 29:DH:149:GLU:HB3 | 2.33 | 0.49 |
| 30:DI:53:LEU:HG | 30:DI:82:LYS:HE2 | 1.93 | 0.49 |
| 47:DZ:14:ILE:HG22 | 47:DZ:15:GLY:N | 2.27 | 0.49 |
| 1:AA:149:A:C2 | 1:AA:150:U:C2 | 3.00 | 0.49 |
| 1:AA:299:G:H2' | 1:AA:300:A:C8 | 2.47 | 0.49 |
| 1:AA:402:G:C6 | 1:AA:403:C:C4 | 3.00 | 0.49 |
| 1:AA:760:G:N7 | 1:AA:761:G:N7 | 2.59 | 0.49 |
| 1:AA:923:A:O4' | 1:AA:1398:A:C2 | 2.65 | 0.49 |
| 1:AA:1314:C:H41 | 19:AS:4:SER:HA | 1.77 | 0.49 |
| 1:AA:1349:A:C2 | 1:AA:1374:A:C5 | 3.00 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1539:C:H5'' | 21:AU:18:ARG:HG3 | 1.93 | 0.49 |
| 2:AB:133:GLU:O | 2:AB:137:ARG:HB2 | 2.11 | 0.49 |
| 3:AC:3:GLN:OE1 | 3:AC:3:GLN:N | 2.45 | 0.49 |
| 7:AG:27:VAL:HG23 | 7:AG:28:ASN:N | 2.28 | 0.49 |
| 7:AG:71:PRO:O | 7:AG:96:ARG:HG3 | 2.12 | 0.49 |
| 11:AK:31:ILE:O | 11:AK:31:ILE:HG13 | 2.12 | 0.49 |
| 16:AP:79:ASN:O | 16:AP:80:LYS:HE3 | 2.13 | 0.49 |
| 22:BA:437:U:H2' | 22:BA:438:G:C8 | 2.46 | 0.49 |
| 22:BA:1026:G:H1' | 22:BA:1134:A:C2 | 2.48 | 0.49 |
| 22:BA:1586:A:C8 | 22:BA:1587:G:C8 | 3.00 | 0.49 |
| 22:BA:1846:G:H2' | 22:BA:1847:A:C4 | 2.47 | 0.49 |
| 22:BA:2131:U:OP2 | 22:BA:2132:U:C6 | 2.66 | 0.49 |
| 22:BA:2532:G:N2 | 22:BA:2663:G:O2' | 2.46 | 0.49 |
| 25:BD:85:ALA:O | 25:BD:86:GLU:C | 2.50 | 0.49 |
| 29:BH:123:ARG:HD3 | 1:CA:358:U:OP1 | 2.12 | 0.49 |
| 35:BN:25:ALA:HB1 | 35:BN:48:VAL:HG22 | 1.93 | 0.49 |
| 39:BR:49:ILE:CB | 39:BR:52:PRO:C | 2.79 | 0.49 |
| 48:B0:30:VAL:HG12 | 48:B0:35:GLY:HA2 | 1.95 | 0.49 |
| 1:CA:411:A:C6 | 1:CA:429:U:C5 | 3.00 | 0.49 |
| 1:CA:579:A:C4 | 1:CA:763:G:N2 | 2.80 | 0.49 |
| 1:CA:794:A:H2' | 1:CA:795:C:C6 | 2.47 | 0.49 |
| 1:CA:945:G:H2' | 1:CA:945:G:N3 | 2.26 | 0.49 |
| 1:CA:1014:A:N7 | 1:CA:1015:G:C6 | 2.80 | 0.49 |
| 1:CA:1463:U:H2' | 1:CA:1464:U:C6 | 2.47 | 0.49 |
| 1:CA:1486:G:H2' | 1:CA:1487:G:O4' | 2.12 | 0.49 |
| 3:CC:77:ILE:HA | 3:CC:84:VAL:HG23 | 1.94 | 0.49 |
| 4:CD:46:PRO:O | 4:CD:48:LEU:N | 2.45 | 0.49 |
| 5:CE:11:LEU:HG | 5:CE:12:GLN:N | 2.28 | 0.49 |
| 14:CN:10:GLU:O | 14:CN:11:VAL:C | 2.49 | 0.49 |
| 20:CT:9:LYS:O | 20:CT:12:ILE:HG12 | 2.12 | 0.49 |
| 22:DA:1127:A:C3' | 22:DA:1128:G:H5'' | 2.43 | 0.49 |
| 22:DA:1176:U:H2' | 22:DA:1177:G:C8 | 2.47 | 0.49 |
| 22:DA:2184:A:H2' | 22:DA:2185:U:C6 | 2.47 | 0.49 |
| 22:DA:2386:A:H2' | 22:DA:2387:U:C6 | 2.48 | 0.49 |
| 22:DA:2537:U:H2' | 22:DA:2538:C:C6 | 2.47 | 0.49 |
| 22:DA:2854:G:N2 | 22:DA:2864:G:N3 | 2.61 | 0.49 |
| 26:DE:61:ARG:O | 26:DE:63:LYS:N | 2.45 | 0.49 |
| 28:DG:95:ARG:HA | 28:DG:128:GLN:O | 2.11 | 0.49 |
| 29:DH:112:LYS:CG | 29:DH:113:SER:N | 2.76 | 0.49 |
| 34:DM:120:ALA:O | 34:DM:124:LEU:HD23 | 2.12 | 0.49 |
| 46:DY:21:LEU:HA | 46:DY:25:GLN:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 52:D4:19:ARG:O | 52:D4:20:ASP:HB2 | 2.11 | 0.49 |
| 1:AA:188:C:O2 | 1:AA:188:C:C2' | 2.61 | 0.49 |
| 1:AA:345:C:N3 | 32:BK:117:SER:OG | 2.46 | 0.49 |
| 1:AA:472:U:C4 | 1:AA:473:U:O4 | 2.66 | 0.49 |
| 1:AA:1226:C:O2' | 13:AM:110:LYS:NZ | 2.45 | 0.49 |
| 1:AA:1243:C:H2' | 1:AA:1244:G:C8 | 2.48 | 0.49 |
| 2:AB:46:THR:CG2 | 2:AB:201:PRO:HB2 | 2.42 | 0.49 |
| 10:AJ:73:LEU:O | 10:AJ:74:VAL:CB | 2.61 | 0.49 |
| 22:BA:603:A:C8 | 22:BA:655:A:C6 | 3.00 | 0.49 |
| 22:BA:687:C:H2' | 22:BA:688:U:O4' | 2.11 | 0.49 |
| 22:BA:830:G:H4' | 22:BA:831:G:OP2 | 2.13 | 0.49 |
| 22:BA:1084:A:C5 | 22:BA:1085:A:C6 | 3.00 | 0.49 |
| 22:BA:1477:A:N6 | 22:BA:1514:G:O2' | 2.44 | 0.49 |
| 22:BA:1791:A:O3' | 24:BC:204:VAL:O | 2.31 | 0.49 |
| 22:BA:1832:C:N4 | 22:BA:1833:C:C4 | 2.81 | 0.49 |
| 22:BA:2298:A:N6 | 22:BA:2318:G:H1' | 2.28 | 0.49 |
| 23:BB:43:C:O2 | 27:BF:92:ARG:NH2 | 2.42 | 0.49 |
| 24:BC:82:GLU:OE1 | 24:BC:103:TYR:OH | 2.23 | 0.49 |
| 24:BC:246:THR:N | 24:BC:250:VAL:O | 2.40 | 0.49 |
| 27:BF:40:VAL:CG1 | 27:BF:41:GLY:N | 2.75 | 0.49 |
| 33:BL:68:SER:O | 33:BL:69:ARG:HG3 | 2.12 | 0.49 |
| 49:B1:6:ARG:HG2 | 49:B1:24:THR:HB | 1.95 | 0.49 |
| 1:CA:53:A:C2 | 1:CA:359:G:C6 | 3.00 | 0.49 |
| 1:CA:840:C:N3 | 1:CA:842:U:H4' | 2.28 | 0.49 |
| 1:CA:983:A:C2' | 1:CA:983:A:N3 | 2.76 | 0.49 |
| 1:CA:1105:A:H2' | 1:CA:1106:G:H8 | 1.78 | 0.49 |
| 1:CA:1213:A:C5 | 1:CA:1215:G:C4 | 3.01 | 0.49 |
| 1:CA:1337:G:C5' | 1:CA:1338:G:OP1 | 2.60 | 0.49 |
| 1:CA:1361:G:H3' | 1:CA:1362:A:H5'' | 1.94 | 0.49 |
| 9:CI:49:ARG:C | 9:CI:49:ARG:HD3 | 2.32 | 0.49 |
| 10:CJ:57:VAL:HG22 | 10:CJ:58:ASN:H | 1.76 | 0.49 |
| 12:CL:28:PRO:HB2 | 12:CL:29:GLN:OE1 | 2.13 | 0.49 |
| 16:CP:23:ASP:OD2 | 16:CP:25:ARG:HG2 | 2.12 | 0.49 |
| 22:DA:197:A:C8 | 22:DA:2430:A:C8 | 3.01 | 0.49 |
| 22:DA:410:G:C6 | 22:DA:2407:A:N6 | 2.81 | 0.49 |
| 22:DA:570:G:H2' | 22:DA:571:U:H5' | 1.93 | 0.49 |
| 22:DA:1931:U:OP2 | 22:DA:1968:G:N1 | 2.43 | 0.49 |
| 22:DA:2057:G:H2' | 22:DA:2058:A:O4' | 2.13 | 0.49 |
| 22:DA:2283:C:H2' | 22:DA:2284:A:H5' | 1.95 | 0.49 |
| 22:DA:2862:G:C6 | 22:DA:2863:C:N4 | 2.81 | 0.49 |
| 34:DM:57:VAL:HG11 | 34:DM:105:MET:SD | 2.52 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 35:DN:48:VAL:N | 35:DN:50:PRO:HD2 | 2.27 | 0.49 |
| 41:DT:61:LEU:HD12 | 41:DT:62:VAL:N | 2.27 | 0.49 |
| 1:AA:705:G:C5 | 1:AA:706:A:C8 | 3.01 | 0.49 |
| 1:AA:850:U:H2' | 1:AA:851:G:O5' | 2.13 | 0.49 |
| 1:AA:1030:U:OP2 | 1:AA:1031:C:C5 | 2.66 | 0.49 |
| 1:AA:1048:G:N3 | 1:AA:1050:G:N7 | 2.60 | 0.49 |
| 1:AA:1417:G:C6 | 1:AA:1482:G:C6 | 3.01 | 0.49 |
| 4:AD:173:VAL:HG13 | 4:AD:174:ASP:N | 2.28 | 0.49 |
| 19:AS:23:VAL:HG12 | 19:AS:24:GLU:N | 2.28 | 0.49 |
| 22:BA:1487:U:C2 | 22:BA:1503:A:C2 | 3.00 | 0.49 |
| 22:BA:2006:C:O2' | 22:BA:2823:A:O2' | 2.27 | 0.49 |
| 22:BA:2267:A:H5'' | 22:BA:2268:A:H5' | 1.94 | 0.49 |
| 22:BA:2452:C:N3 | 56:BA:3001:DOL:H131 | 2.28 | 0.49 |
| 27:BF:8:TYR:HA | 27:BF:12:VAL:CG2 | 2.41 | 0.49 |
| 34:BM:49:ALA:HB1 | 34:BM:120:ALA:HB1 | 1.95 | 0.49 |
| 39:BR:49:ILE:HB | 39:BR:52:PRO:CA | 2.43 | 0.49 |
| 41:BT:1:MET:O | 41:BT:2:ILE:CG1 | 2.61 | 0.49 |
| 51:B3:45:ARG:N | 51:B3:46:PRO:HD2 | 2.27 | 0.49 |
| 1:CA:154:U:C2 | 1:CA:168:G:N2 | 2.81 | 0.49 |
| 1:CA:890:G:N2 | 1:CA:906:A:H2' | 2.28 | 0.49 |
| 1:CA:1361:G:H3' | 1:CA:1362:A:C5' | 2.41 | 0.49 |
| 1:CA:1437:A:C2 | 1:CA:1465:A:C2 | 3.01 | 0.49 |
| 6:CF:78:PHE:CD2 | 6:CF:78:PHE:N | 2.81 | 0.49 |
| 21:CU:44:GLU:OE1 | 21:CU:45:ARG:NH1 | 2.46 | 0.49 |
| 22:DA:49:A:N6 | 22:DA:177:G:C5 | 2.81 | 0.49 |
| 22:DA:411:G:OP1 | 22:DA:2407:A:OP2 | 2.29 | 0.49 |
| 22:DA:569:U:H5'' | 22:DA:821:A:C2 | 2.48 | 0.49 |
| 22:DA:1071:G:O2' | 22:DA:1072:C:O4' | 2.23 | 0.49 |
| 22:DA:1248:G:C4 | 38:DQ:3:ARG:HG3 | 2.47 | 0.49 |
| 22:DA:1250:G:H5' | 38:DQ:6:ARG:HD3 | 1.95 | 0.49 |
| 22:DA:1779:U:C5 | 22:DA:1784:A:N7 | 2.80 | 0.49 |
| 22:DA:2599:G:N7 | 24:DC:236:GLU:CB | 2.76 | 0.49 |
| 22:DA:2842:G:H2' | 22:DA:2843:G:O4' | 2.11 | 0.49 |
| 22:DA:2848:G:OP2 | 37:DP:95:ALA:N | 2.46 | 0.49 |
| 22:DA:2849:U:H4' | 22:DA:2868:A:C2 | 2.47 | 0.49 |
| 23:DB:109:A:C6 | 23:DB:110:C:C4 | 3.00 | 0.49 |
| 34:DM:22:GLN:O | 34:DM:24:THR:N | 2.46 | 0.49 |
| 41:DT:7:LEU:HD21 | 41:DT:45:ALA:HB3 | 1.95 | 0.49 |
| 42:DU:16:GLY:O | 42:DU:17:LYS:HB2 | 2.12 | 0.49 |
| 42:DU:98:SER:O | 42:DU:99:ASN:CB | 2.60 | 0.49 |
| 1:AA:82:G:N2 | 1:AA:89:U:OP1 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:455:G:C2 | 1:AA:478:A:C2 | 3.00 | 0.49 |
| 1:AA:652:U:C4 | 1:AA:752:G:N3 | 2.81 | 0.49 |
| 1:AA:1182:G:C3' | 1:AA:1183:U:H5' | 2.43 | 0.49 |
| 1:AA:1381:U:C2 | 7:AG:78:ARG:NH1 | 2.80 | 0.49 |
| 2:AB:166:ALA:HB2 | 2:AB:187:VAL:HG12 | 1.94 | 0.49 |
| 11:AK:30:THR:HG21 | 11:AK:91:PRO:O | 2.13 | 0.49 |
| 14:AN:43:ASN:C | 14:AN:45:VAL:N | 2.64 | 0.49 |
| 22:BA:58:G:OP1 | 41:BT:78:SER:HB2 | 2.13 | 0.49 |
| 22:BA:360:U:C4 | 22:BA:361:G:C6 | 3.00 | 0.49 |
| 22:BA:1088:A:N3 | 22:BA:1088:A:H5'' | 2.27 | 0.49 |
| 22:BA:1419:A:HO2' | 22:BA:1421:G:H8 | 1.57 | 0.49 |
| 22:BA:1747:U:H2' | 22:BA:1748:C:C6 | 2.47 | 0.49 |
| 22:BA:2014:A:H2' | 22:BA:2015:A:C8 | 2.48 | 0.49 |
| 22:BA:2190:G:N1 | 22:BA:2191:A:C4 | 2.81 | 0.49 |
| 24:BC:15:HIS:O | 24:BC:204:VAL:CG2 | 2.61 | 0.49 |
| 25:BD:101:PHE:C | 25:BD:103:ASP:N | 2.66 | 0.49 |
| 30:BI:86:ILE:N | 30:BI:86:ILE:HD12 | 2.28 | 0.49 |
| 31:BJ:60:ASP:HA | 31:BJ:97:PRO:HB3 | 1.95 | 0.49 |
| 53:B5:215:VAL:O | 53:B5:216:THR:CB | 2.61 | 0.49 |
| 1:CA:597:G:C8 | 1:CA:598:U:C5 | 3.01 | 0.49 |
| 1:CA:1000:A:C2 | 1:CA:1041:G:C2 | 3.01 | 0.49 |
| 5:CE:38:VAL:HG12 | 5:CE:117:VAL:HG21 | 1.94 | 0.49 |
| 12:CL:40:THR:HG22 | 12:CL:41:THR:N | 2.28 | 0.49 |
| 19:CS:73:GLU:HB2 | 19:CS:74:PHE:CD1 | 2.47 | 0.49 |
| 22:DA:182:A:N6 | 22:DA:214:G:O6 | 2.45 | 0.49 |
| 22:DA:508:A:C3' | 22:DA:509:C:H5' | 2.42 | 0.49 |
| 22:DA:792:A:O2' | 22:DA:2440:C:N3 | 2.36 | 0.49 |
| 22:DA:1361:G:C5 | 22:DA:1362:C:C5 | 3.01 | 0.49 |
| 22:DA:1504:A:N6 | 22:DA:1505:A:C6 | 2.81 | 0.49 |
| 22:DA:1814:G:C6 | 22:DA:1815:A:C6 | 3.00 | 0.49 |
| 22:DA:1973:G:C5 | 22:DA:1974:C:C4 | 3.00 | 0.49 |
| 22:DA:2111:U:O4 | 22:DA:2147:A:C2 | 2.66 | 0.49 |
| 22:DA:2146:C:H4' | 22:DA:2147:A:C8 | 2.47 | 0.49 |
| 22:DA:2307:G:N2 | 22:DA:2312:U:N3 | 2.60 | 0.49 |
| 22:DA:2371:G:C2 | 22:DA:2372:U:C5 | 3.00 | 0.49 |
| 29:DH:72:ILE:O | 29:DH:141:LYS:O | 2.30 | 0.49 |
| 32:DK:31:ARG:HB2 | 32:DK:32:TYR:CD2 | 2.47 | 0.49 |
| 37:DP:28:VAL:HG21 | 37:DP:74:PHE:CE2 | 2.48 | 0.49 |
| 1:AA:130:A:C8 | 17:AQ:65:ARG:HB2 | 2.47 | 0.49 |
| 1:AA:438:U:C2 | 1:AA:494:G:C6 | 3.00 | 0.49 |
| 1:AA:501:C:H2' | 1:AA:502:A:C8 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1308:U:O2' | 1:AA:1309:G:H5' | 2.13 | 0.49 |
| 3:AC:19:ASN:OD1 | 3:AC:19:ASN:N | 2.45 | 0.49 |
| 5:AE:137:VAL:O | 5:AE:138:ARG:CB | 2.60 | 0.49 |
| 8:AH:125:ILE:O | 8:AH:125:ILE:CG1 | 2.60 | 0.49 |
| 22:BA:2177:C:N4 | 22:BA:2178:C:O2 | 2.46 | 0.49 |
| 22:BA:2287:A:OP1 | 49:B1:30:LYS:NZ | 2.35 | 0.49 |
| 25:BD:166:GLY:O | 25:BD:167:ASN:HB3 | 2.13 | 0.49 |
| 26:BE:108:ILE:HG13 | 26:BE:109:LEU:N | 2.28 | 0.49 |
| 28:BG:80:THR:CG2 | 28:BG:81:GLU:N | 2.75 | 0.49 |
| 30:BI:105:GLN:O | 30:BI:106:LEU:HB2 | 2.13 | 0.49 |
| 36:BO:25:ARG:HG3 | 36:BO:27:VAL:HG12 | 1.94 | 0.49 |
| 42:BU:13:VAL:HG12 | 42:BU:19:LYS:HA | 1.95 | 0.49 |
| 48:B0:13:ARG:O | 48:B0:17:ARG:HG3 | 2.12 | 0.49 |
| 53:B5:65:LEU:O | 53:B5:67:HIS:N | 2.45 | 0.49 |
| 1:CA:215:C:H2' | 1:CA:216:U:O4' | 2.13 | 0.49 |
| 1:CA:218:U:H2' | 1:CA:219:U:O4' | 2.13 | 0.49 |
| 1:CA:846:G:C2 | 1:CA:847:G:C8 | 3.01 | 0.49 |
| 1:CA:1061:G:N7 | 1:CA:1062:U:C5 | 2.81 | 0.49 |
| 1:CA:1157:A:H4' | 1:CA:1158:C:O5' | 2.13 | 0.49 |
| 1:CA:1211:U:H1' | 1:CA:1213:A:C2 | 2.48 | 0.49 |
| 2:CB:58:ASN:CG | 2:CB:220:THR:O | 2.51 | 0.49 |
| 2:CB:62:SER:HA | 2:CB:224:GLY:HA3 | 1.94 | 0.49 |
| 4:CD:174:ASP:OD1 | 4:CD:177:LYS:N | 2.46 | 0.49 |
| 7:CG:88:PRO:HD2 | 7:CG:152:ALA:HA | 1.94 | 0.49 |
| 11:CK:110:ILE:HG22 | 21:CU:17:ARG:NH1 | 2.28 | 0.49 |
| 12:CL:38:TYR:HB3 | 12:CL:52:VAL:HG13 | 1.94 | 0.49 |
| 22:DA:58:G:C2 | 22:DA:70:G:C2 | 3.01 | 0.49 |
| 22:DA:430:A:H2' | 22:DA:431:U:H5' | 1.95 | 0.49 |
| 22:DA:636:G:O2' | 22:DA:638:G:O2' | 2.29 | 0.49 |
| 22:DA:856:G:C2 | 22:DA:922:C:N3 | 2.81 | 0.49 |
| 22:DA:878:A:C2 | 22:DA:900:A:C4 | 3.01 | 0.49 |
| 22:DA:1993:U:H4' | 25:DD:133:THR:CG2 | 2.43 | 0.49 |
| 22:DA:2231:U:H2' | 22:DA:2232:C:C6 | 2.48 | 0.49 |
| 22:DA:2360:G:H1' | 33:DL:60:ARG:HD3 | 1.94 | 0.49 |
| 22:DA:2586:U:C5 | 22:DA:2587:A:C8 | 3.01 | 0.49 |
| 23:DB:37:C:C5 | 23:DB:38:C:C4 | 3.01 | 0.49 |
| 30:DI:76:ALA:HB2 | 30:DI:129:ILE:HG23 | 1.95 | 0.49 |
| 31:DJ:31:GLU:OE2 | 31:DJ:35:ARG:NH1 | 2.46 | 0.49 |
| 35:DN:87:PHE:O | 35:DN:88:ALA:C | 2.52 | 0.49 |
| 42:DU:85:PHE:N | 42:DU:85:PHE:CD1 | 2.81 | 0.49 |
| 46:DY:20:ASN:O | 46:DY:24:GLU:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:D4:16:ILE:HD13 | 52:D4:25:VAL:HG22 | 1.95 | 0.49 |
| 1:AA:71:A:N3 | 1:AA:72:A:C8 | 2.81 | 0.49 |
| 1:AA:375:U:C4 | 1:AA:376:G:N7 | 2.81 | 0.49 |
| 1:AA:872:A:C8 | 1:AA:874:G:C8 | 3.01 | 0.49 |
| 3:AC:42:TYR:CZ | 3:AC:90:VAL:HG21 | 2.48 | 0.49 |
| 10:AJ:53:ILE:HD11 | 14:AN:85:ARG:NH1 | 2.28 | 0.49 |
| 16:AP:45:GLU:O | 16:AP:46:LYS:O | 2.31 | 0.49 |
| 22:BA:250:G:C6 | 22:BA:251:A:C6 | 3.01 | 0.49 |
| 22:BA:1922:G:N3 | 22:BA:1922:G:C2' | 2.76 | 0.49 |
| 22:BA:2560:A:C5 | 22:BA:2561:U:C5 | 3.00 | 0.49 |
| 27:BF:158:THR:CG2 | 27:BF:160:ALA:H | 2.26 | 0.49 |
| 36:BO:100:HIS:O | 36:BO:104:GLN:HB3 | 2.13 | 0.49 |
| 47:BZ:11:ARG:NH1 | 47:BZ:53:PHE:O | 2.46 | 0.49 |
| 1:CA:157:U:O2' | 1:CA:158:G:H5' | 2.12 | 0.49 |
| 1:CA:1007:U:H2' | 1:CA:1008:U:H5'' | 1.93 | 0.49 |
| 1:CA:1149:C:C4 | 1:CA:1150:A:C6 | 3.00 | 0.49 |
| 7:CG:42:ILE:HG21 | 7:CG:116:MET:HG3 | 1.95 | 0.49 |
| 7:CG:92:ARG:NE | 7:CG:93:PRO:HD3 | 2.28 | 0.49 |
| 11:CK:116:ILE:O | 11:CK:116:ILE:HG22 | 2.13 | 0.49 |
| 16:CP:16:PHE:CE1 | 16:CP:38:PHE:HB2 | 2.48 | 0.49 |
| 22:DA:55:G:C2 | 22:DA:56:A:C8 | 3.00 | 0.49 |
| 22:DA:152:A:C2 | 22:DA:175:G:N3 | 2.81 | 0.49 |
| 22:DA:382:A:N1 | 22:DA:383:C:C2 | 2.81 | 0.49 |
| 22:DA:581:C:OP2 | 38:DQ:33:ARG:NE | 2.46 | 0.49 |
| 22:DA:883:G:N2 | 22:DA:894:U:O2 | 2.46 | 0.49 |
| 22:DA:1567:G:C8 | 24:DC:83:TYR:CD1 | 3.00 | 0.49 |
| 22:DA:1638:C:C5' | 22:DA:2710:C:O2' | 2.61 | 0.49 |
| 22:DA:1791:A:C2' | 22:DA:1792:G:H5' | 2.43 | 0.49 |
| 22:DA:1869:G:C2 | 22:DA:1873:G:N1 | 2.81 | 0.49 |
| 22:DA:2054:A:C2 | 22:DA:2616:C:C2 | 3.01 | 0.49 |
| 22:DA:2059:A:H4' | 26:DE:64:GLY:O | 2.13 | 0.49 |
| 22:DA:2428:G:H5'' | 22:DA:2429:G:OP1 | 2.13 | 0.49 |
| 22:DA:2532:G:N2 | 22:DA:2663:G:O2' | 2.46 | 0.49 |
| 22:DA:2729:G:H2' | 22:DA:2730:C:O4' | 2.13 | 0.49 |
| 24:DC:43:ARG:NH2 | 24:DC:49:ILE:HD11 | 2.28 | 0.49 |
| 27:DF:16:LEU:HD11 | 27:DF:169:LEU:CD1 | 2.43 | 0.49 |
| 32:DK:92:GLU:N | 32:DK:92:GLU:OE2 | 2.43 | 0.49 |
| 34:DM:69:PRO:O | 34:DM:70:ASP:HB3 | 2.11 | 0.49 |
| 40:DS:20:VAL:CG2 | 40:DS:39:THR:HG21 | 2.43 | 0.49 |
| 1:AA:144:G:C2 | 1:AA:179:A:N3 | 2.81 | 0.48 |
| 1:AA:411:A:C5 | 1:AA:429:U:C5 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:AA:591:U:P | 8:AH:31:LYS:HD2 | 2.54 | 0.48 |
| 1:AA:709:U:O2' | 1:AA:710:G:H5' | 2.13 | 0.48 |
| 1:AA:1077:G:N2 | 1:AA:1080:A:OP2 | 2.46 | 0.48 |
| 2:AB:79:ALA:O | 2:AB:214:LEU:CD2 | 2.60 | 0.48 |
| 2:AB:82:ASP:O | 2:AB:84:ALA:N | 2.46 | 0.48 |
| 5:AE:149:SER:O | 5:AE:153:VAL:HG12 | 2.13 | 0.48 |
| 10:AJ:41:PRO:O | 10:AJ:42:LEU:CB | 2.61 | 0.48 |
| 11:AK:88:GLY:N | 11:AK:114:THR:HG22 | 2.28 | 0.48 |
| 13:AM:27:LYS:O | 13:AM:31:LYS:HG3 | 2.12 | 0.48 |
| 14:AN:46:LEU:O | 14:AN:47:LYS:C | 2.51 | 0.48 |
| 17:AQ:82:ALA:O | 17:AQ:83:VAL:O | 2.30 | 0.48 |
| 18:AR:34:THR:OG1 | 18:AR:35:GLU:N | 2.46 | 0.48 |
| 22:BA:78:U:H2' | 22:BA:79:C:C6 | 2.48 | 0.48 |
| 22:BA:1206:G:C6 | 22:BA:1207:C:C4 | 3.01 | 0.48 |
| 22:BA:1881:C:H2' | 22:BA:1882:U:O4' | 2.13 | 0.48 |
| 22:BA:2019:A:H4' | 38:BQ:34:VAL:HG21 | 1.94 | 0.48 |
| 22:BA:2553:G:N1 | 22:BA:2554:U:O2 | 2.46 | 0.48 |
| 22:BA:2555:U:C5 | 22:BA:2556:C:C2 | 3.01 | 0.48 |
| 22:BA:2615:U:C2' | 22:BA:2616:C:H5' | 2.42 | 0.48 |
| 29:BH:121:VAL:H | 29:BH:122:LEU:HB2 | 1.77 | 0.48 |
| 29:BH:139:PHE:O | 29:BH:140:ALA:HB2 | 2.13 | 0.48 |
| 30:BI:6:GLN:O | 30:BI:7:ALA:HB3 | 2.13 | 0.48 |
| 1:CA:66:A:H4' | 1:CA:173:U:C5 | 2.47 | 0.48 |
| 1:CA:73:C:HO2' | 1:CA:74:A:P | 2.34 | 0.48 |
| 1:CA:630:A:H2' | 1:CA:631:C:O4' | 2.13 | 0.48 |
| 1:CA:786:G:H2' | 1:CA:786:G:N3 | 2.27 | 0.48 |
| 1:CA:881:G:C6 | 1:CA:882:C:C4 | 3.01 | 0.48 |
| 1:CA:920:U:C2 | 1:CA:921:U:C5 | 3.01 | 0.48 |
| 1:CA:960:U:O2' | 1:CA:1223:C:H4' | 2.13 | 0.48 |
| 1:CA:1537:U:C5 | 1:CA:1538:C:C4 | 3.01 | 0.48 |
| 2:CB:143:LYS:O | 2:CB:147:SER:OG | 2.24 | 0.48 |
| 4:CD:174:ASP:CG | 4:CD:175:ALA:N | 2.65 | 0.48 |
| 5:CE:13:GLU:HB2 | 5:CE:39:VAL:HG12 | 1.94 | 0.48 |
| 7:CG:78:ARG:O | 7:CG:79:ARG:HB2 | 2.12 | 0.48 |
| 9:CI:24:GLY:N | 9:CI:61:LEU:HA | 2.29 | 0.48 |
| 13:CM:46:SER:O | 13:CM:47:GLU:HB3 | 2.11 | 0.48 |
| 17:CQ:45:HIS:O | 17:CQ:71:LYS:HA | 2.13 | 0.48 |
| 19:CS:51:VAL:O | 19:CS:58:VAL:HG13 | 2.13 | 0.48 |
| 22:DA:477:A:H2' | 22:DA:478:A:O5' | 2.13 | 0.48 |
| 22:DA:591:U:H1' | 51:D3:2:PRO:HD2 | 1.94 | 0.48 |
| 22:DA:771:G:O2' | 22:DA:1355:G:O2' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:933:A:C5' | 22:DA:934:U:OP2 | 2.61 | 0.48 |
| 22:DA:1029:A:N7 | 22:DA:1030:C:C2 | 2.81 | 0.48 |
| 22:DA:1076:C:H1' | 30:DI:93:PRO:HG2 | 1.95 | 0.48 |
| 22:DA:1569:A:C6 | 22:DA:1570:A:C2 | 3.01 | 0.48 |
| 22:DA:1773:A:N3 | 22:DA:1978:A:C2 | 2.81 | 0.48 |
| 22:DA:1981:A:H5'' | 22:DA:1982:U:OP2 | 2.12 | 0.48 |
| 22:DA:2119:A:N1 | 22:DA:2169:A:H2' | 2.28 | 0.48 |
| 22:DA:2502:G:H5' | 22:DA:2503:A:H5'' | 1.94 | 0.48 |
| 23:DB:34:A:N6 | 23:DB:44:G:H1' | 2.28 | 0.48 |
| 31:DJ:84:ILE:O | 31:DJ:84:ILE:CG1 | 2.61 | 0.48 |
| 41:DT:62:VAL:HG12 | 41:DT:63:VAL:N | 2.28 | 0.48 |
| 45:DX:54:LYS:HA | 45:DX:57:ARG:HB2 | 1.94 | 0.48 |
| 47:DZ:7:ILE:N | 47:DZ:36:VAL:O | 2.45 | 0.48 |
| 47:DZ:41:THR:HB | 47:DZ:42:PRO:HD2 | 1.95 | 0.48 |
| 1:AA:72:A:H2' | 1:AA:73:C:H5' | 1.94 | 0.48 |
| 1:AA:215:C:H2' | 1:AA:216:U:O4' | 2.13 | 0.48 |
| 1:AA:451:A:H4' | 1:AA:452:A:O4' | 2.13 | 0.48 |
| 1:AA:586:C:O3' | 8:AH:81:PRO:HB3 | 2.13 | 0.48 |
| 1:AA:721:G:H4' | 1:AA:722:G:O4' | 2.13 | 0.48 |
| 2:AB:40:ILE:N | 2:AB:40:ILE:HD13 | 2.27 | 0.48 |
| 3:AC:37:PHE:O | 3:AC:41:GLN:HB2 | 2.13 | 0.48 |
| 6:AF:93:LYS:CG | 6:AF:93:LYS:O | 2.61 | 0.48 |
| 8:AH:125:ILE:O | 8:AH:125:ILE:HG13 | 2.13 | 0.48 |
| 9:AI:57:MET:CG | 9:AI:58:VAL:N | 2.76 | 0.48 |
| 12:AL:44:LYS:HB2 | 12:AL:45:PRO:CD | 2.42 | 0.48 |
| 21:AU:20:LYS:CE | 21:AU:20:LYS:HA | 2.42 | 0.48 |
| 22:BA:749:A:C6 | 22:BA:1618:A:C2 | 3.01 | 0.48 |
| 22:BA:1188:U:H2' | 22:BA:1189:A:H5' | 1.94 | 0.48 |
| 22:BA:1421:G:N2 | 22:BA:1495:A:N1 | 2.58 | 0.48 |
| 22:BA:1583:A:HO2' | 22:BA:1584:U:P | 2.37 | 0.48 |
| 22:BA:1820:U:OP1 | 24:BC:177:ARG:NH2 | 2.46 | 0.48 |
| 22:BA:2419:U:OP1 | 51:B3:41:LYS:HE2 | 2.13 | 0.48 |
| 1:CA:183:C:HO2' | 1:CA:184:G:P | 2.35 | 0.48 |
| 1:CA:211:G:O2' | 1:CA:212:G:H4' | 2.14 | 0.48 |
| 1:CA:1259:C:N4 | 1:CA:1260:G:C4 | 2.81 | 0.48 |
| 1:CA:1311:A:C2 | 1:CA:1327:C:N3 | 2.81 | 0.48 |
| 1:CA:1408:A:N1 | 1:CA:1494:G:C5 | 2.81 | 0.48 |
| 4:CD:168:PRO:HB2 | 4:CD:171:LEU:HD12 | 1.95 | 0.48 |
| 12:CL:4:VAL:HG22 | 12:CL:5:ASN:N | 2.27 | 0.48 |
| 20:CT:21:ASN:O | 20:CT:25:ARG:HB3 | 2.12 | 0.48 |
| 20:CT:36:TYR:CG | 20:CT:37:ALA:N | 2.82 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:CU:12:PHE:CD1 | 21:CU:13:ASP:N | 2.81 | 0.48 |
| 22:DA:223:A:H2' | 22:DA:408:G:N3 | 2.28 | 0.48 |
| 22:DA:248:G:H5' | 22:DA:250:G:N7 | 2.28 | 0.48 |
| 22:DA:470:A:C2 | 22:DA:471:A:C4 | 3.01 | 0.48 |
| 22:DA:581:C:OP2 | 38:DQ:33:ARG:CZ | 2.61 | 0.48 |
| 22:DA:796:C:H2' | 22:DA:797:G:C8 | 2.48 | 0.48 |
| 22:DA:1331:G:O2' | 22:DA:1332:G:H5' | 2.13 | 0.48 |
| 22:DA:1866:A:N3 | 22:DA:1876:A:C6 | 2.81 | 0.48 |
| 22:DA:2073:C:H5'' | 24:DC:228:VAL:CB | 2.43 | 0.48 |
| 22:DA:2819:G:H2' | 22:DA:2821:A:N7 | 2.29 | 0.48 |
| 29:DH:21:VAL:CG2 | 29:DH:22:LYS:N | 2.76 | 0.48 |
| 30:DI:54:PRO:HG2 | 30:DI:78:VAL:HB | 1.95 | 0.48 |
| 35:DN:85:PRO:O | 35:DN:86:ARG:C | 2.51 | 0.48 |
| 1:AA:64:G:C8 | 1:AA:99:C:C4 | 3.01 | 0.48 |
| 1:AA:471:U:H2' | 1:AA:472:U:O4' | 2.14 | 0.48 |
| 1:AA:872:A:C4 | 1:AA:874:G:N7 | 2.81 | 0.48 |
| 1:AA:1373:G:H5'' | 7:AG:36:LYS:HB2 | 1.95 | 0.48 |
| 2:AB:32:PHE:CG | 2:AB:32:PHE:O | 2.66 | 0.48 |
| 3:AC:79:LYS:O | 3:AC:81:GLY:N | 2.46 | 0.48 |
| 5:AE:80:THR:OG1 | 5:AE:81:LEU:N | 2.45 | 0.48 |
| 5:AE:109:GLY:O | 5:AE:110:ALA:HB2 | 2.12 | 0.48 |
| 14:AN:41:ARG:HD3 | 14:AN:42:TRP:CH2 | 2.49 | 0.48 |
| 17:AQ:12:VAL:O | 17:AQ:13:VAL:CB | 2.61 | 0.48 |
| 21:AU:4:ILE:N | 21:AU:19:PHE:CD1 | 2.80 | 0.48 |
| 22:BA:186:G:O2' | 22:BA:187:G:H5' | 2.13 | 0.48 |
| 22:BA:877:A:O2' | 22:BA:900:A:N6 | 2.45 | 0.48 |
| 22:BA:1838:C:C5 | 22:BA:1899:A:C5 | 3.00 | 0.48 |
| 32:BK:4:GLU:O | 32:BK:5:GLN:CB | 2.61 | 0.48 |
| 33:BL:81:ASP:O | 33:BL:83:ALA:N | 2.39 | 0.48 |
| 34:BM:132:THR:CG2 | 34:BM:133:LYS:N | 2.77 | 0.48 |
| 37:BP:31:TRP:CE2 | 37:BP:40:LEU:HD11 | 2.48 | 0.48 |
| 53:B5:40:GLU:O | 53:B5:42:VAL:N | 2.45 | 0.48 |
| 1:CA:145:G:N2 | 1:CA:146:G:C4 | 2.81 | 0.48 |
| 1:CA:246:A:C4 | 1:CA:279:A:C6 | 3.01 | 0.48 |
| 1:CA:458:U:H2' | 1:CA:459:A:C8 | 2.48 | 0.48 |
| 1:CA:946:A:H2' | 1:CA:947:G:C8 | 2.48 | 0.48 |
| 1:CA:963:G:C2 | 1:CA:973:G:C6 | 3.01 | 0.48 |
| 1:CA:1060:U:H5' | 10:CJ:53:ILE:HG23 | 1.95 | 0.48 |
| 4:CD:97:ARG:O | 4:CD:101:VAL:HG23 | 2.14 | 0.48 |
| 4:CD:107:PHE:N | 4:CD:107:PHE:CD1 | 2.80 | 0.48 |
| 5:CE:150:PRO:C | 5:CE:152:MET:H | 2.15 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:86:TYR:CD2 | 8:CH:124:GLU:HB2 | 2.48 | 0.48 |
| 9:CI:17:ALA:HA | 9:CI:67:VAL:HA | 1.94 | 0.48 |
| 17:CQ:21:ILE:HB | 17:CQ:48:ASP:OD1 | 2.12 | 0.48 |
| 21:CU:32:VAL:O | 21:CU:32:VAL:HG12 | 2.11 | 0.48 |
| 22:DA:193:U:C5 | 22:DA:194:G:N7 | 2.82 | 0.48 |
| 22:DA:242:G:N7 | 51:D3:3:LYS:O | 2.46 | 0.48 |
| 22:DA:449:A:H2' | 22:DA:450:G:H5' | 1.95 | 0.48 |
| 22:DA:655:A:H4' | 22:DA:656:G:OP1 | 2.11 | 0.48 |
| 22:DA:661:A:H2' | 22:DA:662:G:O4' | 2.12 | 0.48 |
| 22:DA:1011:G:O2' | 22:DA:1013:C:H5'' | 2.14 | 0.48 |
| 22:DA:1068:G:H2' | 22:DA:1096:A:C5' | 2.43 | 0.48 |
| 22:DA:1095:A:C2 | 22:DA:1096:A:C2 | 3.01 | 0.48 |
| 22:DA:2727:A:N1 | 22:DA:2728:U:C4 | 2.81 | 0.48 |
| 56:DA:3001:DOL:C43 | 56:DA:3001:DOL:C1 | 2.91 | 0.48 |
| 23:DB:50:A:H2' | 23:DB:51:G:O4' | 2.13 | 0.48 |
| 28:DG:96:ALA:N | 28:DG:128:GLN:O | 2.46 | 0.48 |
| 35:DN:106:ASP:O | 35:DN:107:ASN:C | 2.52 | 0.48 |
| 40:DS:70:LYS:O | 40:DS:107:VAL:HG23 | 2.14 | 0.48 |
| 42:DU:12:ILE:HG21 | 42:DU:80:ALA:HB2 | 1.95 | 0.48 |
| 1:AA:32:A:C2 | 1:AA:33:A:C5 | 3.01 | 0.48 |
| 1:AA:259:G:C2 | 1:AA:260:G:H1' | 2.48 | 0.48 |
| 1:AA:958:A:C6 | 1:AA:959:A:N1 | 2.82 | 0.48 |
| 1:AA:983:A:H5'' | 1:AA:984:C:OP2 | 2.13 | 0.48 |
| 1:AA:988:G:C6 | 1:AA:989:U:C4 | 3.01 | 0.48 |
| 1:AA:1210:C:C4 | 1:AA:1211:U:C4 | 3.02 | 0.48 |
| 1:AA:1362:A:H5'' | 1:AA:1363:A:OP2 | 2.14 | 0.48 |
| 2:AB:68:LEU:HD21 | 2:AB:92:VAL:HG23 | 1.95 | 0.48 |
| 2:AB:82:ASP:C | 2:AB:84:ALA:N | 2.64 | 0.48 |
| 3:AC:97:VAL:HB | 3:AC:98:PRO:HD2 | 1.94 | 0.48 |
| 3:AC:150:LYS:HG3 | 3:AC:201:TRP:CE3 | 2.48 | 0.48 |
| 6:AF:3:HIS:H | 6:AF:92:THR:HG23 | 1.78 | 0.48 |
| 9:AI:57:MET:C | 9:AI:59:GLU:H | 2.17 | 0.48 |
| 10:AJ:42:LEU:HG | 10:AJ:43:PRO:HD2 | 1.94 | 0.48 |
| 10:AJ:61:ALA:O | 10:AJ:62:ARG:HB2 | 2.11 | 0.48 |
| 14:AN:90:ARG:NH1 | 14:AN:92:GLU:OE2 | 2.46 | 0.48 |
| 19:AS:29:LYS:CB | 19:AS:30:PRO:HD2 | 2.43 | 0.48 |
| 21:AU:16:LEU:HA | 21:AU:18:ARG:CZ | 2.42 | 0.48 |
| 22:BA:589:U:H2' | 22:BA:590:A:C8 | 2.49 | 0.48 |
| 22:BA:1353:A:O2' | 22:BA:1354:A:H5' | 2.13 | 0.48 |
| 22:BA:1746:A:H2' | 22:BA:1747:U:H6 | 1.75 | 0.48 |
| 22:BA:2825:G:C3' | 22:BA:2826:A:H5' | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BC:36:LYS:O | 24:BC:37:ASN:CB | 2.62 | 0.48 |
| 26:BE:77:ILE:O | 26:BE:77:ILE:HG13 | 2.13 | 0.48 |
| 32:BK:41:ILE:HD11 | 32:BK:58:LEU:CD2 | 2.44 | 0.48 |
| 36:BO:15:ARG:NE | 36:BO:93:ASP:OD1 | 2.45 | 0.48 |
| 1:CA:169:C:H2' | 1:CA:170:U:C6 | 2.47 | 0.48 |
| 1:CA:195:A:C6 | 1:CA:196:A:N1 | 2.81 | 0.48 |
| 1:CA:457:G:C6 | 1:CA:458:U:N3 | 2.81 | 0.48 |
| 1:CA:805:C:C2 | 1:CA:806:C:C5 | 3.02 | 0.48 |
| 1:CA:932:C:OP1 | 7:CG:4:ARG:HB3 | 2.13 | 0.48 |
| 2:CB:91:PHE:CD2 | 2:CB:150:GLY:HA3 | 2.47 | 0.48 |
| 2:CB:141:LEU:O | 2:CB:142:GLU:C | 2.52 | 0.48 |
| 3:CC:62:LYS:O | 3:CC:97:VAL:HB | 2.14 | 0.48 |
| 5:CE:149:SER:OG | 5:CE:152:MET:HB2 | 2.13 | 0.48 |
| 12:CL:86:ARG:NH1 | 12:CL:88:LYS:HA | 2.28 | 0.48 |
| 17:CQ:13:VAL:HG13 | 17:CQ:22:VAL:HG13 | 1.94 | 0.48 |
| 17:CQ:52:GLU:CD | 17:CQ:75:LEU:HD21 | 2.34 | 0.48 |
| 22:DA:116:C:O2' | 22:DA:126:A:C2' | 2.61 | 0.48 |
| 22:DA:158:U:C4 | 22:DA:159:G:C5 | 3.01 | 0.48 |
| 22:DA:801:G:C8 | 26:DE:49:ARG:HG3 | 2.49 | 0.48 |
| 22:DA:1223:G:N2 | 22:DA:1225:G:H3' | 2.28 | 0.48 |
| 22:DA:1355:G:C5 | 22:DA:1377:G:N2 | 2.81 | 0.48 |
| 22:DA:1568:G:N3 | 24:DC:58:HIS:CE1 | 2.81 | 0.48 |
| 22:DA:2199:A:C5 | 22:DA:2225:A:N1 | 2.82 | 0.48 |
| 22:DA:2409:G:H2' | 22:DA:2410:G:O4' | 2.13 | 0.48 |
| 22:DA:2451:A:C2 | 56:DA:3001:DOL:C12 | 2.97 | 0.48 |
| 22:DA:2656:U:OP2 | 22:DA:2664:G:N1 | 2.41 | 0.48 |
| 22:DA:2693:G:N2 | 22:DA:2717:C:C2 | 2.81 | 0.48 |
| 22:DA:2784:U:H4' | 25:DD:42:ASN:O | 2.13 | 0.48 |
| 25:DD:28:GLU:HA | 25:DD:185:ASN:O | 2.13 | 0.48 |
| 31:DJ:84:ILE:O | 31:DJ:84:ILE:HG13 | 2.13 | 0.48 |
| 49:D1:39:PHE:CG | 49:D1:40:ASP:N | 2.82 | 0.48 |
| 1:AA:57:G:H2' | 1:AA:58:C:C6 | 2.48 | 0.48 |
| 1:AA:104:G:C2 | 1:AA:105:G:C5 | 3.02 | 0.48 |
| 1:AA:765:G:C6 | 1:AA:812:G:C4 | 3.01 | 0.48 |
| 1:AA:781:A:C5 | 1:AA:802:A:C2 | 3.01 | 0.48 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.48 | 0.48 |
| 1:AA:1394:A:C5 | 1:AA:1501:C:H4' | 2.48 | 0.48 |
| 1:AA:1401:G:C2 | 1:AA:1402:C:H1' | 2.49 | 0.48 |
| 4:AD:36:GLN:O | 4:AD:37:ALA:HB2 | 2.13 | 0.48 |
| 7:AG:48:GLU:O | 7:AG:51:ALA:HB3 | 2.12 | 0.48 |
| 11:AK:22:HIS:N | 11:AK:33:THR:O | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AN:46:LEU:C | 14:AN:46:LEU:HD12 | 2.34 | 0.48 |
| 15:AO:70:LEU:HD21 | 15:AO:77:ARG:HB2 | 1.96 | 0.48 |
| 16:AP:77:GLU:C | 16:AP:79:ASN:H | 2.16 | 0.48 |
| 19:AS:42:PRO:O | 19:AS:45:ILE:HG13 | 2.13 | 0.48 |
| 20:AT:66:LEU:HD12 | 20:AT:66:LEU:C | 2.34 | 0.48 |
| 22:BA:39:G:H2' | 22:BA:40:U:C6 | 2.48 | 0.48 |
| 22:BA:141:G:N1 | 41:BT:1:MET:CE | 2.77 | 0.48 |
| 22:BA:1132:U:C3' | 22:BA:1133:A:H5'' | 2.42 | 0.48 |
| 22:BA:1289:C:O2' | 22:BA:1330:C:H4' | 2.13 | 0.48 |
| 22:BA:2355:G:O3' | 44:BW:24:LYS:NZ | 2.45 | 0.48 |
| 29:BH:97:ARG:HD3 | 1:CA:370:C:H5' | 1.95 | 0.48 |
| 37:BP:58:ALA:HB1 | 37:BP:74:PHE:O | 2.13 | 0.48 |
| 53:B5:83:LYS:HB3 | 53:B5:87:ALA:CB | 2.44 | 0.48 |
| 1:CA:509:A:N3 | 1:CA:543:U:O2' | 2.39 | 0.48 |
| 1:CA:860:A:N6 | 1:CA:861:G:C2 | 2.81 | 0.48 |
| 1:CA:1361:G:H2' | 1:CA:1362:A:H5'' | 1.96 | 0.48 |
| 2:CB:19:GLN:O | 2:CB:38:VAL:HG23 | 2.13 | 0.48 |
| 5:CE:96:MET:HE3 | 5:CE:111:MET:HE3 | 1.95 | 0.48 |
| 7:CG:65:ALA:O | 7:CG:127:ALA:HB1 | 2.14 | 0.48 |
| 8:CH:86:TYR:CE2 | 8:CH:124:GLU:HB2 | 2.49 | 0.48 |
| 10:CJ:7:ARG:HD3 | 10:CJ:75:ASP:OD1 | 2.13 | 0.48 |
| 21:CU:40:LYS:N | 21:CU:41:PRO:CD | 2.76 | 0.48 |
| 22:DA:249:C:P | 22:DA:2394:C:HO2' | 2.36 | 0.48 |
| 22:DA:410:G:H2' | 22:DA:2407:A:C8 | 2.47 | 0.48 |
| 22:DA:543:G:C2 | 22:DA:551:G:C5 | 3.01 | 0.48 |
| 22:DA:1350:C:C2 | 22:DA:1382:G:C2 | 3.01 | 0.48 |
| 22:DA:1596:A:C6 | 22:DA:1597:A:C6 | 3.01 | 0.48 |
| 22:DA:1688:U:H1' | 22:DA:1701:A:C6 | 2.49 | 0.48 |
| 22:DA:2134:A:N3 | 22:DA:2159:G:H1' | 2.28 | 0.48 |
| 22:DA:2562:U:C2' | 22:DA:2563:U:H5' | 2.43 | 0.48 |
| 24:DC:252:THR:HG22 | 24:DC:253:LYS:N | 2.28 | 0.48 |
| 28:DG:89:LEU:CD1 | 28:DG:162:VAL:HG22 | 2.44 | 0.48 |
| 29:DH:127:GLU:HG3 | 29:DH:144:VAL:O | 2.13 | 0.48 |
| 31:DJ:71:ASP:O | 31:DJ:73:VAL:CG2 | 2.62 | 0.48 |
| 36:DO:79:ALA:O | 36:DO:83:LEU:HG | 2.13 | 0.48 |
| 41:DT:35:ALA:O | 41:DT:36:LYS:C | 2.51 | 0.48 |
| 1:AA:119:A:C4 | 1:AA:240:G:N7 | 2.81 | 0.48 |
| 1:AA:895:G:H2' | 1:AA:896:C:C6 | 2.49 | 0.48 |
| 1:AA:1004:A:H2' | 1:AA:1005:A:O4' | 2.14 | 0.48 |
| 1:AA:1064:G:O4' | 1:AA:1066:C:C6 | 2.66 | 0.48 |
| 1:AA:1157:A:C2 | 1:AA:1181:G:C4 | 3.02 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:64:LYS:C | 2:AB:64:LYS:HD3 | 2.34 | 0.48 |
| 4:AD:124:MET:HG3 | 4:AD:146:ARG:HG2 | 1.96 | 0.48 |
| 6:AF:3:HIS:N | 6:AF:92:THR:HG23 | 2.29 | 0.48 |
| 8:AH:18:GLN:O | 8:AH:21:ASN:N | 2.47 | 0.48 |
| 10:AJ:35:GLN:OE1 | 10:AJ:35:GLN:HA | 2.14 | 0.48 |
| 12:AL:22:PRO:C | 12:AL:24:LEU:N | 2.67 | 0.48 |
| 22:BA:181:A:C2 | 22:BA:182:A:C4 | 3.01 | 0.48 |
| 22:BA:1866:A:C6 | 22:BA:1876:A:N7 | 2.82 | 0.48 |
| 22:BA:2591:C:H2' | 22:BA:2592:G:C8 | 2.49 | 0.48 |
| 22:BA:2847:U:C2' | 22:BA:2848:G:H5' | 2.44 | 0.48 |
| 24:BC:22:PRO:C | 24:BC:24:LEU:H | 2.17 | 0.48 |
| 35:BN:45:ARG:HG2 | 35:BN:95:THR:HG21 | 1.96 | 0.48 |
| 39:BR:14:VAL:HG11 | 39:BR:98:ILE:HG13 | 1.95 | 0.48 |
| 39:BR:49:ILE:CG2 | 39:BR:52:PRO:C | 2.82 | 0.48 |
| 39:BR:74:ILE:N | 39:BR:74:ILE:CD1 | 2.77 | 0.48 |
| 42:BU:96:PHE:O | 42:BU:100:SER:HA | 2.13 | 0.48 |
| 48:B0:48:TYR:CZ | 48:B0:53:LYS:HD2 | 2.48 | 0.48 |
| 1:CA:309:A:O2' | 1:CA:607:A:N1 | 2.33 | 0.48 |
| 1:CA:1114:C:C2 | 1:CA:1187:G:N2 | 2.82 | 0.48 |
| 1:CA:1240:U:H5' | 1:CA:1241:G:C8 | 2.48 | 0.48 |
| 1:CA:1259:C:N4 | 1:CA:1260:G:C5 | 2.82 | 0.48 |
| 1:CA:1302:C:C4 | 13:CM:17:ILE:CD1 | 2.97 | 0.48 |
| 1:CA:1328:C:H5'' | 13:CM:28:THR:HG21 | 1.94 | 0.48 |
| 1:CA:1394:A:C5 | 1:CA:1501:C:H4' | 2.48 | 0.48 |
| 9:CI:25:ASN:O | 9:CI:27:LYS:N | 2.45 | 0.48 |
| 12:CL:22:PRO:O | 12:CL:24:LEU:N | 2.41 | 0.48 |
| 16:CP:70:ARG:O | 16:CP:74:LEU:HD23 | 2.14 | 0.48 |
| 16:CP:78:VAL:HG22 | 16:CP:78:VAL:O | 2.14 | 0.48 |
| 20:CT:25:ARG:HD2 | 20:CT:29:ARG:NH1 | 2.29 | 0.48 |
| 22:DA:517:C:O2' | 22:DA:518:G:O5' | 2.30 | 0.48 |
| 22:DA:654:A:H3' | 22:DA:654:A:N3 | 2.27 | 0.48 |
| 22:DA:842:U:C4 | 22:DA:843:G:N7 | 2.81 | 0.48 |
| 22:DA:919:U:H2' | 22:DA:920:A:O4' | 2.13 | 0.48 |
| 22:DA:1338:G:H4' | 41:DT:18:GLU:OE2 | 2.13 | 0.48 |
| 22:DA:1344:U:HO2' | 22:DA:1345:C:P | 2.32 | 0.48 |
| 22:DA:1906:G:C8 | 22:DA:1929:G:H2' | 2.49 | 0.48 |
| 22:DA:2062:A:C8 | 54:D6:1:MHW:CD | 2.97 | 0.48 |
| 22:DA:2223:G:C2' | 22:DA:2224:G:H5' | 2.43 | 0.48 |
| 22:DA:2520:C:O2' | 22:DA:2565:A:O2' | 2.25 | 0.48 |
| 22:DA:2815:C:HO2' | 48:D0:41:HIS:CE1 | 2.31 | 0.48 |
| 22:DA:2840:C:H2' | 22:DA:2841:C:C6 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DB:76:G:OP1 | 43:DV:9:ARG:NH2 | 2.47 | 0.48 |
| 24:DC:107:PRO:HB3 | 24:DC:142:HIS:CE1 | 2.49 | 0.48 |
| 25:DD:15:PHE:CD2 | 37:DP:78:SER:HA | 2.49 | 0.48 |
| 33:DL:116:VAL:O | 33:DL:116:VAL:HG13 | 2.13 | 0.48 |
| 40:DS:7:HIS:HB2 | 40:DS:50:VAL:HG21 | 1.96 | 0.48 |
| 45:DX:54:LYS:O | 45:DX:57:ARG:N | 2.46 | 0.48 |
| 49:D1:9:ILE:CG2 | 49:D1:25:LYS:HB3 | 2.43 | 0.48 |
| 1:AA:82:G:O6 | 1:AA:87:C:N4 | 2.46 | 0.48 |
| 1:AA:1084:G:C5 | 1:AA:1085:U:C4 | 3.01 | 0.48 |
| 1:AA:1441:A:H2' | 1:AA:1442:G:O5' | 2.13 | 0.48 |
| 2:AB:91:PHE:CE2 | 2:AB:150:GLY:CA | 2.96 | 0.48 |
| 3:AC:7:PRO:HG2 | 3:AC:184:TYR:CG | 2.48 | 0.48 |
| 4:AD:191:LEU:O | 4:AD:192:SER:HB3 | 2.13 | 0.48 |
| 4:AD:197:GLU:O | 4:AD:200:ILE:N | 2.46 | 0.48 |
| 10:AJ:44:THR:HG22 | 10:AJ:70:HIS:HA | 1.95 | 0.48 |
| 17:AQ:17:MET:HB2 | 17:AQ:20:SER:HB3 | 1.95 | 0.48 |
| 22:BA:48:G:N2 | 22:BA:49:A:N1 | 2.61 | 0.48 |
| 22:BA:735:A:N7 | 22:BA:761:A:H2 | 2.10 | 0.48 |
| 22:BA:1798:U:OP2 | 24:BC:271:ARG:NH2 | 2.45 | 0.48 |
| 22:BA:2298:A:C6 | 22:BA:2321:U:O4 | 2.66 | 0.48 |
| 22:BA:2584:U:H2' | 22:BA:2585:U:H5' | 1.95 | 0.48 |
| 25:BD:26:VAL:HG22 | 25:BD:188:LEU:CD2 | 2.44 | 0.48 |
| 27:BF:48:LYS:O | 27:BF:51:ASP:HB2 | 2.14 | 0.48 |
| 27:BF:63:GLN:OE1 | 27:BF:95:ARG:HD2 | 2.14 | 0.48 |
| 30:BI:127:ARG:HA | 30:BI:130:GLU:CG | 2.44 | 0.48 |
| 31:BJ:42:ALA:O | 38:BQ:64:ARG:HG2 | 2.14 | 0.48 |
| 32:BK:20:MET:C | 32:BK:41:ILE:HG22 | 2.34 | 0.48 |
| 1:CA:32:A:C2 | 1:CA:33:A:C4 | 3.01 | 0.48 |
| 1:CA:585:G:C6 | 1:CA:586:C:C4 | 3.02 | 0.48 |
| 1:CA:722:G:H3' | 1:CA:722:G:N3 | 2.29 | 0.48 |
| 1:CA:745:G:H5'' | 1:CA:851:G:O2' | 2.13 | 0.48 |
| 1:CA:772:U:O2' | 1:CA:773:G:H5' | 2.14 | 0.48 |
| 1:CA:1088:G:C5 | 1:CA:1089:G:N7 | 2.82 | 0.48 |
| 1:CA:1306:A:H1' | 1:CA:1332:A:C5 | 2.49 | 0.48 |
| 3:CC:36:ASP:O | 3:CC:40:ARG:HG3 | 2.14 | 0.48 |
| 3:CC:61:ALA:O | 3:CC:62:LYS:HB2 | 2.14 | 0.48 |
| 5:CE:133:PRO:HA | 5:CE:136:VAL:HG13 | 1.96 | 0.48 |
| 7:CG:123:GLU:OE1 | 7:CG:123:GLU:HA | 2.13 | 0.48 |
| 13:CM:81:MET:O | 13:CM:83:LEU:N | 2.46 | 0.48 |
| 18:CR:32:TYR:CD2 | 18:CR:55:LEU:HD21 | 2.49 | 0.48 |
| 22:DA:396:G:OP2 | 45:DX:10:LYS:HG2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:532:A:N7 | 22:DA:2021:C:C2' | 2.77 | 0.48 |
| 22:DA:532:A:H2' | 22:DA:532:A:N3 | 2.27 | 0.48 |
| 22:DA:640:C:C4 | 22:DA:641:U:C5 | 3.02 | 0.48 |
| 22:DA:646:U:H3' | 22:DA:647:G:C4' | 2.44 | 0.48 |
| 22:DA:740:C:C5' | 22:DA:1784:A:H3' | 2.44 | 0.48 |
| 22:DA:769:U:C2 | 22:DA:770:G:C8 | 3.02 | 0.48 |
| 22:DA:1361:G:C6 | 22:DA:1371:G:C2 | 3.01 | 0.48 |
| 22:DA:1365:A:N3 | 22:DA:1365:A:H2' | 2.27 | 0.48 |
| 22:DA:1373:A:N6 | 22:DA:1374:G:C2 | 2.82 | 0.48 |
| 22:DA:1598:A:H2' | 22:DA:1599:U:C6 | 2.49 | 0.48 |
| 22:DA:1754:A:N6 | 22:DA:1755:A:C6 | 2.82 | 0.48 |
| 22:DA:1830:C:H5' | 24:DC:15:HIS:CD2 | 2.48 | 0.48 |
| 22:DA:2839:G:N2 | 22:DA:2880:C:C2 | 2.81 | 0.48 |
| 24:DC:157:SER:HB2 | 24:DC:160:THR:HG21 | 1.95 | 0.48 |
| 25:DD:104:VAL:O | 25:DD:105:LYS:HB2 | 2.13 | 0.48 |
| 25:DD:151:THR:HG22 | 25:DD:152:PRO:N | 2.29 | 0.48 |
| 26:DE:18:THR:HG22 | 26:DE:19:PHE:CD2 | 2.48 | 0.48 |
| 28:DG:158:LYS:O | 28:DG:159:GLY:C | 2.51 | 0.48 |
| 30:DI:49:ILE:O | 30:DI:50:GLU:HB2 | 2.13 | 0.48 |
| 35:DN:28:LEU:O | 35:DN:28:LEU:CG | 2.62 | 0.48 |
| 35:DN:38:LEU:HB3 | 35:DN:39:PRO:HD3 | 1.95 | 0.48 |
| 36:DO:115:LEU:O | 36:DO:117:PHE:N | 2.41 | 0.48 |
| 42:DU:7:ARG:CG | 42:DU:8:ASP:N | 2.76 | 0.48 |
| 45:DX:43:GLU:O | 45:DX:44:LYS:C | 2.52 | 0.48 |
| 49:D1:26:ASN:O | 49:D1:27:LYS:C | 2.52 | 0.48 |
| 1:AA:57:G:C5 | 1:AA:58:C:C4 | 3.01 | 0.48 |
| 1:AA:652:U:O2' | 1:AA:653:U:OP2 | 2.27 | 0.48 |
| 1:AA:1462:C:H2' | 1:AA:1463:U:O4' | 2.14 | 0.48 |
| 2:AB:15:HIS:ND1 | 2:AB:15:HIS:C | 2.66 | 0.48 |
| 2:AB:70:VAL:O | 2:AB:163:VAL:HA | 2.13 | 0.48 |
| 3:AC:206:GLU:O | 3:AC:207:ILE:HG22 | 2.14 | 0.48 |
| 13:AM:6:GLY:C | 13:AM:8:ASN:N | 2.66 | 0.48 |
| 14:AN:16:LEU:N | 14:AN:16:LEU:HD23 | 2.29 | 0.48 |
| 17:AQ:16:LYS:C | 17:AQ:17:MET:HE3 | 2.34 | 0.48 |
| 17:AQ:50:ASN:O | 17:AQ:51:ASN:C | 2.52 | 0.48 |
| 22:BA:55:G:C2 | 22:BA:56:A:C8 | 3.02 | 0.48 |
| 22:BA:528:A:C8 | 22:BA:528:A:C3' | 2.97 | 0.48 |
| 22:BA:1064:C:H4' | 30:BI:90:SER:HB2 | 1.94 | 0.48 |
| 22:BA:1080:A:H2' | 22:BA:1080:A:N3 | 2.28 | 0.48 |
| 22:BA:1086:A:O2' | 22:BA:1087:G:N7 | 2.47 | 0.48 |
| 22:BA:1319:C:C2' | 22:BA:1320:C:H5' | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1402:U:C2' | 22:BA:1403:A:O5' | 2.62 | 0.48 |
| 22:BA:1452:G:C4 | 22:BA:2702:G:C6 | 3.02 | 0.48 |
| 22:BA:1820:U:O4 | 24:BC:198:ALA:HB1 | 2.13 | 0.48 |
| 22:BA:2256:G:O2' | 22:BA:2257:U:H5' | 2.14 | 0.48 |
| 22:BA:2615:U:C2 | 48:B0:4:GLN:HA | 2.49 | 0.48 |
| 22:BA:2851:A:H2' | 22:BA:2852:G:O4' | 2.14 | 0.48 |
| 27:BF:121:SER:HB2 | 27:BF:128:TYR:CE1 | 2.49 | 0.48 |
| 37:BP:64:ILE:O | 37:BP:64:ILE:HG22 | 2.13 | 0.48 |
| 46:BY:45:GLN:O | 46:BY:46:VAL:CB | 2.62 | 0.48 |
| 49:B1:17:THR:HG22 | 49:B1:42:VAL:HG11 | 1.96 | 0.48 |
| 53:B5:100:ILE:HG22 | 53:B5:104:ILE:CB | 2.43 | 0.48 |
| 53:B5:122:GLY:CA | 53:B5:146:VAL:CB | 2.92 | 0.48 |
| 1:CA:374:A:H5'' | 1:CA:452:A:C2 | 2.47 | 0.48 |
| 1:CA:414:A:H2' | 1:CA:415:A:O4' | 2.14 | 0.48 |
| 1:CA:456:A:H2' | 1:CA:457:G:O4' | 2.14 | 0.48 |
| 1:CA:604:G:N7 | 1:CA:605:U:C5 | 2.82 | 0.48 |
| 1:CA:1123:U:O2' | 10:CJ:39:PRO:O | 2.28 | 0.48 |
| 1:CA:1134:G:H2' | 1:CA:1135:U:O4' | 2.14 | 0.48 |
| 1:CA:1490:U:C2' | 1:CA:1491:G:O4' | 2.62 | 0.48 |
| 2:CB:102:THR:HB | 2:CB:175:GLU:CG | 2.44 | 0.48 |
| 4:CD:29:ASP:O | 4:CD:30:THR:C | 2.52 | 0.48 |
| 4:CD:148:LYS:CD | 4:CD:148:LYS:H | 2.27 | 0.48 |
| 7:CG:46:ALA:HA | 7:CG:121:ALA:HB2 | 1.96 | 0.48 |
| 7:CG:71:PRO:HD2 | 7:CG:96:ARG:O | 2.14 | 0.48 |
| 9:CI:12:ARG:CZ | 9:CI:107:ASP:OD2 | 2.60 | 0.48 |
| 10:CJ:52:LEU:HB2 | 14:CN:81:ARG:HD2 | 1.96 | 0.48 |
| 22:DA:83:A:C2 | 22:DA:103:A:N7 | 2.82 | 0.48 |
| 22:DA:591:U:C2 | 22:DA:592:A:C8 | 3.02 | 0.48 |
| 22:DA:663:G:C6 | 22:DA:664:G:C5 | 3.02 | 0.48 |
| 22:DA:683:U:OP1 | 50:D2:26:ASN:HB3 | 2.14 | 0.48 |
| 22:DA:833:A:H2' | 22:DA:834:G:C8 | 2.48 | 0.48 |
| 22:DA:1668:A:C4 | 22:DA:1674:G:C8 | 3.02 | 0.48 |
| 22:DA:1845:G:P | 24:DC:256:LYS:HZ3 | 2.37 | 0.48 |
| 22:DA:2283:C:N3 | 22:DA:2389:G:C2 | 2.82 | 0.48 |
| 26:DE:23:PHE:CG | 26:DE:111:GLU:HG3 | 2.49 | 0.48 |
| 38:DQ:78:LYS:HE2 | 38:DQ:117:LEU:HD21 | 1.96 | 0.48 |
| 40:DS:58:ALA:O | 40:DS:62:ASP:O | 2.31 | 0.48 |
| 41:DT:77:ARG:O | 41:DT:78:SER:HB2 | 2.14 | 0.48 |
| 42:DU:82:ARG:O | 42:DU:97:LYS:HB2 | 2.14 | 0.48 |
| 43:DV:38:LEU:HD23 | 43:DV:40:ILE:CD1 | 2.43 | 0.48 |
| 1:AA:72:A:C2' | 1:AA:73:C:H5' | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:115:G:H1' | 1:AA:116:A:N7 | 2.29 | 0.48 |
| 1:AA:484:G:C5 | 1:AA:486:U:H1' | 2.48 | 0.48 |
| 1:AA:652:U:C2 | 1:AA:752:G:N2 | 2.81 | 0.48 |
| 1:AA:785:G:N2 | 1:AA:798:U:C2 | 2.81 | 0.48 |
| 1:AA:1108:G:H5' | 3:AC:176:HIS:CE1 | 2.49 | 0.48 |
| 1:AA:1157:A:C5 | 1:AA:1180:A:C6 | 3.01 | 0.48 |
| 1:AA:1210:C:N4 | 1:AA:1211:U:C4 | 2.82 | 0.48 |
| 1:AA:1348:U:C5 | 1:AA:1373:G:N2 | 2.81 | 0.48 |
| 3:AC:11:ARG:O | 3:AC:12:LEU:C | 2.53 | 0.48 |
| 4:AD:4:TYR:O | 4:AD:5:LEU:CB | 2.60 | 0.48 |
| 4:AD:103:TYR:HB2 | 4:AD:114:ALA:CB | 2.43 | 0.48 |
| 5:AE:133:PRO:HA | 5:AE:136:VAL:CG1 | 2.44 | 0.48 |
| 7:AG:68:ASN:O | 7:AG:138:ARG:HD3 | 2.14 | 0.48 |
| 7:AG:130:ASN:HA | 7:AG:135:VAL:HG11 | 1.96 | 0.48 |
| 10:AJ:30:LYS:HA | 10:AJ:34:ALA:HA | 1.95 | 0.48 |
| 10:AJ:56:HIS:C | 10:AJ:57:VAL:HG12 | 2.34 | 0.48 |
| 17:AQ:45:HIS:CG | 17:AQ:70:THR:CG2 | 2.97 | 0.48 |
| 21:AU:40:LYS:N | 21:AU:41:PRO:HD2 | 2.29 | 0.48 |
| 22:BA:585:G:H5'' | 22:BA:586:A:OP1 | 2.14 | 0.48 |
| 22:BA:1870:C:H2' | 22:BA:1871:A:C2 | 2.48 | 0.48 |
| 22:BA:2534:A:C2' | 22:BA:2535:G:O5' | 2.62 | 0.48 |
| 22:BA:2649:C:H2' | 22:BA:2650:U:C6 | 2.48 | 0.48 |
| 29:BH:103:VAL:HG21 | 29:BH:132:PHE:CZ | 2.49 | 0.48 |
| 46:BY:57:LEU:O | 46:BY:58:ASN:HB2 | 2.14 | 0.48 |
| 1:CA:29:U:H5' | 1:CA:296:U:OP1 | 2.14 | 0.48 |
| 1:CA:55:A:C6 | 1:CA:56:U:C2 | 3.01 | 0.48 |
| 1:CA:546:A:P | 4:CD:69:GLU:HB3 | 2.53 | 0.48 |
| 1:CA:749:A:O2' | 1:CA:750:C:H5' | 2.13 | 0.48 |
| 1:CA:1161:C:O2 | 1:CA:1176:A:C2 | 2.67 | 0.48 |
| 4:CD:192:SER:O | 4:CD:193:ALA:HB3 | 2.14 | 0.48 |
| 6:CF:6:ILE:HD12 | 6:CF:6:ILE:N | 2.28 | 0.48 |
| 13:CM:91:HIS:CD2 | 13:CM:97:VAL:HG21 | 2.49 | 0.48 |
| 14:CN:25:ALA:O | 14:CN:28:LYS:HG2 | 2.14 | 0.48 |
| 17:CQ:15:ASP:OD1 | 17:CQ:54:GLY:HA2 | 2.13 | 0.48 |
| 18:CR:57:ARG:HG2 | 18:CR:58:ALA:N | 2.27 | 0.48 |
| 21:CU:36:GLU:OE1 | 21:CU:36:GLU:HA | 2.13 | 0.48 |
| 22:DA:142:A:H2' | 22:DA:143:C:C6 | 2.48 | 0.48 |
| 22:DA:228:C:N3 | 22:DA:418:C:C4' | 2.77 | 0.48 |
| 22:DA:284:U:H2' | 22:DA:284:U:O2 | 2.13 | 0.48 |
| 22:DA:323:C:O2 | 22:DA:323:C:O4' | 2.32 | 0.48 |
| 22:DA:379:G:C6 | 22:DA:396:G:C6 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:487:C:C2 | 22:DA:494:G:N2 | 2.82 | 0.48 |
| 22:DA:593:U:N3 | 22:DA:594:U:C4 | 2.82 | 0.48 |
| 22:DA:600:G:C5' | 26:DE:27:LEU:HD22 | 2.43 | 0.48 |
| 22:DA:782:A:H4' | 22:DA:783:A:O5' | 2.14 | 0.48 |
| 22:DA:846:U:HO2' | 22:DA:847:U:P | 2.37 | 0.48 |
| 22:DA:1097:U:H1' | 30:DI:9:VAL:HG11 | 1.95 | 0.48 |
| 22:DA:1250:G:C5' | 38:DQ:6:ARG:HD2 | 2.44 | 0.48 |
| 22:DA:1470:A:H2' | 22:DA:1471:G:H5' | 1.96 | 0.48 |
| 22:DA:1675:C:N4 | 22:DA:1676:A:C2 | 2.82 | 0.48 |
| 22:DA:1870:C:C3' | 22:DA:1871:A:H5' | 2.44 | 0.48 |
| 22:DA:2234:G:C5 | 22:DA:2235:G:C8 | 3.02 | 0.48 |
| 22:DA:2507:C:C4 | 22:DA:2508:G:C5 | 3.02 | 0.48 |
| 23:DB:27:C:C5 | 23:DB:28:C:C4 | 3.02 | 0.48 |
| 23:DB:109:A:C5 | 23:DB:110:C:C4 | 3.01 | 0.48 |
| 26:DE:1:MET:HB2 | 26:DE:16:GLU:HA | 1.95 | 0.48 |
| 26:DE:25:GLU:OE1 | 33:DL:6:LEU:HA | 2.14 | 0.48 |
| 30:DI:114:ALA:O | 30:DI:115:ALA:HB2 | 2.13 | 0.48 |
| 33:DL:82:LEU:O | 33:DL:82:LEU:HG | 2.14 | 0.48 |
| 35:DN:36:THR:OG1 | 35:DN:37:THR:N | 2.46 | 0.48 |
| 36:DO:58:ILE:HG22 | 36:DO:58:ILE:O | 2.13 | 0.48 |
| 41:DT:2:ILE:HG23 | 41:DT:4:GLU:N | 2.28 | 0.48 |
| 46:DY:36:GLN:O | 46:DY:37:LEU:C | 2.52 | 0.48 |
| 1:AA:90:C:O2' | 1:AA:91:U:P | 2.72 | 0.48 |
| 1:AA:261:U:C5 | 20:AT:74:ARG:NH1 | 2.81 | 0.48 |
| 1:AA:448:A:C4 | 1:AA:487:A:C2 | 3.01 | 0.48 |
| 1:AA:509:A:O5' | 58:AA:1721:HOH:O | 2.20 | 0.48 |
| 1:AA:1018:G:N2 | 1:AA:1019:A:C8 | 2.81 | 0.48 |
| 1:AA:1387:G:C6 | 1:AA:1388:C:C4 | 3.02 | 0.48 |
| 2:AB:99:GLY:O | 2:AB:103:ASN:N | 2.46 | 0.48 |
| 4:AD:150:LYS:O | 4:AD:151:LYS:C | 2.51 | 0.48 |
| 5:AE:69:ARG:O | 5:AE:70:ASN:C | 2.52 | 0.48 |
| 8:AH:51:VAL:O | 8:AH:51:VAL:CG2 | 2.62 | 0.48 |
| 9:AI:81:HIS:NE2 | 9:AI:104:VAL:O | 2.46 | 0.48 |
| 10:AJ:49:PHE:N | 10:AJ:49:PHE:CD1 | 2.81 | 0.48 |
| 21:AU:15:ALA:O | 21:AU:16:LEU:HB2 | 2.14 | 0.48 |
| 22:BA:191:A:H2' | 22:BA:192:C:C6 | 2.49 | 0.48 |
| 22:BA:228:C:H4' | 22:BA:229:C:H5'' | 1.96 | 0.48 |
| 22:BA:503:A:C6 | 22:BA:505:A:C6 | 3.02 | 0.48 |
| 22:BA:523:C:O2' | 22:BA:524:G:H5' | 2.13 | 0.48 |
| 22:BA:1064:C:H4' | 30:BI:90:SER:CB | 2.43 | 0.48 |
| 22:BA:1352:U:O2' | 22:BA:1353:A:H5' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1406:U:C2 | 22:BA:1407:G:C8 | 3.01 | 0.48 |
| 22:BA:2151:U:H2' | 22:BA:2152:G:N7 | 2.28 | 0.48 |
| 22:BA:2451:A:C2 | 56:BA:3001:DOL:C8 | 2.97 | 0.48 |
| 22:BA:2555:U:H5'' | 22:BA:2556:C:OP2 | 2.14 | 0.48 |
| 34:BM:12:MET:HE3 | 34:BM:71:LYS:HG3 | 1.95 | 0.48 |
| 51:B3:15:LYS:HD3 | 51:B3:23:LYS:HE2 | 1.95 | 0.48 |
| 1:CA:119:A:H4' | 1:CA:120:A:O5' | 2.14 | 0.48 |
| 1:CA:509:A:C6 | 1:CA:510:A:N1 | 2.82 | 0.48 |
| 1:CA:620:C:C6 | 4:CD:132:ILE:HD13 | 2.49 | 0.48 |
| 1:CA:966:G:O2' | 9:CI:130:ARG:O | 2.31 | 0.48 |
| 7:CG:46:ALA:HB2 | 7:CG:117:ALA:HA | 1.95 | 0.48 |
| 10:CJ:41:PRO:O | 10:CJ:42:LEU:HB2 | 2.13 | 0.48 |
| 12:CL:42:PRO:HD3 | 12:CL:48:ALA:O | 2.14 | 0.48 |
| 17:CQ:13:VAL:CG1 | 17:CQ:22:VAL:HG13 | 2.44 | 0.48 |
| 20:CT:3:ASN:N | 20:CT:8:LYS:HD3 | 2.29 | 0.48 |
| 20:CT:67:ILE:HD12 | 20:CT:71:LYS:HE3 | 1.95 | 0.48 |
| 22:DA:7:G:H4' | 31:DJ:15:TRP:CH2 | 2.48 | 0.48 |
| 22:DA:126:A:C8 | 22:DA:127:A:C2 | 3.01 | 0.48 |
| 22:DA:183:C:O2' | 22:DA:432:A:O2' | 2.23 | 0.48 |
| 22:DA:200:U:C5 | 22:DA:201:C:C5 | 3.02 | 0.48 |
| 22:DA:218:A:C2 | 22:DA:219:A:C4 | 3.02 | 0.48 |
| 22:DA:306:U:O4 | 22:DA:307:G:C6 | 2.66 | 0.48 |
| 22:DA:457:A:N1 | 22:DA:470:A:H5'' | 2.29 | 0.48 |
| 22:DA:704:G:H1' | 22:DA:726:G:H22 | 1.79 | 0.48 |
| 22:DA:738:G:C6 | 22:DA:739:A:N1 | 2.82 | 0.48 |
| 22:DA:1124:G:O2' | 52:D4:37:GLN:O | 2.32 | 0.48 |
| 22:DA:1272:A:C6 | 22:DA:1618:A:H1' | 2.49 | 0.48 |
| 22:DA:1794:A:H1' | 22:DA:1900:A:C2 | 2.49 | 0.48 |
| 22:DA:1891:G:H2' | 22:DA:1892:C:O4' | 2.14 | 0.48 |
| 22:DA:2031:A:C6 | 22:DA:2498:C:H1' | 2.48 | 0.48 |
| 22:DA:2233:U:H2' | 22:DA:2234:G:C8 | 2.49 | 0.48 |
| 22:DA:2321:U:H5' | 22:DA:2322:A:OP2 | 2.14 | 0.48 |
| 22:DA:2415:G:C2 | 22:DA:2416:C:C2 | 3.02 | 0.48 |
| 22:DA:2562:U:H2' | 22:DA:2563:U:H5' | 1.95 | 0.48 |
| 22:DA:2755:C:C4 | 52:D4:19:ARG:NH1 | 2.82 | 0.48 |
| 33:DL:78:ARG:HB3 | 33:DL:113:ALA:CB | 2.44 | 0.48 |
| 1:AA:19:A:C2 | 1:AA:917:G:C5 | 3.02 | 0.47 |
| 1:AA:39:G:C2 | 1:AA:40:C:C6 | 3.02 | 0.47 |
| 1:AA:195:A:H1' | 1:AA:222:C:O2' | 2.13 | 0.47 |
| 1:AA:601:G:C2 | 1:AA:602:A:C4 | 3.02 | 0.47 |
| 1:AA:1012:A:C2 | 1:AA:1018:G:N7 | 2.82 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:164:ILE:O | 2:AB:186:ILE:HG12 | 2.13 | 0.47 |
| 5:AE:81:LEU:N | 5:AE:81:LEU:HD13 | 2.29 | 0.47 |
| 6:AF:53:LYS:O | 6:AF:54:LEU:CD1 | 2.62 | 0.47 |
| 9:AI:80:ARG:NH1 | 9:AI:103:PHE:CD1 | 2.82 | 0.47 |
| 14:AN:20:TYR:O | 14:AN:24:ARG:N | 2.47 | 0.47 |
| 15:AO:89:ARG:NH1 | 22:BA:714:U:C5 | 2.82 | 0.47 |
| 22:BA:164:C:H2' | 22:BA:165:A:O4' | 2.14 | 0.47 |
| 22:BA:608:A:C6 | 22:BA:609:A:C6 | 3.02 | 0.47 |
| 22:BA:609:A:H2' | 22:BA:610:C:O4' | 2.14 | 0.47 |
| 22:BA:726:G:O2' | 22:BA:727:A:OP2 | 2.28 | 0.47 |
| 22:BA:1250:G:H5'' | 38:BQ:6:ARG:HD3 | 1.96 | 0.47 |
| 22:BA:2187:U:H2' | 22:BA:2188:U:O4' | 2.14 | 0.47 |
| 22:BA:2849:U:N3 | 22:BA:2867:G:O4' | 2.43 | 0.47 |
| 28:BG:121:ILE:CD1 | 28:BG:141:ILE:HG22 | 2.43 | 0.47 |
| 29:BH:135:HIS:CD2 | 29:BH:137:GLU:HG3 | 2.48 | 0.47 |
| 36:BO:53:THR:HG23 | 36:BO:74:VAL:HG21 | 1.95 | 0.47 |
| 39:BR:51:VAL:CG2 | 39:BR:52:PRO:HD2 | 2.43 | 0.47 |
| 40:BS:8:ARG:O | 40:BS:9:HIS:HB2 | 2.14 | 0.47 |
| 41:BT:1:MET:HG3 | 41:BT:2:ILE:N | 2.29 | 0.47 |
| 49:B1:25:LYS:HD3 | 49:B1:52:ALA:O | 2.13 | 0.47 |
| 1:CA:203:G:N2 | 1:CA:215:C:C2 | 2.82 | 0.47 |
| 1:CA:429:U:O3' | 4:CD:22:LYS:HE3 | 2.14 | 0.47 |
| 1:CA:1201:A:H1' | 1:CA:1202:U:OP2 | 2.14 | 0.47 |
| 3:CC:81:GLY:O | 3:CC:83:ASP:N | 2.47 | 0.47 |
| 6:CF:4:TYR:CD2 | 6:CF:71:ILE:HG21 | 2.49 | 0.47 |
| 8:CH:78:VAL:N | 8:CH:126:ILE:O | 2.47 | 0.47 |
| 12:CL:44:LYS:HB3 | 12:CL:45:PRO:CD | 2.43 | 0.47 |
| 13:CM:43:VAL:HG23 | 13:CM:43:VAL:O | 2.14 | 0.47 |
| 13:CM:81:MET:O | 13:CM:82:ASP:C | 2.52 | 0.47 |
| 17:CQ:52:GLU:HG2 | 17:CQ:53:CYS:N | 2.29 | 0.47 |
| 22:DA:38:A:C2 | 22:DA:39:G:C4 | 3.02 | 0.47 |
| 22:DA:580:U:H4' | 38:DQ:31:VAL:HG11 | 1.96 | 0.47 |
| 22:DA:1544:A:C6 | 22:DA:1545:A:C6 | 3.02 | 0.47 |
| 22:DA:1682:G:C2 | 22:DA:1757:A:O4' | 2.67 | 0.47 |
| 22:DA:1845:G:P | 24:DC:256:LYS:NZ | 2.87 | 0.47 |
| 22:DA:2305:U:O4 | 22:DA:2306:C:N4 | 2.47 | 0.47 |
| 22:DA:2478:A:C8 | 22:DA:2529:G:C5 | 3.02 | 0.47 |
| 22:DA:2557:G:H2' | 22:DA:2558:C:C6 | 2.49 | 0.47 |
| 24:DC:108:LYS:HA | 24:DC:196:GLY:CA | 2.44 | 0.47 |
| 31:DJ:42:ALA:O | 38:DQ:64:ARG:HD3 | 2.14 | 0.47 |
| 36:DO:49:VAL:HG12 | 36:DO:50:ALA:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:DO:71:ALA:HB2 | 36:DO:102:ARG:HB2 | 1.96 | 0.47 |
| 36:DO:117:PHE:CD1 | 36:DO:117:PHE:C | 2.87 | 0.47 |
| 42:DU:60:GLU:HG2 | 42:DU:60:GLU:O | 2.14 | 0.47 |
| 1:AA:9:G:OP2 | 5:AE:126:LYS:HG3 | 2.14 | 0.47 |
| 1:AA:162:A:H1' | 1:AA:348:G:O2' | 2.14 | 0.47 |
| 1:AA:667:G:OP1 | 1:AA:732:C:O2' | 2.21 | 0.47 |
| 1:AA:923:A:N6 | 1:AA:1392:G:O6 | 2.46 | 0.47 |
| 1:AA:971:G:H1' | 1:AA:1365:G:O2' | 2.14 | 0.47 |
| 1:AA:1034:G:C6 | 1:AA:1035:A:C2 | 3.02 | 0.47 |
| 1:AA:1053:G:H4' | 1:AA:1054:C:H5'' | 1.96 | 0.47 |
| 1:AA:1123:U:O2' | 10:AJ:39:PRO:O | 2.30 | 0.47 |
| 6:AF:99:ALA:O | 6:AF:100:SER:CB | 2.62 | 0.47 |
| 8:AH:30:SER:OG | 8:AH:33:LYS:HG3 | 2.14 | 0.47 |
| 9:AI:26:GLY:N | 9:AI:59:GLU:HA | 2.29 | 0.47 |
| 20:AT:71:LYS:HD2 | 20:AT:74:ARG:HH21 | 1.80 | 0.47 |
| 22:BA:118:A:N3 | 22:BA:178:G:H1' | 2.29 | 0.47 |
| 22:BA:2038:G:H2' | 22:BA:2039:U:O4' | 2.13 | 0.47 |
| 22:BA:2192:U:C5 | 22:BA:2193:G:C8 | 3.02 | 0.47 |
| 22:BA:2748:A:H1' | 28:BG:67:THR:HG22 | 1.95 | 0.47 |
| 24:BC:44:ASN:C | 24:BC:44:ASN:OD1 | 2.51 | 0.47 |
| 25:BD:12:THR:HG21 | 37:BP:9:GLU:OE2 | 2.13 | 0.47 |
| 26:BE:48:THR:HG22 | 26:BE:86:ALA:HB3 | 1.96 | 0.47 |
| 26:BE:111:GLU:HG2 | 26:BE:114:ARG:NH1 | 2.30 | 0.47 |
| 27:BF:152:LEU:HD12 | 27:BF:153:ASP:N | 2.29 | 0.47 |
| 27:BF:175:PHE:HD1 | 27:BF:177:PHE:CE1 | 2.32 | 0.47 |
| 29:BH:117:LEU:HD23 | 29:BH:121:VAL:HA | 1.95 | 0.47 |
| 40:BS:59:GLU:HA | 40:BS:64:ALA:HB2 | 1.96 | 0.47 |
| 1:CA:1084:G:C5 | 1:CA:1085:U:C4 | 3.01 | 0.47 |
| 1:CA:1364:U:O2 | 1:CA:1364:U:C2' | 2.61 | 0.47 |
| 1:CA:1377:A:C6 | 7:CG:7:ILE:HD12 | 2.49 | 0.47 |
| 6:CF:37:HIS:CD2 | 6:CF:65:GLU:HB2 | 2.49 | 0.47 |
| 14:CN:51:LEU:HB3 | 14:CN:52:PRO:HD2 | 1.95 | 0.47 |
| 18:CR:37:GLY:O | 18:CR:63:ARG:NH2 | 2.48 | 0.47 |
| 19:CS:34:TRP:HA | 19:CS:52:HIS:HB2 | 1.96 | 0.47 |
| 22:DA:228:C:O2 | 22:DA:418:C:H4' | 2.15 | 0.47 |
| 22:DA:305:C:C2 | 22:DA:313:G:N1 | 2.82 | 0.47 |
| 22:DA:574:A:H4' | 22:DA:575:A:C5' | 2.43 | 0.47 |
| 22:DA:1027:A:C5 | 22:DA:1126:A:C2 | 3.02 | 0.47 |
| 22:DA:1250:G:H4' | 38:DQ:6:ARG:HD2 | 1.96 | 0.47 |
| 22:DA:1464:G:C2 | 22:DA:1465:G:C4 | 3.02 | 0.47 |
| 22:DA:1645:G:H5'' | 22:DA:1646:C:C5' | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1783:A:H5' | 22:DA:2608:G:H4' | 1.97 | 0.47 |
| 22:DA:1855:U:C4 | 22:DA:1856:U:C4 | 3.02 | 0.47 |
| 22:DA:2110:G:C6 | 22:DA:2120:G:C8 | 3.02 | 0.47 |
| 22:DA:2119:A:C6 | 22:DA:2170:A:C5 | 3.02 | 0.47 |
| 22:DA:2216:G:H2' | 22:DA:2217:G:C8 | 2.49 | 0.47 |
| 22:DA:2258:C:O2' | 22:DA:2427:C:OP2 | 2.27 | 0.47 |
| 22:DA:2301:C:C2 | 22:DA:2316:G:N2 | 2.82 | 0.47 |
| 22:DA:2747:G:O2' | 28:DG:67:THR:HG22 | 2.14 | 0.47 |
| 22:DA:2814:A:C6 | 22:DA:2815:C:C4 | 3.01 | 0.47 |
| 29:DH:117:LEU:HD11 | 29:DH:130:VAL:HG22 | 1.95 | 0.47 |
| 44:DW:49:ALA:O | 44:DW:50:ASN:HB2 | 2.13 | 0.47 |
| 1:AA:66:A:C2 | 1:AA:104:G:H1' | 2.49 | 0.47 |
| 1:AA:292:G:N7 | 1:AA:293:G:H1' | 2.30 | 0.47 |
| 1:AA:901:A:C5 | 1:AA:902:G:H1' | 2.50 | 0.47 |
| 1:AA:980:C:C5 | 1:AA:981:U:C5 | 3.02 | 0.47 |
| 1:AA:1418:A:N6 | 1:AA:1482:G:O2' | 2.46 | 0.47 |
| 3:AC:89:LYS:HG2 | 3:AC:90:VAL:N | 2.28 | 0.47 |
| 4:AD:107:PHE:CD1 | 4:AD:145:ILE:HD13 | 2.49 | 0.47 |
| 9:AI:30:ILE:O | 9:AI:33:ARG:N | 2.48 | 0.47 |
| 10:AJ:15:HIS:O | 10:AJ:17:LEU:N | 2.40 | 0.47 |
| 10:AJ:15:HIS:CG | 10:AJ:16:ARG:N | 2.83 | 0.47 |
| 10:AJ:63:ASP:HB3 | 10:AJ:65:TYR:CE2 | 2.50 | 0.47 |
| 15:AO:48:LYS:O | 15:AO:50:HIS:N | 2.47 | 0.47 |
| 19:AS:5:LEU:C | 19:AS:6:LYS:HG3 | 2.34 | 0.47 |
| 22:BA:196:A:N3 | 22:BA:196:A:H2' | 2.29 | 0.47 |
| 22:BA:1251:C:OP2 | 38:BQ:6:ARG:HD2 | 2.14 | 0.47 |
| 22:BA:1539:U:H2' | 22:BA:1540:G:C8 | 2.48 | 0.47 |
| 22:BA:1916:A:H2' | 22:BA:1917:U:H1' | 1.96 | 0.47 |
| 22:BA:2339:C:H2' | 22:BA:2340:A:H8 | 1.78 | 0.47 |
| 22:BA:2364:C:OP1 | 44:BW:55:ARG:NH1 | 2.47 | 0.47 |
| 22:BA:2721:A:C2 | 22:BA:2873:A:C5 | 3.02 | 0.47 |
| 22:BA:2747:G:O2' | 28:BG:67:THR:HB | 2.14 | 0.47 |
| 27:BF:88:LYS:HG3 | 27:BF:89:VAL:N | 2.29 | 0.47 |
| 38:BQ:24:TYR:O | 38:BQ:25:TYR:CB | 2.62 | 0.47 |
| 39:BR:43:ASN:N | 39:BR:45:GLU:O | 2.47 | 0.47 |
| 1:CA:552:U:N3 | 1:CA:553:A:N7 | 2.62 | 0.47 |
| 1:CA:1001:C:H2' | 1:CA:1002:G:C8 | 2.48 | 0.47 |
| 1:CA:1088:G:C6 | 1:CA:1089:G:N7 | 2.82 | 0.47 |
| 2:CB:102:THR:HB | 2:CB:175:GLU:HG3 | 1.97 | 0.47 |
| 8:CH:64:LYS:HE2 | 8:CH:71:VAL:HG21 | 1.96 | 0.47 |
| 9:CI:71:GLY:O | 9:CI:75:GLN:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:CK:24:HIS:O | 11:CK:30:THR:HA | 2.14 | 0.47 |
| 11:CK:92:GLY:O | 11:CK:93:ARG:C | 2.53 | 0.47 |
| 22:DA:56:A:C2 | 22:DA:115:C:C2 | 3.01 | 0.47 |
| 22:DA:89:A:C2 | 22:DA:90:U:C2 | 3.02 | 0.47 |
| 22:DA:523:C:H2' | 22:DA:524:G:C8 | 2.49 | 0.47 |
| 22:DA:616:A:OP2 | 58:DA:3291:HOH:O | 2.20 | 0.47 |
| 22:DA:792:A:H2' | 22:DA:2440:C:O2 | 2.13 | 0.47 |
| 22:DA:1131:G:OP1 | 31:DJ:82:GLY:HA2 | 2.13 | 0.47 |
| 22:DA:1203:U:OP2 | 22:DA:1204:A:H2' | 2.14 | 0.47 |
| 22:DA:1607:C:H4' | 22:DA:1608:A:C5' | 2.45 | 0.47 |
| 22:DA:1665:A:H5'' | 32:DK:66:LYS:HG3 | 1.95 | 0.47 |
| 22:DA:1692:U:O2' | 22:DA:1693:U:H2' | 2.14 | 0.47 |
| 22:DA:2199:A:C6 | 22:DA:2225:A:C5 | 3.01 | 0.47 |
| 22:DA:2432:A:N1 | 45:DX:21:ALA:HA | 2.29 | 0.47 |
| 22:DA:2505:G:OP2 | 56:DA:3001:DOL:C17 | 2.62 | 0.47 |
| 22:DA:2718:G:C2 | 22:DA:2719:G:H1' | 2.49 | 0.47 |
| 24:DC:67:PHE:CE2 | 24:DC:156:ARG:CZ | 2.97 | 0.47 |
| 29:DH:62:LEU:O | 29:DH:62:LEU:HD22 | 2.14 | 0.47 |
| 31:DJ:117:ALA:HA | 31:DJ:120:ARG:HD2 | 1.95 | 0.47 |
| 43:DV:9:ARG:HG2 | 43:DV:41:GLU:HB3 | 1.95 | 0.47 |
| 1:AA:631:C:C5' | 1:AA:632:U:O5' | 2.62 | 0.47 |
| 1:AA:720:C:H5'' | 18:AR:41:PRO:HA | 1.97 | 0.47 |
| 1:AA:1035:A:H2' | 1:AA:1036:A:C8 | 2.49 | 0.47 |
| 1:AA:1307:U:H2' | 1:AA:1308:U:C6 | 2.50 | 0.47 |
| 3:AC:175:LEU:HD12 | 3:AC:175:LEU:O | 2.14 | 0.47 |
| 7:AG:99:LEU:O | 7:AG:101:MET:N | 2.46 | 0.47 |
| 16:AP:50:THR:O | 16:AP:50:THR:CG2 | 2.56 | 0.47 |
| 20:AT:81:ALA:O | 20:AT:85:LYS:HG2 | 2.14 | 0.47 |
| 22:BA:416:U:H2' | 22:BA:417:C:C6 | 2.48 | 0.47 |
| 22:BA:851:C:O2' | 47:BZ:46:GLY:HA3 | 2.15 | 0.47 |
| 22:BA:1072:C:C2 | 22:BA:1093:G:O6 | 2.67 | 0.47 |
| 29:BH:116:ARG:O | 29:BH:118:PRO:HD3 | 2.14 | 0.47 |
| 30:BI:57:VAL:HG22 | 30:BI:58:VAL:N | 2.29 | 0.47 |
| 41:BT:88:LYS:O | 41:BT:89:GLU:CB | 2.63 | 0.47 |
| 49:B1:28:ARG:HG2 | 49:B1:28:ARG:O | 2.14 | 0.47 |
| 53:B5:172:ILE:O | 53:B5:173:HIS:CB | 2.62 | 0.47 |
| 1:CA:307:C:H5'' | 1:CA:308:C:OP2 | 2.15 | 0.47 |
| 1:CA:811:C:N4 | 1:CA:812:G:C6 | 2.82 | 0.47 |
| 2:CB:100:MET:HA | 2:CB:107:VAL:HG21 | 1.97 | 0.47 |
| 3:CC:87:LEU:HA | 3:CC:90:VAL:HG22 | 1.97 | 0.47 |
| 9:CI:42:GLU:O | 9:CI:45:ARG:NE | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:CM:22:ILE:HB | 13:CM:25:VAL:CG1 | 2.45 | 0.47 |
| 16:CP:75:ILE:HA | 16:CP:78:VAL:HG12 | 1.96 | 0.47 |
| 22:DA:291:G:N2 | 22:DA:350:G:C5 | 2.83 | 0.47 |
| 22:DA:500:G:N2 | 22:DA:502:A:C8 | 2.82 | 0.47 |
| 22:DA:579:G:C5' | 22:DA:2018:G:OP2 | 2.63 | 0.47 |
| 22:DA:586:A:N1 | 22:DA:809:G:O2' | 2.35 | 0.47 |
| 22:DA:830:G:C4 | 22:DA:2448:A:C5 | 3.03 | 0.47 |
| 22:DA:971:G:O2' | 22:DA:983:A:N3 | 2.43 | 0.47 |
| 22:DA:1016:G:C2 | 22:DA:1147:A:C2 | 3.02 | 0.47 |
| 22:DA:1046:A:O2' | 22:DA:1047:G:OP1 | 2.25 | 0.47 |
| 22:DA:1277:G:C6 | 22:DA:1294:U:C2 | 3.02 | 0.47 |
| 22:DA:1569:A:N1 | 22:DA:1570:A:C2 | 2.82 | 0.47 |
| 22:DA:1598:A:C6 | 22:DA:1599:U:N3 | 2.83 | 0.47 |
| 22:DA:1819:A:H4' | 22:DA:1820:U:H5'' | 1.96 | 0.47 |
| 22:DA:2110:G:N1 | 22:DA:2120:G:C8 | 2.82 | 0.47 |
| 32:DK:28:SER:O | 32:DK:29:HIS:HB2 | 2.13 | 0.47 |
| 33:DL:76:GLU:HG3 | 33:DL:76:GLU:O | 2.14 | 0.47 |
| 35:DN:58:ASP:HA | 35:DN:80:PHE:CD1 | 2.50 | 0.47 |
| 39:DR:68:ARG:HG3 | 39:DR:92:TRP:CZ3 | 2.49 | 0.47 |
| 48:D0:48:TYR:CE2 | 48:D0:53:LYS:HD3 | 2.50 | 0.47 |
| 1:AA:5:U:C6 | 1:AA:5:U:OP1 | 2.68 | 0.47 |
| 1:AA:19:A:C2 | 1:AA:917:G:C4 | 3.02 | 0.47 |
| 1:AA:704:A:C6 | 1:AA:705:G:C5 | 3.02 | 0.47 |
| 1:AA:858:G:O6 | 1:AA:869:G:C8 | 2.67 | 0.47 |
| 1:AA:1124:G:H2' | 1:AA:1145:A:C6 | 2.49 | 0.47 |
| 1:AA:1399:C:H4' | 1:AA:1400:C:H5'' | 1.96 | 0.47 |
| 2:AB:34:ALA:O | 2:AB:35:ARG:C | 2.52 | 0.47 |
| 3:AC:140:ASN:O | 3:AC:141:ALA:HB2 | 2.15 | 0.47 |
| 5:AE:155:ALA:HB1 | 8:AH:66:PHE:CE2 | 2.49 | 0.47 |
| 9:AI:99:ARG:O | 9:AI:102:GLY:N | 2.48 | 0.47 |
| 11:AK:89:PRO:HG3 | 21:AU:29:LEU:HD21 | 1.95 | 0.47 |
| 12:AL:22:PRO:C | 12:AL:24:LEU:H | 2.17 | 0.47 |
| 16:AP:75:ILE:HG22 | 16:AP:80:LYS:CE | 2.44 | 0.47 |
| 22:BA:449:A:H2' | 22:BA:450:G:O5' | 2.13 | 0.47 |
| 22:BA:511:U:C5 | 22:BA:512:G:C5 | 3.03 | 0.47 |
| 22:BA:1003:G:N2 | 22:BA:1004:U:C2 | 2.82 | 0.47 |
| 22:BA:1045:C:C4' | 22:BA:1046:A:H5' | 2.45 | 0.47 |
| 22:BA:1124:G:H1' | 52:B4:38:GLY:OXT | 2.14 | 0.47 |
| 22:BA:1959:G:C2' | 22:BA:1960:A:O5' | 2.62 | 0.47 |
| 22:BA:2228:G:H2' | 22:BA:2229:U:C6 | 2.50 | 0.47 |
| 22:BA:2344:U:H4' | 22:BA:2345:G:OP1 | 2.12 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BF:108:VAL:HG13 | 27:BF:114:PHE:CE2 | 2.49 | 0.47 |
| 28:BG:19:ILE:HD12 | 28:BG:45:HIS:HB2 | 1.96 | 0.47 |
| 33:BL:109:LYS:HG2 | 33:BL:126:ARG:HB2 | 1.96 | 0.47 |
| 34:BM:68:PHE:C | 34:BM:68:PHE:CD2 | 2.88 | 0.47 |
| 35:BN:116:VAL:O | 35:BN:116:VAL:HG13 | 2.14 | 0.47 |
| 48:B0:43:ILE:HG22 | 48:B0:49:TYR:HB2 | 1.96 | 0.47 |
| 1:CA:976:G:C8 | 1:CA:1361:G:O6 | 2.68 | 0.47 |
| 1:CA:1009:U:C2 | 1:CA:1021:A:N6 | 2.82 | 0.47 |
| 4:CD:102:VAL:HG13 | 4:CD:107:PHE:HB2 | 1.95 | 0.47 |
| 11:CK:61:PHE:C | 11:CK:61:PHE:CD2 | 2.88 | 0.47 |
| 11:CK:112:ASP:HB3 | 21:CU:4:ILE:CG2 | 2.44 | 0.47 |
| 12:CL:107:VAL:HG23 | 12:CL:117:TYR:HB3 | 1.97 | 0.47 |
| 13:CM:22:ILE:HB | 13:CM:25:VAL:HG12 | 1.96 | 0.47 |
| 22:DA:167:A:C2 | 22:DA:168:G:H1' | 2.50 | 0.47 |
| 22:DA:200:U:C6 | 22:DA:201:C:C6 | 3.02 | 0.47 |
| 22:DA:249:C:O2 | 51:D3:12:LYS:NZ | 2.48 | 0.47 |
| 22:DA:320:A:H4' | 22:DA:322:A:C8 | 2.50 | 0.47 |
| 22:DA:498:G:C2 | 22:DA:499:U:C6 | 3.03 | 0.47 |
| 22:DA:749:A:C6 | 22:DA:750:A:N7 | 2.82 | 0.47 |
| 22:DA:1096:A:OP2 | 22:DA:1096:A:C8 | 2.67 | 0.47 |
| 22:DA:1153:C:H5' | 38:DQ:62:ILE:HD13 | 1.95 | 0.47 |
| 22:DA:1257:C:C4 | 22:DA:1258:U:C4 | 3.02 | 0.47 |
| 22:DA:1361:G:N3 | 22:DA:1362:C:C6 | 2.82 | 0.47 |
| 22:DA:1565:C:C5 | 22:DA:1567:G:C6 | 3.02 | 0.47 |
| 22:DA:1662:U:O2 | 22:DA:2687:U:H5'' | 2.14 | 0.47 |
| 22:DA:1683:U:O5' | 22:DA:1683:U:H6 | 1.98 | 0.47 |
| 22:DA:1760:C:H2' | 22:DA:1761:C:O4' | 2.15 | 0.47 |
| 22:DA:1782:U:O4 | 22:DA:2586:U:H5 | 1.97 | 0.47 |
| 22:DA:2062:A:N7 | 54:D6:1:MHW:CD | 2.77 | 0.47 |
| 22:DA:2685:G:C4 | 22:DA:2686:G:C8 | 3.02 | 0.47 |
| 22:DA:2802:G:C6 | 22:DA:2803:G:C5 | 3.02 | 0.47 |
| 22:DA:2885:G:N2 | 48:D0:32:LYS:HA | 2.29 | 0.47 |
| 23:DB:66:A:N6 | 23:DB:107:G:H2' | 2.30 | 0.47 |
| 25:DD:176:ASP:HB2 | 25:DD:190:LYS:HB3 | 1.95 | 0.47 |
| 26:DE:5:LEU:O | 26:DE:6:LYS:C | 2.52 | 0.47 |
| 27:DF:117:LEU:HB3 | 27:DF:130:MET:SD | 2.54 | 0.47 |
| 30:DI:86:ILE:HD13 | 30:DI:89:GLY:N | 2.29 | 0.47 |
| 34:DM:53:MET:HG3 | 34:DM:54:THR:N | 2.30 | 0.47 |
| 40:DS:55:ILE:CG2 | 40:DS:66:ILE:CD1 | 2.93 | 0.47 |
| 1:AA:212:G:N2 | 1:AA:213:G:C4 | 2.82 | 0.47 |
| 1:AA:577:G:C8 | 1:AA:816:A:C6 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:21:ARG:HA | 2:AB:21:ARG:NE | 2.28 | 0.47 |
| 3:AC:146:ALA:C | 3:AC:148:GLY:H | 2.18 | 0.47 |
| 4:AD:68:LEU:N | 4:AD:68:LEU:CD2 | 2.77 | 0.47 |
| 5:AE:82:GLN:HG2 | 5:AE:150:PRO:HB3 | 1.96 | 0.47 |
| 6:AF:41:ASP:O | 6:AF:43:GLY:N | 2.47 | 0.47 |
| 7:AG:120:LEU:O | 7:AG:124:LEU:HD23 | 2.14 | 0.47 |
| 10:AJ:28:THR:O | 10:AJ:28:THR:HG22 | 2.15 | 0.47 |
| 20:AT:5:LYS:O | 20:AT:6:SER:C | 2.52 | 0.47 |
| 20:AT:83:ILE:HD12 | 20:AT:84:ASN:N | 2.29 | 0.47 |
| 22:BA:140:C:O4' | 22:BA:140:C:O2 | 2.33 | 0.47 |
| 22:BA:388:G:N7 | 22:BA:390:U:H2' | 2.29 | 0.47 |
| 22:BA:1199:U:H1' | 38:BQ:4:VAL:HG22 | 1.97 | 0.47 |
| 22:BA:1224:U:H4' | 39:BR:88:GLY:O | 2.14 | 0.47 |
| 22:BA:2040:G:H2' | 22:BA:2041:U:O4' | 2.13 | 0.47 |
| 22:BA:2063:C:O2 | 22:BA:2450:A:N1 | 2.47 | 0.47 |
| 22:BA:2131:U:OP2 | 22:BA:2132:U:C5 | 2.68 | 0.47 |
| 22:BA:2311:A:N7 | 27:BF:77:PHE:CD2 | 2.83 | 0.47 |
| 23:BB:37:C:C5 | 23:BB:38:C:C5 | 3.03 | 0.47 |
| 24:BC:161:TYR:CD2 | 24:BC:194:GLU:HG2 | 2.49 | 0.47 |
| 24:BC:250:VAL:HG12 | 24:BC:251:GLN:N | 2.30 | 0.47 |
| 25:BD:36:GLN:OE1 | 25:BD:67:HIS:HE1 | 1.97 | 0.47 |
| 29:BH:14:SER:O | 29:BH:15:LEU:CB | 2.61 | 0.47 |
| 29:BH:111:ALA:O | 29:BH:114:GLU:HB2 | 2.13 | 0.47 |
| 35:BN:32:GLU:HA | 35:BN:115:LEU:HD12 | 1.96 | 0.47 |
| 35:BN:65:LEU:HD11 | 35:BN:69:ARG:HH21 | 1.76 | 0.47 |
| 36:BO:41:ALA:HB2 | 36:BO:48:LEU:HD21 | 1.97 | 0.47 |
| 46:BY:46:VAL:O | 46:BY:49:ASP:N | 2.48 | 0.47 |
| 49:B1:19:HIS:HE1 | 49:B1:21:TYR:CE2 | 2.33 | 0.47 |
| 1:CA:74:A:C2 | 1:CA:75:G:C8 | 3.02 | 0.47 |
| 1:CA:155:A:C2 | 1:CA:167:A:C5 | 3.03 | 0.47 |
| 1:CA:782:A:N7 | 1:CA:783:C:C5 | 2.82 | 0.47 |
| 1:CA:991:U:H4' | 1:CA:992:U:H5'' | 1.96 | 0.47 |
| 1:CA:1007:U:C4 | 1:CA:1008:U:C5 | 3.02 | 0.47 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:C8 | 3.02 | 0.47 |
| 3:CC:130:PHE:CZ | 3:CC:131:ARG:HD2 | 2.50 | 0.47 |
| 9:CI:26:GLY:N | 9:CI:61:LEU:O | 2.48 | 0.47 |
| 12:CL:34:CYS:O | 12:CL:76:GLU:O | 2.33 | 0.47 |
| 22:DA:881:G:C2 | 22:DA:882:G:N7 | 2.83 | 0.47 |
| 22:DA:957:C:C4 | 22:DA:2459:A:H1' | 2.49 | 0.47 |
| 22:DA:1250:G:H5' | 38:DQ:6:ARG:CD | 2.45 | 0.47 |
| 22:DA:1306:C:C2 | 22:DA:1307:A:C8 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 22:DA:1574:C:N4 | 58:DA:3620:HOH:O | 2.47 | 0.47 |
| 22:DA:2164:C:H2' | 22:DA:2165:C:C5 | 2.50 | 0.47 |
| 22:DA:2202:U:H5'' | 22:DA:2203:U:OP1 | 2.14 | 0.47 |
| 22:DA:2847:U:O4 | 22:DA:2848:G:C6 | 2.67 | 0.47 |
| 26:DE:109:LEU:O | 26:DE:112:LEU:HB2 | 2.14 | 0.47 |
| 33:DL:90:VAL:HB | 33:DL:122:VAL:HA | 1.96 | 0.47 |
| 36:DO:78:VAL:HA | 36:DO:81:ARG:HB2 | 1.96 | 0.47 |
| 40:DS:15:GLN:NE2 | 48:D0:17:ARG:NH2 | 2.63 | 0.47 |
| 45:DX:56:MET:O | 45:DX:60:ASP:N | 2.44 | 0.47 |
| 1:AA:350:G:O2' | 1:AA:351:G:H5' | 2.15 | 0.47 |
| 1:AA:445:G:C4 | 1:AA:446:G:C8 | 3.03 | 0.47 |
| 1:AA:729:A:H2' | 1:AA:730:G:O4' | 2.14 | 0.47 |
| 1:AA:922:G:C6 | 1:AA:923:A:C6 | 3.02 | 0.47 |
| 1:AA:958:A:N1 | 19:AS:54:GLY:HA3 | 2.29 | 0.47 |
| 1:AA:1277:C:O2' | 1:AA:1279:G:C8 | 2.67 | 0.47 |
| 1:AA:1324:A:C2 | 1:AA:1325:C:C2 | 3.03 | 0.47 |
| 1:AA:1355:G:O2' | 1:AA:1356:G:H5' | 2.15 | 0.47 |
| 6:AF:92:THR:O | 6:AF:93:LYS:HG2 | 2.14 | 0.47 |
| 8:AH:7:ILE:HD12 | 8:AH:7:ILE:N | 2.29 | 0.47 |
| 11:AK:25:ALA:HA | 11:AK:30:THR:HG22 | 1.96 | 0.47 |
| 20:AT:67:ILE:CG1 | 20:AT:71:LYS:HG2 | 2.45 | 0.47 |
| 22:BA:136:G:N2 | 22:BA:144:A:C6 | 2.83 | 0.47 |
| 22:BA:197:A:N6 | 22:BA:2430:A:H2' | 2.29 | 0.47 |
| 22:BA:599:A:O2' | 22:BA:600:G:H5' | 2.15 | 0.47 |
| 22:BA:731:C:P | 58:BA:3693:HOH:O | 2.51 | 0.47 |
| 22:BA:864:G:C6 | 22:BA:865:C:N4 | 2.82 | 0.47 |
| 22:BA:877:A:N6 | 22:BA:899:A:C6 | 2.83 | 0.47 |
| 22:BA:877:A:C6 | 22:BA:899:A:C6 | 3.02 | 0.47 |
| 22:BA:983:A:N6 | 22:BA:984:A:C2 | 2.83 | 0.47 |
| 22:BA:1074:G:H2' | 22:BA:1075:C:C6 | 2.49 | 0.47 |
| 22:BA:1153:C:N4 | 22:BA:1154:G:N1 | 2.62 | 0.47 |
| 22:BA:1169:A:H2' | 22:BA:1170:C:O4' | 2.15 | 0.47 |
| 22:BA:1237:A:H4' | 22:BA:1238:G:OP1 | 2.15 | 0.47 |
| 22:BA:1259:G:O2' | 22:BA:1260:A:H5' | 2.15 | 0.47 |
| 22:BA:1421:G:N3 | 22:BA:1421:G:H2' | 2.29 | 0.47 |
| 22:BA:1696:G:C6 | 22:BA:1697:G:C4 | 3.02 | 0.47 |
| 22:BA:1794:A:H2' | 22:BA:1795:C:C6 | 2.48 | 0.47 |
| 22:BA:2056:G:C2 | 22:BA:2057:G:C8 | 3.02 | 0.47 |
| 22:BA:2393:U:H2' | 22:BA:2394:C:O5' | 2.14 | 0.47 |
| 56:BA:3001:DOL:H452 | 56:BA:3001:DOL:H483 | 1.54 | 0.47 |
| 23:BB:14:U:O2 | 23:BB:107:G:H4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BC:182:ARG:NH2 | 24:BC:266:PHE:HB3 | 2.30 | 0.47 |
| 25:BD:133:THR:CG2 | 25:BD:134:HIS:CD2 | 2.98 | 0.47 |
| 26:BE:155:GLU:OE1 | 26:BE:155:GLU:HA | 2.15 | 0.47 |
| 27:BF:104:ILE:HG22 | 27:BF:176:PRO:CD | 2.44 | 0.47 |
| 32:BK:41:ILE:HD11 | 32:BK:58:LEU:HD22 | 1.96 | 0.47 |
| 33:BL:14:LYS:HG2 | 33:BL:15:ALA:N | 2.29 | 0.47 |
| 33:BL:53:GLY:O | 33:BL:54:GLN:C | 2.52 | 0.47 |
| 33:BL:100:ILE:O | 33:BL:100:ILE:HG13 | 2.14 | 0.47 |
| 35:BN:14:SER:HA | 35:BN:17:ARG:NH1 | 2.30 | 0.47 |
| 35:BN:117:ASP:O | 35:BN:119:SER:N | 2.47 | 0.47 |
| 36:BO:31:THR:HG22 | 36:BO:34:HIS:H | 1.79 | 0.47 |
| 36:BO:67:ASN:HA | 36:BO:102:ARG:HD3 | 1.96 | 0.47 |
| 38:BQ:40:ILE:O | 38:BQ:44:GLN:HG3 | 2.15 | 0.47 |
| 39:BR:46:GLU:OE1 | 39:BR:46:GLU:O | 2.32 | 0.47 |
| 42:BU:39:ILE:CG2 | 42:BU:40:ASN:N | 2.78 | 0.47 |
| 43:BV:65:VAL:O | 43:BV:66:ASP:C | 2.53 | 0.47 |
| 46:BY:26:PHE:CE1 | 46:BY:30:MET:HG3 | 2.49 | 0.47 |
| 49:B1:39:PHE:HB2 | 49:B1:46:HIS:CE1 | 2.50 | 0.47 |
| 1:CA:91:U:C4 | 1:CA:92:U:C5 | 3.03 | 0.47 |
| 1:CA:161:A:H2' | 1:CA:162:A:C8 | 2.49 | 0.47 |
| 1:CA:369:G:OP2 | 1:CA:388:G:N1 | 2.45 | 0.47 |
| 1:CA:509:A:C6 | 1:CA:510:A:C6 | 3.03 | 0.47 |
| 1:CA:568:G:O6 | 12:CL:2:ALA:HB2 | 2.15 | 0.47 |
| 1:CA:771:G:C4 | 1:CA:809:G:N2 | 2.83 | 0.47 |
| 1:CA:920:U:H2' | 1:CA:921:U:H6 | 1.78 | 0.47 |
| 1:CA:957:U:O2 | 1:CA:959:A:C8 | 2.68 | 0.47 |
| 1:CA:991:U:H4' | 1:CA:992:U:OP1 | 2.15 | 0.47 |
| 1:CA:1151:A:H1' | 1:CA:1152:A:C8 | 2.49 | 0.47 |
| 1:CA:1202:U:N3 | 14:CN:82:ILE:HG21 | 2.29 | 0.47 |
| 1:CA:1224:U:N3 | 1:CA:1322:C:O2 | 2.47 | 0.47 |
| 1:CA:1288:A:N1 | 1:CA:1371:G:H1' | 2.29 | 0.47 |
| 1:CA:1458:G:O3' | 20:CT:23:SER:HA | 2.14 | 0.47 |
| 5:CE:13:GLU:OE1 | 5:CE:68:ARG:NH1 | 2.48 | 0.47 |
| 6:CF:9:MET:CE | 6:CF:59:TYR:CE1 | 2.98 | 0.47 |
| 9:CI:88:MET:O | 9:CI:88:MET:CG | 2.63 | 0.47 |
| 9:CI:95:ARG:HG2 | 9:CI:104:VAL:HG11 | 1.97 | 0.47 |
| 15:CO:27:VAL:O | 15:CO:31:LEU:HD13 | 2.15 | 0.47 |
| 18:CR:25:ASP:C | 18:CR:27:ALA:N | 2.67 | 0.47 |
| 22:DA:66:C:C4 | 22:DA:67:U:C5 | 3.03 | 0.47 |
| 22:DA:81:G:N7 | 22:DA:82:U:C4 | 2.83 | 0.47 |
| 22:DA:301:G:C2 | 22:DA:302:C:N3 | 2.83 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:686:U:H2' | 22:DA:788:A:N1 | 2.30 | 0.47 |
| 22:DA:703:U:C5 | 22:DA:704:G:C6 | 3.03 | 0.47 |
| 22:DA:770:G:C2 | 22:DA:771:G:C8 | 3.03 | 0.47 |
| 22:DA:915:C:N4 | 22:DA:916:G:C6 | 2.83 | 0.47 |
| 22:DA:1034:G:C6 | 22:DA:1035:U:N3 | 2.82 | 0.47 |
| 22:DA:1184:U:OP1 | 47:DZ:30:ARG:HD2 | 2.14 | 0.47 |
| 22:DA:1258:U:H2' | 22:DA:1259:G:C8 | 2.49 | 0.47 |
| 22:DA:1287:A:C2' | 22:DA:1288:G:H5' | 2.45 | 0.47 |
| 22:DA:1340:U:O2 | 22:DA:1340:U:H2' | 2.15 | 0.47 |
| 22:DA:1445:G:C2 | 22:DA:1547:C:N3 | 2.83 | 0.47 |
| 22:DA:1678:A:C4 | 22:DA:1679:A:C8 | 3.02 | 0.47 |
| 22:DA:1831:G:C5 | 22:DA:1832:C:C4 | 3.02 | 0.47 |
| 22:DA:2040:G:C6 | 22:DA:2041:U:C4 | 3.02 | 0.47 |
| 22:DA:2122:U:H2' | 22:DA:2123:G:O4' | 2.15 | 0.47 |
| 22:DA:2345:G:C6 | 22:DA:2347:C:N4 | 2.82 | 0.47 |
| 22:DA:2392:A:C8 | 22:DA:2429:G:C2 | 3.03 | 0.47 |
| 22:DA:2677:G:C2 | 22:DA:2731:G:C2 | 3.03 | 0.47 |
| 22:DA:2822:G:H2' | 22:DA:2823:A:H5'' | 1.97 | 0.47 |
| 25:DD:35:THR:O | 25:DD:36:GLN:HB3 | 2.15 | 0.47 |
| 25:DD:109:VAL:CG1 | 25:DD:201:LEU:HD22 | 2.44 | 0.47 |
| 26:DE:106:LYS:HG3 | 26:DE:200:LEU:HD23 | 1.95 | 0.47 |
| 29:DH:5:LEU:HD13 | 29:DH:13:GLY:HA3 | 1.96 | 0.47 |
| 32:DK:41:ILE:HD11 | 32:DK:86:LEU:HD22 | 1.97 | 0.47 |
| 33:DL:108:ALA:HB3 | 33:DL:125:LEU:HG | 1.96 | 0.47 |
| 37:DP:46:VAL:HG12 | 37:DP:47:VAL:N | 2.30 | 0.47 |
| 47:DZ:7:ILE:O | 47:DZ:36:VAL:N | 2.48 | 0.47 |
| 52:D4:1:MET:SD | 52:D4:34:LYS:HG2 | 2.54 | 0.47 |
| 1:AA:66:A:C6 | 1:AA:67:C:C5 | 3.03 | 0.47 |
| 1:AA:189:A:H2' | 1:AA:190:A:O4' | 2.15 | 0.47 |
| 1:AA:444:G:C6 | 1:AA:445:G:C5 | 3.02 | 0.47 |
| 1:AA:591:U:H2' | 1:AA:592:G:C8 | 2.50 | 0.47 |
| 1:AA:927:G:N1 | 1:AA:1391:U:C2 | 2.82 | 0.47 |
| 1:AA:947:G:C2 | 1:AA:948:C:C2 | 3.02 | 0.47 |
| 2:AB:188:ASP:HB2 | 2:AB:204:ASP:OD1 | 2.14 | 0.47 |
| 3:AC:47:LEU:HB3 | 3:AC:50:ALA:HB3 | 1.96 | 0.47 |
| 4:AD:51:TYR:CE2 | 4:AD:55:LEU:HD12 | 2.50 | 0.47 |
| 5:AE:39:VAL:HG22 | 5:AE:67:ALA:HB1 | 1.97 | 0.47 |
| 6:AF:92:THR:HG22 | 6:AF:93:LYS:N | 2.29 | 0.47 |
| 7:AG:56:LYS:O | 7:AG:57:SER:HB3 | 2.14 | 0.47 |
| 8:AH:10:MET:O | 8:AH:12:THR:N | 2.47 | 0.47 |
| 9:AI:58:VAL:O | 9:AI:59:GLU:HG2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:AL:39:THR:O | 12:AL:39:THR:OG1 | 2.23 | 0.47 |
| 16:AP:29:ASN:N | 16:AP:29:ASN:OD1 | 2.48 | 0.47 |
| 20:AT:57:ILE:HD12 | 20:AT:60:ARG:HD2 | 1.97 | 0.47 |
| 21:AU:18:ARG:HD2 | 21:AU:18:ARG:H | 1.80 | 0.47 |
| 22:BA:137:U:H2' | 22:BA:140:C:N1 | 2.30 | 0.47 |
| 22:BA:223:A:C4 | 22:BA:422:A:C8 | 3.03 | 0.47 |
| 22:BA:528:A:H2 | 22:BA:2043:C:C5' | 2.27 | 0.47 |
| 22:BA:591:U:HO2' | 51:B3:2:PRO:N | 2.12 | 0.47 |
| 22:BA:622:G:P | 58:BA:3293:HOH:O | 2.66 | 0.47 |
| 22:BA:975:A:C8 | 22:BA:990:A:N6 | 2.83 | 0.47 |
| 22:BA:1554:U:H3' | 22:BA:1555:G:C8 | 2.49 | 0.47 |
| 22:BA:1554:U:H4' | 22:BA:1555:G:OP2 | 2.15 | 0.47 |
| 22:BA:1946:U:H2' | 22:BA:1947:C:C6 | 2.50 | 0.47 |
| 22:BA:2323:G:C2' | 22:BA:2324:U:H5' | 2.45 | 0.47 |
| 22:BA:2714:G:C5 | 22:BA:2715:C:C5 | 3.03 | 0.47 |
| 25:BD:142:VAL:HB | 25:BD:143:PRO:HD2 | 1.97 | 0.47 |
| 28:BG:54:PRO:HG3 | 28:BG:62:TRP:NE1 | 2.30 | 0.47 |
| 33:BL:78:ARG:HG2 | 33:BL:113:ALA:HB3 | 1.97 | 0.47 |
| 34:BM:20:LEU:HD12 | 43:BV:81:PRO:HG2 | 1.96 | 0.47 |
| 34:BM:59:ARG:HG3 | 34:BM:59:ARG:O | 2.14 | 0.47 |
| 41:BT:17:SER:O | 41:BT:18:GLU:C | 2.53 | 0.47 |
| 53:B5:78:ILE:HG22 | 53:B5:123:ALA:HA | 1.96 | 0.47 |
| 1:CA:121:U:H3' | 1:CA:122:G:H5' | 1.97 | 0.47 |
| 1:CA:172:A:C5 | 1:CA:174:A:N7 | 2.83 | 0.47 |
| 1:CA:247:G:C6 | 1:CA:278:G:C2 | 3.03 | 0.47 |
| 1:CA:339:C:O2 | 1:CA:351:G:N2 | 2.47 | 0.47 |
| 1:CA:376:G:OP1 | 16:CP:6:LEU:N | 2.46 | 0.47 |
| 1:CA:653:U:C2 | 8:CH:56:LYS:HG2 | 2.49 | 0.47 |
| 1:CA:662:U:H2' | 1:CA:663:A:C8 | 2.50 | 0.47 |
| 1:CA:818:G:O2' | 1:CA:819:A:H5' | 2.14 | 0.47 |
| 1:CA:1000:A:C2 | 1:CA:1041:G:N2 | 2.83 | 0.47 |
| 1:CA:1262:C:C2' | 1:CA:1263:C:H5' | 2.45 | 0.47 |
| 3:CC:64:ILE:CG1 | 3:CC:66:VAL:HG23 | 2.45 | 0.47 |
| 22:DA:310:A:H5'' | 42:DU:15:THR:HB | 1.96 | 0.47 |
| 22:DA:396:G:H5'' | 45:DX:13:VAL:HG21 | 1.95 | 0.47 |
| 22:DA:511:U:O4 | 22:DA:512:G:N1 | 2.47 | 0.47 |
| 22:DA:1416:G:C4 | 22:DA:1417:C:C5 | 3.03 | 0.47 |
| 22:DA:1832:C:H2' | 22:DA:1833:C:O4' | 2.15 | 0.47 |
| 22:DA:1973:G:O6 | 22:DA:1974:C:N4 | 2.48 | 0.47 |
| 32:DK:97:THR:C | 32:DK:98:ARG:HG2 | 2.36 | 0.47 |
| 33:DL:90:VAL:N | 33:DL:121:THR:O | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:130:A:N7 | 17:AQ:65:ARG:HB2 | 2.29 | 0.47 |
| 1:AA:259:G:H2' | 1:AA:260:G:O4' | 2.15 | 0.47 |
| 1:AA:266:G:H3' | 17:AQ:69:LYS:HB3 | 1.96 | 0.47 |
| 1:AA:507:C:C4 | 1:AA:508:U:C4 | 3.03 | 0.47 |
| 1:AA:1121:U:H2' | 1:AA:1122:U:O4' | 2.15 | 0.47 |
| 1:AA:1122:U:C4 | 1:AA:1123:U:C5 | 3.02 | 0.47 |
| 1:AA:1135:U:H2' | 1:AA:1136:C:O5' | 2.14 | 0.47 |
| 1:AA:1144:G:N1 | 1:AA:1145:A:H2 | 2.13 | 0.47 |
| 1:AA:1157:A:N7 | 1:AA:1180:A:C6 | 2.83 | 0.47 |
| 1:AA:1161:C:H2' | 1:AA:1162:C:H6 | 1.80 | 0.47 |
| 2:AB:42:ASN:O | 2:AB:43:LEU:C | 2.53 | 0.47 |
| 2:AB:79:ALA:O | 2:AB:80:VAL:HG23 | 2.15 | 0.47 |
| 4:AD:29:ASP:C | 4:AD:30:THR:O | 2.51 | 0.47 |
| 4:AD:168:PRO:HB2 | 4:AD:171:LEU:HD11 | 1.97 | 0.47 |
| 5:AE:13:GLU:HB3 | 5:AE:39:VAL:HG12 | 1.97 | 0.47 |
| 5:AE:144:LEU:O | 5:AE:147:MET:HB3 | 2.15 | 0.47 |
| 9:AI:19:VAL:HA | 9:AI:65:ILE:HG22 | 1.97 | 0.47 |
| 10:AJ:36:VAL:HA | 10:AJ:76:ILE:HA | 1.95 | 0.47 |
| 10:AJ:63:ASP:OD1 | 14:AN:85:ARG:HD2 | 2.15 | 0.47 |
| 13:AM:64:VAL:O | 13:AM:64:VAL:CG1 | 2.62 | 0.47 |
| 14:AN:41:ARG:HB2 | 14:AN:42:TRP:CZ3 | 2.50 | 0.47 |
| 16:AP:1:MET:O | 16:AP:1:MET:SD | 2.72 | 0.47 |
| 22:BA:250:G:OP2 | 51:B3:13:ARG:NH1 | 2.47 | 0.47 |
| 22:BA:601:C:O2 | 22:BA:605:G:H4' | 2.15 | 0.47 |
| 22:BA:752:A:C2 | 22:BA:1781:U:C2 | 3.03 | 0.47 |
| 22:BA:1415:U:O2 | 22:BA:1415:U:H2' | 2.15 | 0.47 |
| 22:BA:1747:U:O2' | 22:BA:1748:C:H5' | 2.14 | 0.47 |
| 22:BA:1851:U:C4 | 22:BA:1852:U:C4 | 3.02 | 0.47 |
| 22:BA:1959:G:H2' | 22:BA:1960:A:O4' | 2.15 | 0.47 |
| 22:BA:2436:G:C2 | 22:BA:2437:G:C8 | 3.03 | 0.47 |
| 23:BB:48:U:H2' | 23:BB:49:C:C6 | 2.50 | 0.47 |
| 26:BE:149:ILE:HD12 | 26:BE:149:ILE:C | 2.34 | 0.47 |
| 30:BI:106:LEU:HA | 30:BI:109:ILE:HB | 1.97 | 0.47 |
| 30:BI:117:MET:SD | 30:BI:129:ILE:HD11 | 2.55 | 0.47 |
| 31:BJ:31:GLU:CG | 31:BJ:142:ILE:HD11 | 2.44 | 0.47 |
| 35:BN:32:GLU:OE1 | 35:BN:86:ARG:NH2 | 2.46 | 0.47 |
| 42:BU:12:ILE:CG2 | 42:BU:80:ALA:HB2 | 2.45 | 0.47 |
| 1:CA:160:A:C6 | 1:CA:346:G:O6 | 2.68 | 0.47 |
| 1:CA:179:A:H2' | 1:CA:180:U:C6 | 2.50 | 0.47 |
| 1:CA:740:U:O2' | 1:CA:741:G:H5' | 2.15 | 0.47 |
| 1:CA:1162:C:C2 | 1:CA:1175:G:N2 | 2.82 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1314:C:H2' | 1:CA:1315:U:C6 | 2.50 | 0.47 |
| 3:CC:59:ARG:HB2 | 3:CC:63:SER:O | 2.15 | 0.47 |
| 9:CI:122:ARG:O | 9:CI:124:ARG:N | 2.48 | 0.47 |
| 11:CK:31:ILE:HB | 11:CK:46:THR:HG22 | 1.97 | 0.47 |
| 11:CK:45:ALA:HB3 | 11:CK:70:CYS:HB2 | 1.96 | 0.47 |
| 13:CM:3:ARG:HG2 | 13:CM:7:ILE:HA | 1.97 | 0.47 |
| 13:CM:20:THR:HG22 | 13:CM:20:THR:O | 2.15 | 0.47 |
| 13:CM:45:ILE:HG22 | 13:CM:45:ILE:O | 2.15 | 0.47 |
| 16:CP:52:LEU:HD22 | 16:CP:57:ILE:HD11 | 1.97 | 0.47 |
| 21:CU:5:LYS:HD2 | 21:CU:5:LYS:O | 2.15 | 0.47 |
| 22:DA:279:A:N6 | 22:DA:361:G:C2' | 2.78 | 0.47 |
| 22:DA:302:C:C2 | 22:DA:303:G:C8 | 3.03 | 0.47 |
| 22:DA:389:G:O4' | 22:DA:2413:G:H5' | 2.15 | 0.47 |
| 22:DA:579:G:N2 | 22:DA:1262:A:C4 | 2.83 | 0.47 |
| 22:DA:746:U:O2' | 22:DA:2611:C:O2' | 2.24 | 0.47 |
| 22:DA:779:U:OP1 | 24:DC:49:ILE:HG13 | 2.15 | 0.47 |
| 22:DA:846:U:O2' | 22:DA:847:U:P | 2.73 | 0.47 |
| 22:DA:1076:C:O2' | 30:DI:93:PRO:HD2 | 2.15 | 0.47 |
| 22:DA:1361:G:C6 | 22:DA:1362:C:C5 | 3.03 | 0.47 |
| 22:DA:1532:A:C2 | 22:DA:1540:G:C6 | 3.02 | 0.47 |
| 22:DA:1726:C:H2' | 22:DA:1727:C:C6 | 2.50 | 0.47 |
| 22:DA:1768:C:H2' | 22:DA:1769:U:O4' | 2.15 | 0.47 |
| 22:DA:1783:A:C2 | 22:DA:2588:G:O4' | 2.67 | 0.47 |
| 22:DA:1835:G:C5 | 22:DA:1836:C:C5 | 3.03 | 0.47 |
| 22:DA:1857:G:N2 | 22:DA:1884:G:C4 | 2.83 | 0.47 |
| 22:DA:1980:G:C2 | 22:DA:1982:U:C4 | 3.03 | 0.47 |
| 22:DA:2074:U:O2' | 22:DA:2075:U:H5' | 2.15 | 0.47 |
| 22:DA:2291:U:OP1 | 22:DA:2380:C:O2' | 2.30 | 0.47 |
| 22:DA:2331:G:C6 | 22:DA:2332:C:C4 | 3.03 | 0.47 |
| 22:DA:2372:U:O4' | 49:D1:46:HIS:ND1 | 2.48 | 0.47 |
| 22:DA:2702:G:N7 | 22:DA:2703:C:C5 | 2.83 | 0.47 |
| 22:DA:2736:A:C4 | 22:DA:2737:G:C8 | 3.02 | 0.47 |
| 24:DC:184:VAL:O | 24:DC:185:GLU:C | 2.54 | 0.47 |
| 26:DE:77:ILE:O | 26:DE:77:ILE:HG13 | 2.14 | 0.47 |
| 32:DK:41:ILE:HD11 | 32:DK:86:LEU:CD2 | 2.44 | 0.47 |
| 37:DP:89:ARG:O | 37:DP:112:GLU:HA | 2.15 | 0.47 |
| 40:DS:47:VAL:CG2 | 40:DS:47:VAL:O | 2.63 | 0.47 |
| 40:DS:89:ALA:O | 40:DS:90:LYS:HB2 | 2.15 | 0.47 |
| 42:DU:13:VAL:HG21 | 42:DU:39:ILE:HG23 | 1.96 | 0.47 |
| 50:D2:18:PHE:O | 50:D2:19:ARG:C | 2.54 | 0.47 |
| 1:AA:223:A:C6 | 1:AA:224:U:C4 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1095:U:H2' | 1:AA:1096:C:O4' | 2.14 | 0.47 |
| 2:AB:91:PHE:CD2 | 2:AB:150:GLY:CA | 2.98 | 0.47 |
| 2:AB:144:LEU:O | 2:AB:148:LEU:HB2 | 2.15 | 0.47 |
| 3:AC:113:ALA:HA | 3:AC:200:VAL:HG21 | 1.97 | 0.47 |
| 4:AD:130:VAL:HG11 | 4:AD:135:TYR:CG | 2.50 | 0.47 |
| 5:AE:136:VAL:O | 5:AE:139:ALA:N | 2.47 | 0.47 |
| 7:AG:50:LEU:O | 7:AG:50:LEU:HD13 | 2.14 | 0.47 |
| 21:AU:34:ARG:NE | 21:AU:35:ARG:HB2 | 2.29 | 0.47 |
| 22:BA:277:G:C2' | 22:BA:361:G:O6 | 2.62 | 0.47 |
| 22:BA:630:G:H5'' | 22:BA:631:A:OP2 | 2.14 | 0.47 |
| 22:BA:1098:A:N7 | 22:BA:1099:G:O6 | 2.47 | 0.47 |
| 22:BA:1394:U:C2' | 22:BA:1395:A:O5' | 2.63 | 0.47 |
| 22:BA:1583:A:O2' | 22:BA:1584:U:O5' | 2.31 | 0.47 |
| 22:BA:1793:C:C2' | 22:BA:1794:A:H5' | 2.45 | 0.47 |
| 22:BA:1949:G:C2 | 22:BA:1958:C:O2 | 2.67 | 0.47 |
| 22:BA:2173:A:C8 | 22:BA:2174:C:C5 | 3.02 | 0.47 |
| 22:BA:2318:G:C5 | 22:BA:2319:G:C6 | 3.03 | 0.47 |
| 25:BD:13:ARG:HD2 | 25:BD:15:PHE:CZ | 2.50 | 0.47 |
| 25:BD:101:PHE:C | 25:BD:103:ASP:H | 2.17 | 0.47 |
| 25:BD:103:ASP:OD2 | 25:BD:104:VAL:N | 2.48 | 0.47 |
| 27:BF:25:VAL:O | 27:BF:28:VAL:HG12 | 2.14 | 0.47 |
| 27:BF:135:GLN:OE1 | 27:BF:135:GLN:N | 2.45 | 0.47 |
| 28:BG:155:GLU:OE2 | 28:BG:158:LYS:N | 2.47 | 0.47 |
| 34:BM:28:PHE:N | 34:BM:104:GLU:OE2 | 2.46 | 0.47 |
| 46:BY:6:LEU:HD22 | 46:BY:56:LEU:HD21 | 1.96 | 0.47 |
| 46:BY:21:LEU:O | 46:BY:22:LEU:O | 2.33 | 0.47 |
| 1:CA:202:G:H2' | 1:CA:203:G:O4' | 2.15 | 0.47 |
| 1:CA:445:G:C2 | 1:CA:490:C:C2 | 3.02 | 0.47 |
| 1:CA:734:G:C5 | 1:CA:735:C:C5 | 3.03 | 0.47 |
| 1:CA:802:A:C2 | 1:CA:803:G:C1' | 2.96 | 0.47 |
| 1:CA:892:A:C2 | 1:CA:907:A:C4 | 3.03 | 0.47 |
| 1:CA:927:G:N2 | 1:CA:1391:U:H1' | 2.30 | 0.47 |
| 1:CA:1315:U:O2' | 1:CA:1360:A:N3 | 2.35 | 0.47 |
| 3:CC:22:TRP:CH2 | 3:CC:32:ASN:HB3 | 2.50 | 0.47 |
| 3:CC:130:PHE:CZ | 3:CC:131:ARG:CD | 2.98 | 0.47 |
| 5:CE:157:ARG:HD3 | 5:CE:158:GLY:H | 1.78 | 0.47 |
| 12:CL:3:THR:CB | 12:CL:6:GLN:HG3 | 2.44 | 0.47 |
| 14:CN:35:ASN:O | 14:CN:42:TRP:CH2 | 2.68 | 0.47 |
| 15:CO:35:GLN:NE2 | 15:CO:39:LEU:CD2 | 2.78 | 0.47 |
| 20:CT:67:ILE:CD1 | 20:CT:71:LYS:HE3 | 2.45 | 0.47 |
| 21:CU:36:GLU:HG3 | 21:CU:37:PHE:H | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:185:G:N1 | 22:DA:212:G:C2 | 2.82 | 0.47 |
| 22:DA:711:G:C2 | 22:DA:721:A:N3 | 2.83 | 0.47 |
| 22:DA:1335:C:H2' | 22:DA:1336:A:C8 | 2.49 | 0.47 |
| 22:DA:1343:G:C5 | 22:DA:1344:U:O4 | 2.67 | 0.47 |
| 22:DA:1581:G:C6 | 22:DA:1582:C:N4 | 2.83 | 0.47 |
| 22:DA:1782:U:O4 | 22:DA:2586:U:C5 | 2.68 | 0.47 |
| 22:DA:1835:G:C4 | 22:DA:1836:C:C6 | 3.02 | 0.47 |
| 22:DA:2011:U:H2' | 22:DA:2012:G:O4' | 2.15 | 0.47 |
| 22:DA:2144:G:C2 | 22:DA:2146:C:O2 | 2.68 | 0.47 |
| 22:DA:2297:A:N1 | 22:DA:2321:U:H5 | 2.13 | 0.47 |
| 22:DA:2681:C:C2 | 22:DA:2724:U:O4 | 2.68 | 0.47 |
| 22:DA:2732:G:O2' | 22:DA:2733:A:H5' | 2.15 | 0.47 |
| 24:DC:72:ASP:HA | 24:DC:118:SER:O | 2.15 | 0.47 |
| 24:DC:87:ARG:HB3 | 24:DC:87:ARG:NH1 | 2.30 | 0.47 |
| 24:DC:232:HIS:NE2 | 24:DC:244:PRO:HA | 2.30 | 0.47 |
| 30:DI:28:LEU:HD13 | 30:DI:38:PHE:CD2 | 2.50 | 0.47 |
| 31:DJ:41:LYS:O | 31:DJ:44:TYR:N | 2.43 | 0.47 |
| 34:DM:76:LYS:HE3 | 34:DM:80:VAL:HG12 | 1.97 | 0.47 |
| 41:DT:28:ASN:HB3 | 41:DT:87:LEU:HB2 | 1.96 | 0.47 |
| 42:DU:41:LEU:HD12 | 42:DU:60:GLU:CG | 2.45 | 0.47 |
| 51:D3:7:VAL:O | 51:D3:10:ALA:N | 2.45 | 0.47 |
| 1:AA:132:C:H2' | 1:AA:133:U:O4' | 2.15 | 0.46 |
| 1:AA:542:G:OP1 | 4:AD:10:LYS:HE2 | 2.15 | 0.46 |
| 1:AA:654:G:H2' | 1:AA:655:A:H5' | 1.96 | 0.46 |
| 7:AG:55:GLY:C | 7:AG:57:SER:N | 2.68 | 0.46 |
| 7:AG:69:VAL:HG23 | 7:AG:100:ALA:HB1 | 1.97 | 0.46 |
| 10:AJ:57:VAL:CG2 | 10:AJ:58:ASN:N | 2.78 | 0.46 |
| 11:AK:74:VAL:C | 11:AK:76:GLU:N | 2.66 | 0.46 |
| 12:AL:44:LYS:CB | 12:AL:45:PRO:HD3 | 2.45 | 0.46 |
| 13:AM:114:LYS:CB | 13:AM:115:PRO:CD | 2.91 | 0.46 |
| 22:BA:111:A:N1 | 22:BA:112:U:C2 | 2.83 | 0.46 |
| 22:BA:259:G:O2' | 22:BA:260:G:H5' | 2.14 | 0.46 |
| 22:BA:287:G:C2 | 22:BA:354:A:C2 | 3.03 | 0.46 |
| 22:BA:1174:U:O2 | 22:BA:1174:U:O4' | 2.32 | 0.46 |
| 22:BA:1239:G:H2' | 22:BA:1240:U:O4' | 2.15 | 0.46 |
| 22:BA:1385:A:C2 | 22:BA:1386:C:C2 | 3.04 | 0.46 |
| 22:BA:1491:G:N2 | 22:BA:1500:G:H1' | 2.29 | 0.46 |
| 22:BA:1883:U:O4 | 22:BA:1884:G:N1 | 2.48 | 0.46 |
| 22:BA:2592:G:C6 | 22:BA:2593:U:C4 | 3.03 | 0.46 |
| 22:BA:2847:U:H2' | 22:BA:2848:G:H5' | 1.96 | 0.46 |
| 22:BA:2898:U:O2' | 22:BA:2899:A:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BI:65:ARG:NH1 | 30:BI:66:SER:OG | 2.48 | 0.46 |
| 33:BL:26:GLY:O | 33:BL:27:LEU:HD23 | 2.14 | 0.46 |
| 39:BR:49:ILE:HB | 39:BR:52:PRO:HA | 1.97 | 0.46 |
| 1:CA:93:U:C2' | 1:CA:94:G:H5'' | 2.45 | 0.46 |
| 1:CA:108:G:C6 | 20:CT:10:ARG:HG2 | 2.50 | 0.46 |
| 1:CA:223:A:C6 | 1:CA:224:U:C4 | 3.03 | 0.46 |
| 1:CA:412:A:O2' | 1:CA:414:A:H5' | 2.15 | 0.46 |
| 1:CA:748:G:H2' | 1:CA:749:A:H8 | 1.78 | 0.46 |
| 1:CA:791:G:C5 | 1:CA:792:A:N7 | 2.83 | 0.46 |
| 1:CA:1004:A:C6 | 1:CA:1005:A:N1 | 2.83 | 0.46 |
| 1:CA:1022:A:C5 | 1:CA:1023:U:C5 | 3.03 | 0.46 |
| 1:CA:1130:A:N9 | 1:CA:1146:A:C2 | 2.83 | 0.46 |
| 1:CA:1160:G:O6 | 1:CA:1181:G:C6 | 2.67 | 0.46 |
| 2:CB:164:ILE:O | 2:CB:186:ILE:HG23 | 2.16 | 0.46 |
| 5:CE:137:VAL:O | 5:CE:138:ARG:CG | 2.60 | 0.46 |
| 9:CI:30:ILE:HD13 | 9:CI:39:PHE:CE2 | 2.50 | 0.46 |
| 12:CL:44:LYS:HD3 | 12:CL:44:LYS:N | 2.29 | 0.46 |
| 13:CM:33:ILE:HG22 | 13:CM:56:LEU:HD23 | 1.96 | 0.46 |
| 22:DA:84:A:C2 | 22:DA:103:A:C5 | 3.03 | 0.46 |
| 22:DA:104:A:C8 | 22:DA:105:C:C4 | 3.03 | 0.46 |
| 22:DA:125:A:H3' | 50:D2:19:ARG:HG3 | 1.97 | 0.46 |
| 22:DA:372:G:O2' | 22:DA:400:G:O6 | 2.25 | 0.46 |
| 22:DA:765:C:C4 | 22:DA:766:U:C4 | 3.03 | 0.46 |
| 22:DA:1277:G:N3 | 35:DN:23:ASN:HB3 | 2.30 | 0.46 |
| 22:DA:1343:G:C6 | 22:DA:1344:U:O4 | 2.68 | 0.46 |
| 22:DA:1394:U:H6 | 22:DA:1394:U:H3' | 1.80 | 0.46 |
| 22:DA:1731:G:N1 | 22:DA:1733:G:C4 | 2.83 | 0.46 |
| 22:DA:1805:A:C2 | 22:DA:1813:G:N1 | 2.83 | 0.46 |
| 22:DA:2199:A:C4 | 22:DA:2225:A:N1 | 2.83 | 0.46 |
| 22:DA:2799:A:C6 | 22:DA:2801:G:C4 | 3.03 | 0.46 |
| 23:DB:81:G:C6 | 23:DB:82:U:C4 | 3.03 | 0.46 |
| 24:DC:30:PHE:CD1 | 24:DC:32:PRO:HD2 | 2.50 | 0.46 |
| 26:DE:130:LYS:HB2 | 26:DE:133:LEU:HB3 | 1.97 | 0.46 |
| 38:DQ:36:PHE:CE1 | 38:DQ:40:ILE:HD11 | 2.49 | 0.46 |
| 39:DR:66:HIS:CD2 | 39:DR:94:THR:CG2 | 2.98 | 0.46 |
| 39:DR:68:ARG:HB3 | 39:DR:90:ARG:HG2 | 1.96 | 0.46 |
| 50:D2:30:VAL:O | 50:D2:34:ARG:HG3 | 2.15 | 0.46 |
| 1:AA:474:G:C5 | 1:AA:475:C:C5 | 3.03 | 0.46 |
| 1:AA:1181:G:O2' | 1:AA:1182:G:N7 | 2.48 | 0.46 |
| 2:AB:33:GLY:HA3 | 2:AB:40:ILE:H | 1.79 | 0.46 |
| 4:AD:118:VAL:HA | 4:AD:123:ILE:HD12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AE:20:ARG:HG3 | 5:AE:21:VAL:N | 2.29 | 0.46 |
| 6:AF:66:ALA:HB1 | 6:AF:67:PRO:HD2 | 1.97 | 0.46 |
| 7:AG:8:GLY:O | 7:AG:9:GLN:HB3 | 2.14 | 0.46 |
| 11:AK:112:ASP:HB2 | 21:AU:20:LYS:HD2 | 1.96 | 0.46 |
| 13:AM:12:HIS:HA | 13:AM:44:LYS:HE3 | 1.96 | 0.46 |
| 19:AS:3:ARG:O | 19:AS:4:SER:HB2 | 2.16 | 0.46 |
| 21:AU:25:LYS:O | 21:AU:29:LEU:HB3 | 2.16 | 0.46 |
| 22:BA:1084:A:C2 | 22:BA:1106:G:H1' | 2.50 | 0.46 |
| 22:BA:1839:G:H2' | 22:BA:1840:G:O5' | 2.15 | 0.46 |
| 22:BA:1886:U:C2' | 22:BA:1887:C:H5' | 2.45 | 0.46 |
| 22:BA:1915:U:C4 | 22:BA:1916:A:C5 | 3.03 | 0.46 |
| 22:BA:2820:A:C6 | 25:BD:197:THR:CG2 | 2.98 | 0.46 |
| 22:BA:2871:U:OP1 | 35:BN:69:ARG:NH1 | 2.48 | 0.46 |
| 26:BE:119:ILE:O | 26:BE:187:VAL:HA | 2.15 | 0.46 |
| 33:BL:85:VAL:HB | 33:BL:94:THR:HG23 | 1.97 | 0.46 |
| 42:BU:14:LEU:HD11 | 42:BU:71:ALA:HB2 | 1.96 | 0.46 |
| 1:CA:50:A:H1' | 1:CA:52:C:O4' | 2.15 | 0.46 |
| 1:CA:517:G:H5' | 1:CA:519:C:C2 | 2.51 | 0.46 |
| 1:CA:577:G:C2 | 1:CA:578:C:C5 | 3.03 | 0.46 |
| 1:CA:1019:A:H2' | 1:CA:1020:G:O4' | 2.16 | 0.46 |
| 1:CA:1027:C:N4 | 1:CA:1034:G:N1 | 2.63 | 0.46 |
| 1:CA:1032:G:H2' | 1:CA:1032:G:N3 | 2.31 | 0.46 |
| 1:CA:1237:C:O2 | 1:CA:1334:G:O2' | 2.17 | 0.46 |
| 4:CD:9:LEU:HD11 | 4:CD:29:ASP:OD1 | 2.14 | 0.46 |
| 4:CD:35:GLU:HG3 | 4:CD:36:GLN:HG3 | 1.97 | 0.46 |
| 8:CH:2:SER:C | 8:CH:4:GLN:N | 2.68 | 0.46 |
| 12:CL:47:SER:O | 12:CL:48:ALA:HB2 | 2.12 | 0.46 |
| 14:CN:23:LYS:O | 14:CN:26:GLU:HG3 | 2.15 | 0.46 |
| 21:CU:4:ILE:O | 21:CU:4:ILE:HG22 | 2.15 | 0.46 |
| 22:DA:188:G:C2 | 22:DA:209:C:N3 | 2.84 | 0.46 |
| 22:DA:273:G:H2' | 22:DA:274:C:O4' | 2.14 | 0.46 |
| 22:DA:981:A:H5'' | 58:DA:3588:HOH:O | 2.14 | 0.46 |
| 22:DA:1062:G:C6 | 22:DA:1063:G:O6 | 2.68 | 0.46 |
| 22:DA:1121:C:C2 | 22:DA:1122:G:C8 | 3.03 | 0.46 |
| 22:DA:1317:G:N2 | 22:DA:1336:A:N3 | 2.63 | 0.46 |
| 22:DA:1669:A:O4' | 32:DK:5:GLN:HG3 | 2.15 | 0.46 |
| 22:DA:1954:G:H1' | 22:DA:1956:U:O4 | 2.15 | 0.46 |
| 22:DA:2121:G:C2 | 22:DA:2177:C:O2 | 2.68 | 0.46 |
| 22:DA:2297:A:N7 | 22:DA:2320:U:C4 | 2.83 | 0.46 |
| 22:DA:2405:G:H1' | 22:DA:2412:A:N6 | 2.30 | 0.46 |
| 22:DA:2693:G:N2 | 22:DA:2717:C:O2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2751:G:H4' | 28:DG:4:VAL:HG23 | 1.96 | 0.46 |
| 22:DA:2839:G:C5 | 22:DA:2840:C:C5 | 3.03 | 0.46 |
| 25:DD:133:THR:HG23 | 25:DD:134:HIS:H | 1.81 | 0.46 |
| 26:DE:76:PRO:HA | 26:DE:82:GLY:HA2 | 1.96 | 0.46 |
| 32:DK:105:ARG:N | 32:DK:122:VAL:OXT | 2.48 | 0.46 |
| 34:DM:2:LEU:HD12 | 34:DM:2:LEU:N | 2.30 | 0.46 |
| 1:AA:74:A:C2 | 1:AA:97:G:C6 | 3.03 | 0.46 |
| 1:AA:404:G:H4' | 1:AA:439:U:O2 | 2.16 | 0.46 |
| 1:AA:572:A:H5' | 1:AA:573:A:P | 2.56 | 0.46 |
| 1:AA:596:A:N6 | 1:AA:645:G:N1 | 2.63 | 0.46 |
| 1:AA:663:A:C2 | 1:AA:743:A:C2 | 3.04 | 0.46 |
| 1:AA:737:C:H2' | 1:AA:738:C:C6 | 2.50 | 0.46 |
| 2:AB:94:HIS:O | 2:AB:95:ARG:C | 2.53 | 0.46 |
| 2:AB:103:ASN:O | 2:AB:106:THR:N | 2.47 | 0.46 |
| 2:AB:213:TYR:O | 2:AB:217:VAL:HG23 | 2.15 | 0.46 |
| 3:AC:149:ILE:HG13 | 3:AC:201:TRP:O | 2.15 | 0.46 |
| 4:AD:98:LEU:HD23 | 4:AD:118:VAL:HG11 | 1.98 | 0.46 |
| 12:AL:38:TYR:O | 12:AL:39:THR:HG22 | 2.15 | 0.46 |
| 13:AM:11:ASP:O | 13:AM:12:HIS:CB | 2.62 | 0.46 |
| 20:AT:25:ARG:O | 20:AT:29:ARG:HG2 | 2.14 | 0.46 |
| 22:BA:528:A:C2 | 22:BA:2043:C:C5' | 2.95 | 0.46 |
| 22:BA:1268:A:C2 | 22:BA:2013:A:C4 | 3.03 | 0.46 |
| 22:BA:1489:C:C2 | 22:BA:1501:G:C2 | 3.03 | 0.46 |
| 22:BA:1951:U:H2' | 22:BA:1953:A:OP2 | 2.15 | 0.46 |
| 22:BA:2661:G:H2' | 22:BA:2662:A:C8 | 2.50 | 0.46 |
| 24:BC:144:VAL:HG21 | 24:BC:162:VAL:HG21 | 1.96 | 0.46 |
| 28:BG:87:LEU:N | 28:BG:87:LEU:HD12 | 2.30 | 0.46 |
| 29:BH:80:ILE:HG21 | 29:BH:94:ILE:CG1 | 2.45 | 0.46 |
| 29:BH:132:PHE:CD2 | 29:BH:142:VAL:CG2 | 2.99 | 0.46 |
| 42:BU:26:LYS:O | 42:BU:27:ASN:HB3 | 2.15 | 0.46 |
| 46:BY:46:VAL:O | 46:BY:47:ARG:C | 2.54 | 0.46 |
| 1:CA:81:A:C2 | 1:CA:89:U:C2 | 3.03 | 0.46 |
| 1:CA:182:A:C5 | 1:CA:184:G:C5 | 3.03 | 0.46 |
| 1:CA:496:A:C2 | 1:CA:497:G:C6 | 3.03 | 0.46 |
| 1:CA:517:G:C8 | 1:CA:531:U:C4 | 3.03 | 0.46 |
| 1:CA:543:U:O2' | 1:CA:544:G:H5' | 2.15 | 0.46 |
| 1:CA:578:C:C2 | 1:CA:579:A:C8 | 3.03 | 0.46 |
| 2:CB:34:ALA:O | 2:CB:35:ARG:O | 2.34 | 0.46 |
| 6:CF:32:ALA:O | 6:CF:33:GLU:C | 2.54 | 0.46 |
| 7:CG:91:VAL:HG21 | 7:CG:96:ARG:HA | 1.97 | 0.46 |
| 10:CJ:53:ILE:HD11 | 14:CN:85:ARG:NH1 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:CQ:30:LYS:HB2 | 17:CQ:37:PHE:CZ | 2.50 | 0.46 |
| 22:DA:218:A:H2' | 22:DA:219:A:O4' | 2.15 | 0.46 |
| 22:DA:265:A:H4' | 22:DA:266:G:OP1 | 2.15 | 0.46 |
| 22:DA:487:C:N4 | 22:DA:488:G:C6 | 2.83 | 0.46 |
| 22:DA:570:G:C2' | 22:DA:571:U:H5' | 2.45 | 0.46 |
| 22:DA:997:G:OP1 | 38:DQ:92:ARG:NE | 2.48 | 0.46 |
| 22:DA:1184:U:OP1 | 47:DZ:30:ARG:NH2 | 2.48 | 0.46 |
| 22:DA:1470:A:H2' | 22:DA:1471:G:C5' | 2.45 | 0.46 |
| 22:DA:1734:G:C2 | 22:DA:1735:A:C5 | 3.04 | 0.46 |
| 22:DA:2283:C:C2 | 22:DA:2389:G:C2 | 3.03 | 0.46 |
| 22:DA:2305:U:C4 | 22:DA:2306:C:N4 | 2.83 | 0.46 |
| 22:DA:2682:A:C2 | 25:DD:23:PRO:HB3 | 2.50 | 0.46 |
| 24:DC:247:PRO:HG2 | 24:DC:248:TRP:CZ3 | 2.51 | 0.46 |
| 26:DE:23:PHE:CD1 | 26:DE:111:GLU:HG3 | 2.49 | 0.46 |
| 29:DH:41:LYS:O | 29:DH:44:ILE:HG12 | 2.15 | 0.46 |
| 30:DI:20:PRO:HB2 | 30:DI:23:PRO:HD2 | 1.98 | 0.46 |
| 30:DI:93:PRO:HB3 | 30:DI:136:MET:HA | 1.97 | 0.46 |
| 32:DK:108:ARG:HB2 | 32:DK:116:ILE:HD13 | 1.96 | 0.46 |
| 38:DQ:61:TRP:HB3 | 38:DQ:92:ARG:O | 2.16 | 0.46 |
| 1:AA:818:G:O2' | 1:AA:819:A:H5' | 2.15 | 0.46 |
| 1:AA:1286:U:H2' | 1:AA:1286:U:O2 | 2.15 | 0.46 |
| 3:AC:79:LYS:O | 3:AC:80:LYS:C | 2.54 | 0.46 |
| 20:AT:68:HIS:HB3 | 20:AT:69:LYS:HZ2 | 1.80 | 0.46 |
| 22:BA:146:A:H2' | 22:BA:147:C:O4' | 2.16 | 0.46 |
| 22:BA:322:A:C5 | 22:BA:340:A:C2 | 3.03 | 0.46 |
| 22:BA:1087:G:O2' | 22:BA:1089:A:O4' | 2.29 | 0.46 |
| 22:BA:2018:G:O2' | 22:BA:2019:A:H5' | 2.15 | 0.46 |
| 22:BA:2444:G:OP2 | 26:BE:63:LYS:HD3 | 2.16 | 0.46 |
| 22:BA:2607:G:H2' | 22:BA:2608:G:O4' | 2.16 | 0.46 |
| 24:BC:162:VAL:CG1 | 24:BC:176:LEU:HD23 | 2.45 | 0.46 |
| 28:BG:54:PRO:HG3 | 28:BG:62:TRP:CE2 | 2.50 | 0.46 |
| 29:BH:37:VAL:CG2 | 29:BH:38:PRO:HD2 | 2.45 | 0.46 |
| 39:BR:11:GLN:C | 39:BR:12:HIS:CG | 2.88 | 0.46 |
| 40:BS:74:ILE:HG23 | 40:BS:74:ILE:O | 2.16 | 0.46 |
| 42:BU:72:ILE:HD12 | 42:BU:72:ILE:O | 2.15 | 0.46 |
| 53:B5:200:HIS:O | 53:B5:201:LYS:C | 2.53 | 0.46 |
| 1:CA:651:C:N4 | 1:CA:753:A:OP2 | 2.47 | 0.46 |
| 1:CA:779:C:C2' | 1:CA:780:A:H5' | 2.46 | 0.46 |
| 1:CA:1010:U:C2 | 1:CA:1020:G:C2 | 3.04 | 0.46 |
| 1:CA:1279:G:OP2 | 10:CJ:11:LYS:NZ | 2.44 | 0.46 |
| 1:CA:1307:U:C4 | 1:CA:1308:U:C5 | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1460:C:C4 | 1:CA:1461:G:C5 | 3.03 | 0.46 |
| 3:CC:126:ARG:O | 3:CC:127:ARG:CB | 2.63 | 0.46 |
| 4:CD:161:LEU:HD23 | 4:CD:162:ALA:N | 2.30 | 0.46 |
| 5:CE:70:ASN:N | 5:CE:70:ASN:OD1 | 2.49 | 0.46 |
| 12:CL:61:PHE:N | 12:CL:61:PHE:HD1 | 2.13 | 0.46 |
| 13:CM:23:TYR:CD2 | 13:CM:23:TYR:O | 2.69 | 0.46 |
| 15:CO:45:GLU:O | 15:CO:46:HIS:HB2 | 2.16 | 0.46 |
| 16:CP:19:VAL:HG13 | 16:CP:37:GLY:N | 2.31 | 0.46 |
| 22:DA:295:G:C2 | 22:DA:296:U:C6 | 3.03 | 0.46 |
| 22:DA:771:G:C6 | 22:DA:772:C:C5 | 3.03 | 0.46 |
| 22:DA:813:U:H2' | 22:DA:814:C:C6 | 2.50 | 0.46 |
| 22:DA:881:G:N1 | 22:DA:895:U:O2 | 2.47 | 0.46 |
| 22:DA:1070:A:H2' | 22:DA:1097:U:O5' | 2.16 | 0.46 |
| 22:DA:1330:C:C2' | 22:DA:1331:G:O5' | 2.63 | 0.46 |
| 22:DA:1475:G:H4' | 22:DA:1732:C:C5 | 2.50 | 0.46 |
| 22:DA:1577:C:H2' | 22:DA:1578:U:C1' | 2.46 | 0.46 |
| 22:DA:1845:G:OP1 | 24:DC:256:LYS:NZ | 2.40 | 0.46 |
| 22:DA:1924:C:H2' | 22:DA:1925:C:O4' | 2.16 | 0.46 |
| 22:DA:2015:A:C6 | 48:D0:3:VAL:HG23 | 2.51 | 0.46 |
| 24:DC:226:ASN:HB3 | 24:DC:227:PRO:CD | 2.45 | 0.46 |
| 25:DD:148:GLN:OE1 | 25:DD:148:GLN:N | 2.48 | 0.46 |
| 26:DE:52:VAL:HG21 | 26:DE:81:GLY:HA2 | 1.98 | 0.46 |
| 37:DP:89:ARG:NH1 | 37:DP:115:ASN:OXT | 2.48 | 0.46 |
| 39:DR:52:PRO:O | 39:DR:53:PHE:HB2 | 2.14 | 0.46 |
| 52:D4:25:VAL:HB | 52:D4:35:GLN:HB2 | 1.97 | 0.46 |
| 1:AA:104:G:C2 | 1:AA:105:G:C8 | 3.04 | 0.46 |
| 1:AA:737:C:H2' | 1:AA:738:C:H6 | 1.79 | 0.46 |
| 1:AA:858:G:O2' | 1:AA:859:G:H5' | 2.15 | 0.46 |
| 1:AA:1126:U:O2 | 1:AA:1280:A:C5' | 2.63 | 0.46 |
| 1:AA:1211:U:C2' | 1:AA:1212:U:OP2 | 2.63 | 0.46 |
| 8:AH:11:LEU:N | 8:AH:11:LEU:HD23 | 2.31 | 0.46 |
| 14:AN:49:GLN:OE1 | 14:AN:49:GLN:CA | 2.64 | 0.46 |
| 17:AQ:45:HIS:CB | 17:AQ:70:THR:HG22 | 2.46 | 0.46 |
| 19:AS:63:THR:HB | 19:AS:65:GLU:OE2 | 2.15 | 0.46 |
| 20:AT:71:LYS:HD2 | 20:AT:74:ARG:NH2 | 2.31 | 0.46 |
| 22:BA:578:G:OP1 | 22:BA:1255:U:O2' | 2.29 | 0.46 |
| 22:BA:918:A:H4' | 23:BB:97:C:O2 | 2.16 | 0.46 |
| 22:BA:1564:C:O2' | 22:BA:1565:C:H5' | 2.16 | 0.46 |
| 22:BA:1592:C:C2' | 22:BA:1593:A:H5' | 2.46 | 0.46 |
| 22:BA:1637:A:H5' | 22:BA:1760:C:O2' | 2.15 | 0.46 |
| 22:BA:1958:C:O2' | 22:BA:1959:G:H5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2262:U:OP1 | 22:BA:2387:U:O2' | 2.29 | 0.46 |
| 25:BD:12:THR:HG22 | 37:BP:9:GLU:OE2 | 2.15 | 0.46 |
| 34:BM:95:LEU:C | 34:BM:96:ILE:HD13 | 2.35 | 0.46 |
| 36:BO:7:ARG:HG3 | 36:BO:96:GLY:HA3 | 1.97 | 0.46 |
| 37:BP:26:VAL:CG1 | 37:BP:47:VAL:HG23 | 2.45 | 0.46 |
| 38:BQ:36:PHE:CZ | 38:BQ:40:ILE:HD11 | 2.49 | 0.46 |
| 46:BY:57:LEU:HA | 46:BY:60:LYS:HB3 | 1.96 | 0.46 |
| 1:CA:81:A:H2' | 1:CA:82:G:C8 | 2.50 | 0.46 |
| 1:CA:669:G:N2 | 1:CA:738:C:C2 | 2.84 | 0.46 |
| 1:CA:872:A:C4 | 1:CA:874:G:C8 | 3.03 | 0.46 |
| 1:CA:1134:G:C6 | 1:CA:1135:U:C2 | 3.03 | 0.46 |
| 2:CB:128:LYS:O | 2:CB:129:LEU:HB2 | 2.15 | 0.46 |
| 7:CG:25:LYS:O | 7:CG:29:ILE:HG12 | 2.15 | 0.46 |
| 19:CS:44:MET:HE1 | 19:CS:71:LEU:HD21 | 1.95 | 0.46 |
| 22:DA:72:U:O2' | 22:DA:73:A:O5' | 2.25 | 0.46 |
| 22:DA:197:A:N6 | 22:DA:2430:A:H2' | 2.30 | 0.46 |
| 22:DA:538:A:O2' | 31:DJ:8:PRO:CG | 2.63 | 0.46 |
| 22:DA:571:U:C4 | 22:DA:575:A:C5 | 3.04 | 0.46 |
| 22:DA:678:C:H2' | 22:DA:679:C:C6 | 2.51 | 0.46 |
| 22:DA:989:G:C8 | 47:DZ:14:ILE:HD11 | 2.50 | 0.46 |
| 22:DA:1323:C:C4 | 22:DA:1324:G:N7 | 2.83 | 0.46 |
| 22:DA:1325:U:OP1 | 22:DA:1647:U:O2' | 2.28 | 0.46 |
| 22:DA:1529:G:O6 | 22:DA:1543:G:C2 | 2.68 | 0.46 |
| 22:DA:1753:G:N1 | 22:DA:1756:G:C2 | 2.83 | 0.46 |
| 22:DA:1819:A:H5'' | 24:DC:157:SER:HB2 | 1.98 | 0.46 |
| 22:DA:2420:C:OP1 | 51:D3:34:THR:HB | 2.16 | 0.46 |
| 22:DA:2602:A:H4' | 22:DA:2603:G:C5' | 2.45 | 0.46 |
| 23:DB:71:C:C2 | 23:DB:106:G:C2 | 3.03 | 0.46 |
| 32:DK:31:ARG:HB3 | 32:DK:32:TYR:CD2 | 2.50 | 0.46 |
| 34:DM:56:ALA:C | 34:DM:58:LYS:H | 2.19 | 0.46 |
| 35:DN:67:PHE:O | 35:DN:71:ARG:HD2 | 2.16 | 0.46 |
| 35:DN:84:GLY:N | 35:DN:85:PRO:HD2 | 2.30 | 0.46 |
| 39:DR:87:GLN:HG2 | 39:DR:88:GLY:N | 2.31 | 0.46 |
| 44:DW:52:GLY:HA3 | 44:DW:60:PHE:CE1 | 2.50 | 0.46 |
| 50:D2:34:ARG:HB2 | 50:D2:42:LEU:CD1 | 2.46 | 0.46 |
| 1:AA:36:C:H2' | 1:AA:37:U:O4' | 2.16 | 0.46 |
| 1:AA:509:A:P | 58:AA:1721:HOH:O | 2.73 | 0.46 |
| 1:AA:670:G:C2' | 1:AA:671:G:O5' | 2.63 | 0.46 |
| 1:AA:723:U:OP2 | 1:AA:723:U:H4' | 2.14 | 0.46 |
| 1:AA:1244:G:C2 | 1:AA:1294:G:C2 | 3.03 | 0.46 |
| 2:AB:84:ALA:O | 2:AB:89:GLN:HB2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:AC:144:LEU:HD13 | 3:AC:144:LEU:N | 2.31 | 0.46 |
| 3:AC:203:PHE:CE1 | 3:AC:205:GLY:O | 2.69 | 0.46 |
| 5:AE:88:VAL:HG23 | 5:AE:93:ARG:HG2 | 1.98 | 0.46 |
| 9:AI:30:ILE:O | 9:AI:33:ARG:HB2 | 2.15 | 0.46 |
| 21:AU:20:LYS:HE2 | 21:AU:20:LYS:N | 2.31 | 0.46 |
| 22:BA:526:A:O2' | 22:BA:2043:C:O2 | 2.27 | 0.46 |
| 22:BA:920:A:O2' | 22:BA:921:C:H5' | 2.15 | 0.46 |
| 22:BA:1181:U:H2' | 22:BA:1182:G:C8 | 2.51 | 0.46 |
| 22:BA:2190:G:C6 | 22:BA:2191:A:C6 | 3.04 | 0.46 |
| 22:BA:2648:G:H2' | 22:BA:2649:C:O4' | 2.16 | 0.46 |
| 24:BC:162:VAL:HG11 | 24:BC:174:LEU:HB3 | 1.96 | 0.46 |
| 27:BF:73:SER:HB2 | 27:BF:81:GLN:N | 2.31 | 0.46 |
| 30:BI:62:TYR:O | 30:BI:63:ALA:HB2 | 2.15 | 0.46 |
| 30:BI:116:ASP:O | 30:BI:117:MET:HG2 | 2.15 | 0.46 |
| 33:BL:87:GLY:O | 33:BL:89:VAL:HG12 | 2.16 | 0.46 |
| 51:B3:31:HIS:CD2 | 51:B3:31:HIS:C | 2.88 | 0.46 |
| 1:CA:33:A:H2' | 1:CA:34:C:H6 | 1.81 | 0.46 |
| 1:CA:429:U:H4' | 1:CA:430:A:OP1 | 2.15 | 0.46 |
| 1:CA:429:U:H3' | 4:CD:9:LEU:HD23 | 1.96 | 0.46 |
| 1:CA:541:G:H2' | 1:CA:542:G:O4' | 2.15 | 0.46 |
| 1:CA:620:C:H2' | 1:CA:621:A:O4' | 2.15 | 0.46 |
| 1:CA:681:A:C2 | 1:CA:710:G:C2 | 3.04 | 0.46 |
| 1:CA:748:G:H2' | 1:CA:749:A:C8 | 2.51 | 0.46 |
| 1:CA:846:G:OP2 | 18:CR:48:ARG:NH2 | 2.49 | 0.46 |
| 1:CA:1226:C:N4 | 13:CM:103:LYS:HB2 | 2.31 | 0.46 |
| 4:CD:9:LEU:HG | 4:CD:32:CYS:HB2 | 1.97 | 0.46 |
| 5:CE:16:ILE:N | 5:CE:16:ILE:HD12 | 2.30 | 0.46 |
| 6:CF:8:PHE:N | 6:CF:8:PHE:CD2 | 2.83 | 0.46 |
| 7:CG:31:MET:O | 7:CG:31:MET:HG2 | 2.16 | 0.46 |
| 7:CG:114:LYS:HB2 | 7:CG:118:LEU:HD12 | 1.97 | 0.46 |
| 12:CL:25:GLU:CB | 12:CL:27:CYS:SG | 3.03 | 0.46 |
| 17:CQ:38:ILE:CG2 | 17:CQ:39:LYS:N | 2.79 | 0.46 |
| 20:CT:51:PHE:C | 20:CT:51:PHE:CD1 | 2.88 | 0.46 |
| 22:DA:485:C:C2 | 22:DA:496:G:C2 | 3.04 | 0.46 |
| 22:DA:867:C:C5 | 22:DA:868:U:C5 | 3.03 | 0.46 |
| 22:DA:1131:G:O6 | 22:DA:2024:G:O2' | 2.25 | 0.46 |
| 22:DA:1177:G:H2' | 22:DA:1178:C:H4' | 1.97 | 0.46 |
| 22:DA:1682:G:N3 | 22:DA:1757:A:H1' | 2.31 | 0.46 |
| 22:DA:1940:U:C2 | 22:DA:1965:C:OP2 | 2.68 | 0.46 |
| 22:DA:1957:C:H5' | 22:DA:1984:G:O2' | 2.16 | 0.46 |
| 22:DA:2244:U:H2' | 22:DA:2245:U:O4' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2336:A:N3 | 22:DA:2385:C:H1' | 2.30 | 0.46 |
| 22:DA:2581:G:H2' | 22:DA:2581:G:N3 | 2.30 | 0.46 |
| 22:DA:2741:A:H2' | 22:DA:2742:G:H5' | 1.98 | 0.46 |
| 22:DA:2889:C:C4 | 22:DA:2890:G:C5 | 3.03 | 0.46 |
| 25:DD:122:VAL:HG21 | 25:DD:141:ARG:NH1 | 2.31 | 0.46 |
| 31:DJ:19:ASP:O | 31:DJ:23:LYS:HE3 | 2.16 | 0.46 |
| 31:DJ:124:VAL:O | 31:DJ:124:VAL:HG23 | 2.16 | 0.46 |
| 32:DK:118:LEU:O | 32:DK:119:ALA:HB3 | 2.15 | 0.46 |
| 41:DT:14:PRO:HD2 | 46:DY:33:ALA:HB1 | 1.96 | 0.46 |
| 1:AA:32:A:OP1 | 1:AA:398:U:H1' | 2.15 | 0.46 |
| 1:AA:445:G:H2' | 1:AA:446:G:O4' | 2.15 | 0.46 |
| 1:AA:712:A:C6 | 1:AA:713:G:C6 | 3.04 | 0.46 |
| 1:AA:968:A:H4' | 1:AA:969:A:OP2 | 2.16 | 0.46 |
| 1:AA:978:A:C5 | 1:AA:1318:A:C6 | 3.03 | 0.46 |
| 1:AA:1059:C:N3 | 1:AA:1060:U:C5 | 2.83 | 0.46 |
| 4:AD:34:ILE:O | 4:AD:35:GLU:CB | 2.64 | 0.46 |
| 4:AD:34:ILE:HG12 | 4:AD:35:GLU:N | 2.29 | 0.46 |
| 8:AH:75:ILE:O | 8:AH:75:ILE:HG23 | 2.16 | 0.46 |
| 8:AH:78:VAL:HG11 | 8:AH:125:ILE:CD1 | 2.46 | 0.46 |
| 8:AH:89:LYS:HG3 | 8:AH:90:ASP:N | 2.31 | 0.46 |
| 11:AK:92:GLY:O | 11:AK:96:THR:HB | 2.16 | 0.46 |
| 12:AL:44:LYS:HB3 | 12:AL:45:PRO:HD3 | 1.96 | 0.46 |
| 15:AO:2:SER:O | 15:AO:3:LEU:HB2 | 2.14 | 0.46 |
| 20:AT:54:MET:SD | 20:AT:79:LEU:CD1 | 3.04 | 0.46 |
| 22:BA:281:C:H2' | 22:BA:282:A:C8 | 2.51 | 0.46 |
| 22:BA:851:C:H2' | 22:BA:852:U:H6 | 1.80 | 0.46 |
| 22:BA:1047:G:N2 | 22:BA:1110:G:C4 | 2.84 | 0.46 |
| 22:BA:2293:G:H2' | 22:BA:2294:G:O4' | 2.16 | 0.46 |
| 28:BG:141:ILE:C | 28:BG:141:ILE:HD12 | 2.36 | 0.46 |
| 29:BH:90:LEU:HD23 | 29:BH:93:SER:HA | 1.97 | 0.46 |
| 29:BH:94:ILE:HG23 | 29:BH:98:ASP:HB2 | 1.98 | 0.46 |
| 30:BI:117:MET:CE | 30:BI:129:ILE:HD11 | 2.46 | 0.46 |
| 31:BJ:32:LEU:O | 31:BJ:36:LEU:HG | 2.16 | 0.46 |
| 41:BT:16:VAL:O | 41:BT:17:SER:HB3 | 2.15 | 0.46 |
| 1:CA:3:A:C6 | 1:CA:629:A:H4' | 2.51 | 0.46 |
| 1:CA:73:C:O2' | 1:CA:74:A:P | 2.74 | 0.46 |
| 1:CA:84:U:O2' | 1:CA:85:U:H5' | 2.16 | 0.46 |
| 1:CA:517:G:H5' | 1:CA:519:C:O2 | 2.16 | 0.46 |
| 1:CA:643:C:H5' | 8:CH:32:LEU:HD22 | 1.96 | 0.46 |
| 1:CA:671:G:N1 | 1:CA:672:U:C2 | 2.84 | 0.46 |
| 1:CA:933:G:OP2 | 7:CG:3:ARG:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1170:A:H3' | 1:CA:1171:A:H8 | 1.80 | 0.46 |
| 1:CA:1232:U:OP1 | 9:CI:126:GLN:HG2 | 2.16 | 0.46 |
| 2:CB:219:ALA:O | 2:CB:220:THR:CB | 2.64 | 0.46 |
| 6:CF:36:ILE:HG12 | 6:CF:36:ILE:O | 2.15 | 0.46 |
| 7:CG:30:LEU:HD11 | 7:CG:116:MET:HE2 | 1.98 | 0.46 |
| 9:CI:88:MET:HB2 | 9:CI:92:GLU:CD | 2.36 | 0.46 |
| 12:CL:107:VAL:CG2 | 12:CL:117:TYR:HB3 | 2.45 | 0.46 |
| 20:CT:3:ASN:O | 20:CT:4:ILE:C | 2.53 | 0.46 |
| 21:CU:37:PHE:HD2 | 21:CU:41:PRO:HG3 | 1.80 | 0.46 |
| 22:DA:404:A:C1' | 22:DA:405:U:OP2 | 2.63 | 0.46 |
| 22:DA:415:A:C2 | 22:DA:2409:G:C2 | 3.04 | 0.46 |
| 22:DA:647:G:N7 | 22:DA:648:G:N7 | 2.64 | 0.46 |
| 22:DA:682:G:N3 | 22:DA:682:G:H2' | 2.30 | 0.46 |
| 22:DA:882:G:C2 | 22:DA:883:G:H1' | 2.51 | 0.46 |
| 22:DA:1264:A:C8 | 22:DA:1265:A:C8 | 3.03 | 0.46 |
| 22:DA:1361:G:C6 | 22:DA:1362:C:C4 | 3.04 | 0.46 |
| 22:DA:1437:C:N4 | 22:DA:1438:U:O4 | 2.49 | 0.46 |
| 22:DA:1514:G:H5'' | 22:DA:1515:A:P | 2.56 | 0.46 |
| 22:DA:1806:C:C5 | 22:DA:1807:G:C8 | 3.03 | 0.46 |
| 22:DA:1818:U:H2' | 24:DC:156:ARG:HD3 | 1.98 | 0.46 |
| 22:DA:2114:A:N6 | 22:DA:2119:A:N7 | 2.64 | 0.46 |
| 22:DA:2282:G:N3 | 22:DA:2425:A:N6 | 2.64 | 0.46 |
| 22:DA:2318:G:C6 | 22:DA:2319:G:C6 | 3.02 | 0.46 |
| 22:DA:2330:G:N2 | 22:DA:2386:A:C4 | 2.83 | 0.46 |
| 22:DA:2335:A:N6 | 22:DA:2337:G:H1' | 2.31 | 0.46 |
| 25:DD:65:ALA:O | 25:DD:69:ALA:N | 2.44 | 0.46 |
| 26:DE:40:ARG:CZ | 26:DE:92:HIS:CE1 | 2.99 | 0.46 |
| 26:DE:147:LEU:HD11 | 26:DE:170:ARG:HG2 | 1.97 | 0.46 |
| 29:DH:34:GLY:O | 29:DH:35:LYS:CG | 2.64 | 0.46 |
| 38:DQ:98:ILE:HG22 | 38:DQ:106:PHE:HB2 | 1.98 | 0.46 |
| 41:DT:32:LEU:HD12 | 41:DT:32:LEU:O | 2.15 | 0.46 |
| 43:DV:38:LEU:HD23 | 43:DV:40:ILE:HD11 | 1.96 | 0.46 |
| 1:AA:572:A:H5' | 1:AA:573:A:OP2 | 2.15 | 0.46 |
| 1:AA:1014:A:C2 | 19:AS:34:TRP:CZ2 | 3.04 | 0.46 |
| 1:AA:1124:G:H2' | 1:AA:1145:A:N6 | 2.30 | 0.46 |
| 1:AA:1492:A:OP1 | 12:AL:44:LYS:CA | 2.64 | 0.46 |
| 2:AB:42:ASN:O | 2:AB:45:LYS:N | 2.42 | 0.46 |
| 4:AD:190:ASP:C | 4:AD:191:LEU:HG | 2.36 | 0.46 |
| 6:AF:51:ILE:HD12 | 6:AF:86:ARG:CZ | 2.45 | 0.46 |
| 7:AG:145:ALA:O | 7:AG:146:GLU:HB3 | 2.16 | 0.46 |
| 9:AI:30:ILE:HA | 9:AI:65:ILE:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:43:PRO:O | 10:AJ:71:LEU:HD23 | 2.16 | 0.46 |
| 13:AM:15:ALA:CB | 13:AM:34:LEU:HD21 | 2.45 | 0.46 |
| 20:AT:78:ASN:O | 20:AT:82:GLN:HG2 | 2.15 | 0.46 |
| 21:AU:17:ARG:NH1 | 21:AU:20:LYS:CG | 2.79 | 0.46 |
| 21:AU:22:SER:C | 21:AU:23:CYS:SG | 2.94 | 0.46 |
| 22:BA:380:G:H2' | 22:BA:381:G:O4' | 2.15 | 0.46 |
| 22:BA:723:C:H2' | 22:BA:724:U:C6 | 2.50 | 0.46 |
| 22:BA:996:A:C6 | 22:BA:1160:G:C2 | 3.03 | 0.46 |
| 22:BA:1047:G:N2 | 22:BA:1110:G:O2' | 2.49 | 0.46 |
| 22:BA:1319:C:H2' | 22:BA:1320:C:H5' | 1.98 | 0.46 |
| 22:BA:1394:U:H2' | 22:BA:1395:A:O5' | 2.16 | 0.46 |
| 22:BA:1508:A:H4' | 22:BA:1508:A:OP1 | 2.15 | 0.46 |
| 22:BA:2122:U:C4 | 22:BA:2123:G:N7 | 2.84 | 0.46 |
| 24:BC:252:THR:HG22 | 24:BC:253:LYS:N | 2.30 | 0.46 |
| 25:BD:104:VAL:O | 25:BD:105:LYS:CB | 2.61 | 0.46 |
| 27:BF:108:VAL:HG13 | 27:BF:114:PHE:CZ | 2.51 | 0.46 |
| 28:BG:121:ILE:HD11 | 28:BG:140:VAL:HG12 | 1.98 | 0.46 |
| 30:BI:62:TYR:CD2 | 30:BI:62:TYR:N | 2.83 | 0.46 |
| 32:BK:116:ILE:O | 32:BK:118:LEU:O | 2.34 | 0.46 |
| 33:BL:132:ARG:HG3 | 33:BL:142:ILE:CD1 | 2.45 | 0.46 |
| 39:BR:66:HIS:CE1 | 39:BR:94:THR:HG22 | 2.51 | 0.46 |
| 40:BS:36:LEU:HD13 | 40:BS:48:LYS:CA | 2.46 | 0.46 |
| 42:BU:6:ARG:O | 42:BU:9:ASP:HB2 | 2.16 | 0.46 |
| 1:CA:38:G:N2 | 1:CA:397:A:C4 | 2.84 | 0.46 |
| 1:CA:131:A:O2' | 1:CA:262:A:N3 | 2.40 | 0.46 |
| 1:CA:147:G:N2 | 1:CA:148:G:C6 | 2.84 | 0.46 |
| 1:CA:510:A:H5'' | 1:CA:511:C:P | 2.55 | 0.46 |
| 1:CA:688:G:C5 | 1:CA:700:G:C2 | 3.04 | 0.46 |
| 1:CA:724:G:C2 | 1:CA:725:G:C8 | 3.04 | 0.46 |
| 1:CA:851:G:C2 | 1:CA:852:G:C8 | 3.04 | 0.46 |
| 1:CA:983:A:N3 | 1:CA:983:A:H2' | 2.31 | 0.46 |
| 1:CA:1197:A:H2' | 1:CA:1198:G:H5' | 1.97 | 0.46 |
| 1:CA:1471:U:O2' | 1:CA:1472:U:H5' | 2.16 | 0.46 |
| 2:CB:16:PHE:CD2 | 2:CB:16:PHE:N | 2.84 | 0.46 |
| 4:CD:168:PRO:CB | 4:CD:171:LEU:HD12 | 2.46 | 0.46 |
| 6:CF:51:ILE:O | 6:CF:51:ILE:CG1 | 2.64 | 0.46 |
| 11:CK:52:PHE:HB2 | 11:CK:56:ARG:HB2 | 1.98 | 0.46 |
| 12:CL:3:THR:O | 12:CL:4:VAL:C | 2.52 | 0.46 |
| 14:CN:18:ASP:OD2 | 14:CN:18:ASP:N | 2.49 | 0.46 |
| 16:CP:6:LEU:CD1 | 16:CP:71:VAL:CG2 | 2.93 | 0.46 |
| 22:DA:228:C:C2 | 22:DA:418:C:H4' | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:324:A:C6 | 22:DA:325:G:C4 | 3.04 | 0.46 |
| 22:DA:359:G:H2' | 22:DA:360:U:O4' | 2.16 | 0.46 |
| 22:DA:613:A:O2' | 22:DA:614:A:P | 2.71 | 0.46 |
| 22:DA:1288:G:C4 | 22:DA:1327:A:C2 | 3.04 | 0.46 |
| 22:DA:1352:U:H5 | 22:DA:1377:G:N7 | 2.14 | 0.46 |
| 22:DA:1437:C:C4 | 22:DA:1438:U:O4 | 2.69 | 0.46 |
| 22:DA:1446:C:O2 | 22:DA:1545:A:O2' | 2.32 | 0.46 |
| 22:DA:1570:A:H5' | 24:DC:36:LYS:HB3 | 1.96 | 0.46 |
| 22:DA:1736:U:H2' | 22:DA:1737:G:O4' | 2.16 | 0.46 |
| 22:DA:2283:C:H2' | 22:DA:2284:A:C5' | 2.46 | 0.46 |
| 22:DA:2443:C:H2' | 22:DA:2444:G:O4' | 2.16 | 0.46 |
| 22:DA:2499:C:C4 | 22:DA:2500:U:O4 | 2.69 | 0.46 |
| 22:DA:2574:G:N1 | 22:DA:2575:C:C2 | 2.84 | 0.46 |
| 22:DA:2880:C:N3 | 22:DA:2881:U:C5 | 2.84 | 0.46 |
| 23:DB:8:C:O3' | 36:DO:25:ARG:NH1 | 2.49 | 0.46 |
| 30:DI:9:VAL:HG23 | 30:DI:10:LYS:N | 2.31 | 0.46 |
| 30:DI:46:THR:HG22 | 30:DI:51:LYS:HG3 | 1.98 | 0.46 |
| 34:DM:72:PRO:HB3 | 34:DM:92:TRP:CZ3 | 2.51 | 0.46 |
| 35:DN:71:ARG:HH21 | 35:DN:71:ARG:HG3 | 1.81 | 0.46 |
| 35:DN:92:GLY:HA2 | 35:DN:94:TYR:CZ | 2.51 | 0.46 |
| 45:DX:25:THR:O | 45:DX:25:THR:HG22 | 2.15 | 0.46 |
| 47:DZ:3:LYS:CD | 47:DZ:3:LYS:N | 2.78 | 0.46 |
| 1:AA:263:A:P | 20:AT:74:ARG:NH1 | 2.89 | 0.46 |
| 1:AA:292:G:O2' | 1:AA:608:A:N6 | 2.47 | 0.46 |
| 1:AA:615:G:C2 | 1:AA:616:G:C8 | 3.04 | 0.46 |
| 1:AA:927:G:C6 | 1:AA:1391:U:O2 | 2.69 | 0.46 |
| 1:AA:927:G:N2 | 1:AA:1391:U:H1' | 2.30 | 0.46 |
| 1:AA:1075:U:OP1 | 2:AB:102:THR:HG21 | 2.16 | 0.46 |
| 1:AA:1081:A:P | 5:AE:21:VAL:HG21 | 2.56 | 0.46 |
| 1:AA:1129:C:O2 | 1:AA:1130:A:N6 | 2.49 | 0.46 |
| 1:AA:1133:G:C6 | 1:AA:1142:G:C6 | 3.04 | 0.46 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.51 | 0.46 |
| 1:AA:1458:G:OP1 | 20:AT:30:THR:OG1 | 2.29 | 0.46 |
| 1:AA:1492:A:N7 | 1:AA:1493:A:C2 | 2.84 | 0.46 |
| 2:AB:87:CYS:HB2 | 2:AB:89:GLN:NE2 | 2.30 | 0.46 |
| 2:AB:106:THR:O | 2:AB:107:VAL:CB | 2.64 | 0.46 |
| 3:AC:143:ARG:CG | 3:AC:144:LEU:HD13 | 2.46 | 0.46 |
| 5:AE:136:VAL:HG22 | 5:AE:137:VAL:N | 2.29 | 0.46 |
| 11:AK:69:ARG:HD2 | 22:BA:2146:C:N3 | 2.31 | 0.46 |
| 12:AL:38:TYR:O | 12:AL:39:THR:CG2 | 2.63 | 0.46 |
| 22:BA:374:A:C2 | 22:BA:401:A:C4 | 3.04 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BC:141:VAL:CG1 | 24:BC:190:ALA:HB1 | 2.45 | 0.46 |
| 24:BC:222:GLY:HA3 | 24:BC:230:HIS:CE1 | 2.51 | 0.46 |
| 39:BR:80:ARG:O | 39:BR:80:ARG:HG2 | 2.15 | 0.46 |
| 1:CA:32:A:OP1 | 1:CA:398:U:H1' | 2.16 | 0.46 |
| 1:CA:597:G:C5 | 1:CA:598:U:C6 | 3.04 | 0.46 |
| 1:CA:955:U:H2' | 1:CA:956:U:O4' | 2.16 | 0.46 |
| 1:CA:1041:G:C6 | 1:CA:1042:A:N6 | 2.83 | 0.46 |
| 1:CA:1152:A:H4' | 10:CJ:15:HIS:CD2 | 2.51 | 0.46 |
| 2:CB:49:MET:HG2 | 2:CB:199:VAL:O | 2.16 | 0.46 |
| 2:CB:57:LEU:HD13 | 2:CB:57:LEU:C | 2.36 | 0.46 |
| 12:CL:83:ARG:CG | 12:CL:84:GLY:N | 2.79 | 0.46 |
| 22:DA:208:C:H2' | 22:DA:209:C:C6 | 2.50 | 0.46 |
| 22:DA:320:A:H2' | 26:DE:131:THR:CG2 | 2.46 | 0.46 |
| 22:DA:349:U:C2' | 22:DA:350:G:H5' | 2.45 | 0.46 |
| 22:DA:458:G:O2' | 22:DA:459:U:OP2 | 2.33 | 0.46 |
| 22:DA:476:G:O4' | 22:DA:505:A:C2 | 2.69 | 0.46 |
| 22:DA:1050:A:C2 | 22:DA:2751:G:C5 | 3.03 | 0.46 |
| 22:DA:1265:A:P | 58:DA:3745:HOH:O | 2.74 | 0.46 |
| 22:DA:1404:C:H2' | 22:DA:1405:U:O5' | 2.16 | 0.46 |
| 22:DA:2048:G:H2' | 22:DA:2049:G:O5' | 2.16 | 0.46 |
| 22:DA:2234:G:C4 | 22:DA:2235:G:C8 | 3.04 | 0.46 |
| 22:DA:2279:G:N7 | 44:DW:14:ARG:NH2 | 2.61 | 0.46 |
| 22:DA:2552:U:C2 | 22:DA:2554:U:H5' | 2.51 | 0.46 |
| 22:DA:2896:C:C2' | 22:DA:2897:U:O5' | 2.64 | 0.46 |
| 24:DC:18:LYS:O | 24:DC:19:VAL:HG23 | 2.16 | 0.46 |
| 24:DC:107:PRO:HD2 | 24:DC:110:LEU:HD22 | 1.97 | 0.46 |
| 25:DD:104:VAL:O | 25:DD:105:LYS:HB3 | 2.16 | 0.46 |
| 26:DE:61:ARG:HD2 | 26:DE:63:LYS:O | 2.15 | 0.46 |
| 28:DG:98:VAL:HG22 | 28:DG:125:CYS:SG | 2.55 | 0.46 |
| 29:DH:60:GLU:HA | 29:DH:60:GLU:OE2 | 2.15 | 0.46 |
| 32:DK:32:TYR:CD2 | 32:DK:32:TYR:N | 2.84 | 0.46 |
| 34:DM:31:PHE:CZ | 34:DM:110:GLU:HA | 2.51 | 0.46 |
| 37:DP:91:ALA:HB2 | 37:DP:113:ARG:HG3 | 1.97 | 0.46 |
| 40:DS:55:ILE:HG21 | 40:DS:66:ILE:CD1 | 2.46 | 0.46 |
| 42:DU:34:VAL:O | 42:DU:64:ALA:HA | 2.16 | 0.46 |
| 49:D1:39:PHE:CD2 | 49:D1:40:ASP:N | 2.83 | 0.46 |
| 54:D6:5:MHU:H12 | 54:D6:8:MHT:H8 | 1.98 | 0.46 |
| 1:AA:594:U:C4 | 1:AA:595:A:C6 | 3.03 | 0.46 |
| 1:AA:660:C:OP1 | 15:AO:5:THR:HG21 | 2.16 | 0.46 |
| 1:AA:844:G:N3 | 1:AA:845:A:C8 | 2.83 | 0.46 |
| 1:AA:1086:U:O2' | 1:AA:1087:G:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1250:A:H4' | 9:AI:70:GLY:O | 2.15 | 0.46 |
| 4:AD:85:ASN:OD1 | 4:AD:88:GLU:HG3 | 2.16 | 0.46 |
| 13:AM:3:ARG:O | 13:AM:4:ILE:CG1 | 2.64 | 0.46 |
| 13:AM:37:ALA:CB | 13:AM:56:LEU:HD23 | 2.46 | 0.46 |
| 16:AP:4:ILE:HG13 | 16:AP:21:VAL:CG2 | 2.46 | 0.46 |
| 16:AP:67:ILE:CG2 | 16:AP:71:VAL:HG12 | 2.46 | 0.46 |
| 17:AQ:10:GLY:HA3 | 17:AQ:24:ALA:O | 2.16 | 0.46 |
| 21:AU:14:VAL:CG1 | 21:AU:16:LEU:HD21 | 2.46 | 0.46 |
| 22:BA:340:A:H2' | 22:BA:341:C:C5' | 2.46 | 0.46 |
| 22:BA:464:U:C5 | 22:BA:788:A:C4 | 3.04 | 0.46 |
| 22:BA:1234:U:H2' | 22:BA:1235:G:O4' | 2.16 | 0.46 |
| 22:BA:1316:U:C2 | 22:BA:1337:G:N2 | 2.84 | 0.46 |
| 22:BA:1956:U:H2' | 22:BA:1957:C:H5' | 1.98 | 0.46 |
| 22:BA:1980:G:H4' | 58:BA:3451:HOH:O | 2.14 | 0.46 |
| 22:BA:2133:G:C2' | 22:BA:2134:A:OP2 | 2.64 | 0.46 |
| 22:BA:2469:A:C2 | 22:BA:2482:A:C4 | 3.04 | 0.46 |
| 22:BA:2593:U:C2' | 22:BA:2594:C:O5' | 2.64 | 0.46 |
| 22:BA:2669:G:O2' | 22:BA:2670:A:H5' | 2.16 | 0.46 |
| 25:BD:133:THR:CG2 | 25:BD:134:HIS:N | 2.79 | 0.46 |
| 27:BF:122:PHE:HB3 | 27:BF:163:ASP:CG | 2.36 | 0.46 |
| 28:BG:155:GLU:OE2 | 28:BG:158:LYS:HB2 | 2.16 | 0.46 |
| 29:BH:79:THR:HG23 | 29:BH:147:VAL:HB | 1.98 | 0.46 |
| 29:BH:90:LEU:HD21 | 29:BH:93:SER:HA | 1.97 | 0.46 |
| 36:BO:88:LYS:HA | 36:BO:115:LEU:HD12 | 1.98 | 0.46 |
| 38:BQ:19:LYS:O | 38:BQ:22:LYS:HG3 | 2.16 | 0.46 |
| 39:BR:86:GLN:HG2 | 39:BR:87:GLN:N | 2.31 | 0.46 |
| 1:CA:824:G:H1' | 8:CH:2:SER:HA | 1.97 | 0.46 |
| 1:CA:939:G:C6 | 1:CA:940:C:C4 | 3.04 | 0.46 |
| 1:CA:1006:G:OP1 | 1:CA:1038:C:H5'' | 2.16 | 0.46 |
| 1:CA:1022:A:C5 | 1:CA:1023:U:C4 | 3.04 | 0.46 |
| 1:CA:1071:C:H2' | 1:CA:1072:G:C8 | 2.51 | 0.46 |
| 1:CA:1074:G:O2' | 2:CB:102:THR:HG23 | 2.15 | 0.46 |
| 1:CA:1130:A:C8 | 1:CA:1146:A:N1 | 2.84 | 0.46 |
| 1:CA:1491:G:C5 | 1:CA:1492:A:C6 | 3.04 | 0.46 |
| 8:CH:96:MET:HB2 | 8:CH:99:LEU:O | 2.16 | 0.46 |
| 10:CJ:74:VAL:HG12 | 10:CJ:75:ASP:N | 2.31 | 0.46 |
| 11:CK:113:VAL:HB | 18:CR:73:ARG:NH2 | 2.31 | 0.46 |
| 13:CM:13:LYS:O | 13:CM:14:HIS:CG | 2.69 | 0.46 |
| 22:DA:79:C:C2' | 22:DA:346:A:N3 | 2.79 | 0.46 |
| 22:DA:303:G:C2 | 22:DA:315:G:C6 | 3.04 | 0.46 |
| 22:DA:396:G:H2' | 22:DA:397:U:O5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:532:A:N7 | 22:DA:2021:C:O2' | 2.43 | 0.46 |
| 22:DA:685:A:C2 | 22:DA:689:A:C6 | 3.04 | 0.46 |
| 22:DA:945:A:N7 | 22:DA:2448:A:C2 | 2.84 | 0.46 |
| 22:DA:1304:A:C6 | 22:DA:1305:C:C4 | 3.04 | 0.46 |
| 22:DA:1389:G:N2 | 22:DA:1398:C:N3 | 2.64 | 0.46 |
| 22:DA:1404:C:C2' | 22:DA:1405:U:O5' | 2.63 | 0.46 |
| 22:DA:1551:A:C5 | 22:DA:1552:A:C8 | 3.04 | 0.46 |
| 22:DA:1847:A:H2' | 22:DA:1848:A:OP2 | 2.16 | 0.46 |
| 22:DA:1931:U:OP2 | 22:DA:1968:G:N2 | 2.47 | 0.46 |
| 22:DA:2094:A:C2 | 22:DA:2196:C:C2 | 3.04 | 0.46 |
| 22:DA:2823:A:C5 | 22:DA:2824:C:C5 | 3.04 | 0.46 |
| 27:DF:123:ASP:N | 27:DF:127:ASN:O | 2.49 | 0.46 |
| 30:DI:101:ILE:HG22 | 30:DI:102:SER:N | 2.30 | 0.46 |
| 33:DL:29:LYS:O | 33:DL:30:THR:OG1 | 2.31 | 0.46 |
| 35:DN:90:ARG:NH2 | 35:DN:116:VAL:HG11 | 2.31 | 0.46 |
| 43:DV:42:LEU:HD23 | 43:DV:42:LEU:N | 2.31 | 0.46 |
| 45:DX:65:ASP:O | 45:DX:66:THR:C | 2.54 | 0.46 |
| 1:AA:144:G:C5 | 1:AA:179:A:C2 | 3.04 | 0.45 |
| 1:AA:275:G:H5' | 17:AQ:17:MET:CE | 2.46 | 0.45 |
| 1:AA:575:G:C6 | 1:AA:821:G:N7 | 2.84 | 0.45 |
| 1:AA:674:G:N2 | 1:AA:717:U:O2 | 2.49 | 0.45 |
| 1:AA:949:A:C4 | 1:AA:950:U:C6 | 3.04 | 0.45 |
| 1:AA:1026:G:N1 | 1:AA:1035:A:C2 | 2.84 | 0.45 |
| 1:AA:1202:U:C5 | 1:AA:1203:C:C5 | 3.04 | 0.45 |
| 1:AA:1210:C:C4 | 1:AA:1211:U:C5 | 3.04 | 0.45 |
| 2:AB:32:PHE:CD1 | 2:AB:32:PHE:C | 2.89 | 0.45 |
| 2:AB:62:SER:C | 2:AB:64:LYS:N | 2.69 | 0.45 |
| 5:AE:149:SER:CB | 5:AE:152:MET:HB2 | 2.46 | 0.45 |
| 7:AG:80:VAL:O | 7:AG:81:GLY:C | 2.55 | 0.45 |
| 8:AH:95:VAL:HG12 | 8:AH:96:MET:N | 2.31 | 0.45 |
| 9:AI:91:ASP:OD2 | 9:AI:91:ASP:C | 2.54 | 0.45 |
| 10:AJ:59:LYS:N | 10:AJ:59:LYS:HD2 | 2.31 | 0.45 |
| 11:AK:102:ALA:C | 11:AK:104:GLY:N | 2.69 | 0.45 |
| 15:AO:18:ASP:OD1 | 15:AO:18:ASP:N | 2.49 | 0.45 |
| 20:AT:25:ARG:HG2 | 20:AT:29:ARG:NH1 | 2.31 | 0.45 |
| 22:BA:368:A:N6 | 22:BA:369:U:O4 | 2.49 | 0.45 |
| 22:BA:878:A:H5' | 22:BA:879:G:OP2 | 2.17 | 0.45 |
| 22:BA:1153:C:H2' | 22:BA:1154:G:O4' | 2.16 | 0.45 |
| 22:BA:1413:A:O2' | 22:BA:1414:C:H5' | 2.16 | 0.45 |
| 22:BA:1422:G:C4 | 22:BA:1423:G:C8 | 3.04 | 0.45 |
| 22:BA:1840:G:C6 | 22:BA:1841:U:C4 | 3.05 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1856:U:C4 | 22:BA:1857:G:C6 | 3.04 | 0.45 |
| 22:BA:1875:G:HO2' | 22:BA:1876:A:P | 2.38 | 0.45 |
| 22:BA:2885:G:C2' | 22:BA:2886:A:H5' | 2.46 | 0.45 |
| 32:BK:73:ASP:OD1 | 32:BK:75:SER:OG | 2.30 | 0.45 |
| 33:BL:91:ASP:O | 33:BL:94:THR:HB | 2.16 | 0.45 |
| 35:BN:119:SER:O | 35:BN:120:GLU:C | 2.53 | 0.45 |
| 38:BQ:110:VAL:O | 38:BQ:114:LYS:HG3 | 2.15 | 0.45 |
| 39:BR:49:ILE:O | 39:BR:51:VAL:O | 2.34 | 0.45 |
| 53:B5:191:ARG:O | 53:B5:195:ARG:CB | 2.63 | 0.45 |
| 1:CA:285:C:H2' | 1:CA:286:C:C6 | 2.52 | 0.45 |
| 1:CA:451:A:N6 | 1:CA:480:U:H2' | 2.31 | 0.45 |
| 1:CA:570:G:H5'' | 1:CA:571:U:OP2 | 2.16 | 0.45 |
| 1:CA:711:G:N2 | 1:CA:712:A:C4 | 2.84 | 0.45 |
| 1:CA:1006:G:OP1 | 1:CA:1038:C:C5' | 2.64 | 0.45 |
| 1:CA:1250:A:C2 | 1:CA:1287:A:N1 | 2.84 | 0.45 |
| 1:CA:1255:G:C6 | 1:CA:1279:G:N7 | 2.83 | 0.45 |
| 1:CA:1299:A:H2' | 1:CA:1299:A:N3 | 2.30 | 0.45 |
| 2:CB:18:HIS:O | 2:CB:19:GLN:HB2 | 2.16 | 0.45 |
| 2:CB:30:PHE:CD1 | 2:CB:30:PHE:N | 2.81 | 0.45 |
| 5:CE:15:LEU:C | 5:CE:15:LEU:CD1 | 2.84 | 0.45 |
| 8:CH:2:SER:O | 8:CH:4:GLN:N | 2.49 | 0.45 |
| 10:CJ:15:HIS:CD2 | 10:CJ:15:HIS:C | 2.88 | 0.45 |
| 12:CL:43:LYS:O | 12:CL:44:LYS:O | 2.34 | 0.45 |
| 12:CL:108:LYS:O | 12:CL:109:ASP:HB2 | 2.16 | 0.45 |
| 15:CO:35:GLN:O | 15:CO:38:HIS:N | 2.50 | 0.45 |
| 17:CQ:46:VAL:HG11 | 17:CQ:61:ILE:CG1 | 2.45 | 0.45 |
| 22:DA:371:A:N6 | 22:DA:402:A:OP2 | 2.48 | 0.45 |
| 22:DA:408:G:C6 | 22:DA:409:G:C5 | 3.04 | 0.45 |
| 22:DA:466:A:N1 | 22:DA:795:C:O2' | 2.36 | 0.45 |
| 22:DA:585:G:H2' | 22:DA:586:A:N7 | 2.31 | 0.45 |
| 22:DA:830:G:C2 | 22:DA:2448:A:N7 | 2.84 | 0.45 |
| 22:DA:858:G:H3' | 22:DA:859:G:C8 | 2.51 | 0.45 |
| 22:DA:1208:C:C5 | 22:DA:1209:U:C5 | 3.04 | 0.45 |
| 22:DA:1327:A:N6 | 22:DA:1328:A:C2 | 2.83 | 0.45 |
| 22:DA:2725:A:C5 | 22:DA:2727:A:N7 | 2.84 | 0.45 |
| 24:DC:121:ASP:OD1 | 24:DC:121:ASP:N | 2.50 | 0.45 |
| 25:DD:125:TRP:CE3 | 25:DD:160:LYS:HD3 | 2.50 | 0.45 |
| 29:DH:39:ALA:O | 29:DH:41:LYS:N | 2.47 | 0.45 |
| 33:DL:120:VAL:CG1 | 33:DL:121:THR:N | 2.80 | 0.45 |
| 1:AA:559:A:H2' | 1:AA:559:A:N3 | 2.30 | 0.45 |
| 1:AA:1035:A:H2' | 1:AA:1036:A:C1' | 2.45 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AA:1197:A:OP2 | 58:AA:1785:HOH:O | 2.21 | 0.45 |
| 1:AA:1211:U:O2' | 1:AA:1212:U:P | 2.73 | 0.45 |
| 3:AC:167:TRP:O | 3:AC:168:TYR:HB2 | 2.15 | 0.45 |
| 8:AH:42:GLU:OE1 | 8:AH:42:GLU:CA | 2.65 | 0.45 |
| 10:AJ:57:VAL:O | 10:AJ:58:ASN:HB2 | 2.16 | 0.45 |
| 16:AP:59:HIS:O | 16:AP:63:GLN:HB2 | 2.17 | 0.45 |
| 21:AU:37:PHE:HB3 | 21:AU:41:PRO:HG3 | 1.97 | 0.45 |
| 22:BA:242:G:C8 | 51:B3:5:LYS:HG2 | 2.51 | 0.45 |
| 22:BA:868:U:C4 | 22:BA:869:G:N7 | 2.84 | 0.45 |
| 22:BA:989:G:C8 | 47:BZ:14:ILE:HD11 | 2.51 | 0.45 |
| 22:BA:1008:A:N6 | 22:BA:1136:G:O6 | 2.50 | 0.45 |
| 22:BA:1340:U:OP1 | 41:BT:19:LYS:NZ | 2.50 | 0.45 |
| 22:BA:1464:G:H2' | 22:BA:1465:G:C8 | 2.51 | 0.45 |
| 22:BA:1474:U:C3' | 22:BA:1475:G:H5' | 2.46 | 0.45 |
| 22:BA:1613:G:H4' | 50:B2:3:ARG:HD3 | 1.98 | 0.45 |
| 22:BA:1622:G:C2 | 22:BA:1623:G:C8 | 3.04 | 0.45 |
| 22:BA:1709:U:C2 | 22:BA:1750:G:N2 | 2.85 | 0.45 |
| 22:BA:1820:U:H4' | 22:BA:1821:A:OP2 | 2.16 | 0.45 |
| 22:BA:1949:G:N2 | 22:BA:1958:C:O2 | 2.49 | 0.45 |
| 22:BA:2001:C:H4' | 22:BA:2689:U:H2' | 1.97 | 0.45 |
| 22:BA:2727:A:C6 | 22:BA:2728:U:O4 | 2.70 | 0.45 |
| 24:BC:71:LYS:HB3 | 24:BC:96:TYR:CE2 | 2.50 | 0.45 |
| 30:BI:19:ASN:N | 30:BI:20:PRO:HD2 | 2.31 | 0.45 |
| 33:BL:57:LEU:HA | 33:BL:60:ARG:HD2 | 1.97 | 0.45 |
| 34:BM:2:LEU:HD22 | 34:BM:2:LEU:N | 2.32 | 0.45 |
| 44:BW:41:ARG:HA | 44:BW:41:ARG:HD3 | 1.54 | 0.45 |
| 1:CA:57:G:H2' | 1:CA:58:C:C6 | 2.51 | 0.45 |
| 1:CA:68:G:O4' | 1:CA:171:A:H1' | 2.16 | 0.45 |
| 1:CA:518:C:H2' | 1:CA:530:G:C8 | 2.51 | 0.45 |
| 1:CA:583:A:C2 | 1:CA:759:A:C5 | 3.04 | 0.45 |
| 1:CA:741:G:N1 | 1:CA:742:G:C5 | 2.84 | 0.45 |
| 1:CA:888:G:H4' | 1:CA:1488:G:O2' | 2.16 | 0.45 |
| 1:CA:1087:G:N2 | 1:CA:1099:G:H1' | 2.31 | 0.45 |
| 5:CE:101:GLU:O | 5:CE:103:THR:CA | 2.62 | 0.45 |
| 9:CI:50:GLN:N | 9:CI:51:PRO:HD2 | 2.31 | 0.45 |
| 12:CL:25:GLU:HB2 | 12:CL:27:CYS:SG | 2.57 | 0.45 |
| 21:CU:34:ARG:CD | 21:CU:35:ARG:HB2 | 2.46 | 0.45 |
| 22:DA:183:C:H1' | 22:DA:433:C:H1' | 1.97 | 0.45 |
| 22:DA:189:G:C4 | 22:DA:205:G:N2 | 2.84 | 0.45 |
| 22:DA:230:G:C2 | 22:DA:231:A:N7 | 2.84 | 0.45 |
| 22:DA:414:C:N4 | 22:DA:415:A:N6 | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:1288:G:C5 | 22:DA:1327:A:C2 | 3.04 | 0.45 |
| 22:DA:1649:G:O6 | 22:DA:2009:A:N6 | 2.49 | 0.45 |
| 22:DA:1682:G:H2' | 22:DA:1683:U:C6 | 2.51 | 0.45 |
| 22:DA:1731:G:H2' | 22:DA:1732:C:H3' | 1.98 | 0.45 |
| 22:DA:1797:G:O3' | 24:DC:256:LYS:HA | 2.16 | 0.45 |
| 22:DA:2209:G:C6 | 22:DA:2210:U:O4 | 2.68 | 0.45 |
| 22:DA:2267:A:OP2 | 22:DA:2268:A:H5'' | 2.16 | 0.45 |
| 22:DA:2322:A:H2' | 22:DA:2323:G:O4' | 2.16 | 0.45 |
| 22:DA:2507:C:N4 | 22:DA:2508:G:C6 | 2.84 | 0.45 |
| 22:DA:2552:U:C2 | 22:DA:2554:U:C5' | 2.99 | 0.45 |
| 22:DA:2636:C:H4' | 25:DD:81:GLU:CD | 2.37 | 0.45 |
| 24:DC:266:PHE:N | 24:DC:266:PHE:CD1 | 2.83 | 0.45 |
| 29:DH:112:LYS:HG2 | 29:DH:113:SER:N | 2.32 | 0.45 |
| 33:DL:54:GLN:HG2 | 33:DL:55:MET:N | 2.31 | 0.45 |
| 40:DS:22:ASP:OD2 | 40:DS:22:ASP:N | 2.49 | 0.45 |
| 41:DT:45:ALA:HA | 41:DT:49:LYS:HE3 | 1.98 | 0.45 |
| 1:AA:1028:C:O2 | 1:AA:1034:G:C6 | 2.69 | 0.45 |
| 1:AA:1107:C:N3 | 1:AA:1108:G:C8 | 2.85 | 0.45 |
| 2:AB:47:VAL:O | 2:AB:49:MET:N | 2.50 | 0.45 |
| 2:AB:50:PHE:CD2 | 2:AB:51:ASN:OD1 | 2.70 | 0.45 |
| 7:AG:129:GLU:O | 7:AG:130:ASN:C | 2.55 | 0.45 |
| 22:BA:88:G:C6 | 22:BA:89:A:N7 | 2.84 | 0.45 |
| 22:BA:697:G:H2' | 22:BA:698:C:C6 | 2.51 | 0.45 |
| 22:BA:1138:G:O2' | 31:BJ:107:GLY:HA3 | 2.17 | 0.45 |
| 22:BA:1176:U:OP1 | 22:BA:1176:U:H4' | 2.16 | 0.45 |
| 22:BA:1385:A:H4' | 22:BA:1386:C:OP1 | 2.17 | 0.45 |
| 22:BA:1430:G:C6 | 22:BA:1431:A:C5 | 3.04 | 0.45 |
| 22:BA:2164:C:H3' | 22:BA:2165:C:H5'' | 1.98 | 0.45 |
| 26:BE:147:LEU:HB2 | 26:BE:183:PHE:CD1 | 2.51 | 0.45 |
| 27:BF:158:THR:HG22 | 27:BF:160:ALA:H | 1.81 | 0.45 |
| 29:BH:94:ILE:HG23 | 29:BH:98:ASP:CB | 2.47 | 0.45 |
| 36:BO:64:TYR:O | 36:BO:67:ASN:ND2 | 2.49 | 0.45 |
| 49:B1:26:ASN:OD1 | 49:B1:28:ARG:HB3 | 2.15 | 0.45 |
| 53:B5:78:ILE:HG23 | 53:B5:78:ILE:O | 2.17 | 0.45 |
| 1:CA:128:G:N2 | 1:CA:234:C:C2 | 2.85 | 0.45 |
| 1:CA:219:U:C2 | 1:CA:220:G:C8 | 3.04 | 0.45 |
| 1:CA:230:G:H2' | 1:CA:231:U:O4' | 2.16 | 0.45 |
| 1:CA:369:G:C6 | 1:CA:370:C:C4 | 3.03 | 0.45 |
| 1:CA:575:G:C6 | 1:CA:821:G:C5 | 3.04 | 0.45 |
| 1:CA:798:U:C2' | 1:CA:799:G:O5' | 2.64 | 0.45 |
| 1:CA:821:G:H2' | 1:CA:822:U:H6 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1005:A:N7 | 1:CA:1006:G:C4 | 2.84 | 0.45 |
| 1:CA:1304:G:O2' | 1:CA:1333:A:N6 | 2.41 | 0.45 |
| 1:CA:1377:A:C5 | 7:CG:7:ILE:HD12 | 2.51 | 0.45 |
| 4:CD:11:LEU:HD23 | 4:CD:11:LEU:N | 2.31 | 0.45 |
| 22:DA:33:C:O2 | 22:DA:447:A:N6 | 2.49 | 0.45 |
| 22:DA:308:G:N1 | 22:DA:309:A:C2 | 2.84 | 0.45 |
| 22:DA:649:G:H2' | 22:DA:650:C:C6 | 2.51 | 0.45 |
| 22:DA:1337:G:H2' | 22:DA:1338:G:O4' | 2.15 | 0.45 |
| 22:DA:1355:G:N1 | 22:DA:1356:G:C8 | 2.84 | 0.45 |
| 22:DA:1385:A:C2 | 22:DA:1386:C:C2 | 3.04 | 0.45 |
| 22:DA:1555:G:N1 | 22:DA:1556:C:C2 | 2.84 | 0.45 |
| 22:DA:1666:G:N7 | 22:DA:1667:G:C6 | 2.85 | 0.45 |
| 22:DA:1866:A:N7 | 22:DA:1867:G:C8 | 2.84 | 0.45 |
| 22:DA:2033:A:H4' | 22:DA:2034:U:OP1 | 2.16 | 0.45 |
| 22:DA:2106:U:H2' | 22:DA:2107:G:C8 | 2.51 | 0.45 |
| 22:DA:2148:G:C2 | 22:DA:2149:U:C5 | 3.04 | 0.45 |
| 22:DA:2163:A:OP2 | 22:DA:2171:A:C8 | 2.69 | 0.45 |
| 22:DA:2387:U:H1' | 44:DW:41:ARG:HD2 | 1.99 | 0.45 |
| 22:DA:2655:G:HO2' | 22:DA:2656:U:P | 2.38 | 0.45 |
| 22:DA:2718:G:OP1 | 37:DP:98:TYR:CD1 | 2.70 | 0.45 |
| 22:DA:2748:A:C2 | 22:DA:2757:A:C5 | 3.05 | 0.45 |
| 22:DA:2804:U:C4 | 22:DA:2805:C:C4 | 3.04 | 0.45 |
| 22:DA:2847:U:C2' | 22:DA:2848:G:H5' | 2.46 | 0.45 |
| 22:DA:2896:C:H2' | 22:DA:2897:U:O5' | 2.16 | 0.45 |
| 23:DB:100:G:H2' | 23:DB:101:A:O4' | 2.17 | 0.45 |
| 31:DJ:12:LYS:HE3 | 31:DJ:14:ASP:OD2 | 2.16 | 0.45 |
| 34:DM:69:PRO:O | 34:DM:93:VAL:O | 2.35 | 0.45 |
| 43:DV:42:LEU:HD12 | 43:DV:47:VAL:HG21 | 1.99 | 0.45 |
| 46:DY:46:VAL:O | 46:DY:50:VAL:HG23 | 2.16 | 0.45 |
| 1:AA:351:G:H4' | 1:AA:352:C:OP2 | 2.16 | 0.45 |
| 1:AA:522:C:N4 | 1:AA:523:A:C6 | 2.84 | 0.45 |
| 1:AA:554:A:H2' | 1:AA:555:U:C6 | 2.52 | 0.45 |
| 1:AA:757:U:OP1 | 1:AA:822:U:O2' | 2.28 | 0.45 |
| 1:AA:1162:C:H2' | 1:AA:1163:A:O4' | 2.16 | 0.45 |
| 1:AA:1163:A:C2 | 1:AA:1174:G:C2 | 3.04 | 0.45 |
| 1:AA:1202:U:C2 | 1:AA:1203:C:C6 | 3.05 | 0.45 |
| 1:AA:1241:G:C2 | 1:AA:1242:G:C5 | 3.05 | 0.45 |
| 2:AB:155:GLY:O | 2:AB:157:LEU:N | 2.50 | 0.45 |
| 3:AC:39:VAL:O | 3:AC:43:LEU:HB2 | 2.16 | 0.45 |
| 3:AC:126:ARG:O | 3:AC:127:ARG:CB | 2.64 | 0.45 |
| 5:AE:75:ALA:O | 5:AE:82:GLN:NE2 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AF:29:ILE:HG23 | 6:AF:66:ALA:HB2 | 1.98 | 0.45 |
| 7:AG:67:GLU:HA | 7:AG:70:ARG:HE | 1.82 | 0.45 |
| 7:AG:146:GLU:O | 7:AG:149:LYS:HB2 | 2.16 | 0.45 |
| 9:AI:21:ILE:CG2 | 9:AI:22:LYS:N | 2.78 | 0.45 |
| 12:AL:55:VAL:HG21 | 12:AL:80:ILE:HD11 | 1.99 | 0.45 |
| 16:AP:4:ILE:HG13 | 16:AP:21:VAL:HG22 | 1.99 | 0.45 |
| 16:AP:10:GLY:O | 16:AP:11:ALA:HB2 | 2.16 | 0.45 |
| 21:AU:10:GLU:CB | 21:AU:11:PRO:HD3 | 2.46 | 0.45 |
| 22:BA:790:U:HO2' | 22:BA:791:C:P | 2.37 | 0.45 |
| 22:BA:1403:A:H2' | 22:BA:1404:C:C6 | 2.52 | 0.45 |
| 22:BA:1947:C:O2' | 22:BA:1948:G:H5' | 2.16 | 0.45 |
| 22:BA:2020:A:H5' | 48:B0:9:THR:CG2 | 2.46 | 0.45 |
| 22:BA:2031:A:C6 | 22:BA:2498:C:H1' | 2.51 | 0.45 |
| 22:BA:2077:A:C6 | 22:BA:2435:A:N6 | 2.85 | 0.45 |
| 22:BA:2575:C:O2' | 25:BD:145:SER:HB2 | 2.17 | 0.45 |
| 22:BA:2808:G:C2 | 22:BA:2891:U:C6 | 3.04 | 0.45 |
| 27:BF:175:PHE:O | 27:BF:176:PRO:O | 2.35 | 0.45 |
| 32:BK:41:ILE:CD1 | 32:BK:58:LEU:HD22 | 2.47 | 0.45 |
| 46:BY:53:VAL:O | 46:BY:56:LEU:O | 2.35 | 0.45 |
| 1:CA:299:G:N2 | 1:CA:565:U:O2 | 2.49 | 0.45 |
| 1:CA:607:A:C2 | 1:CA:608:A:C4 | 3.05 | 0.45 |
| 1:CA:819:A:H4' | 1:CA:820:U:OP2 | 2.17 | 0.45 |
| 1:CA:891:U:C5 | 1:CA:906:A:C2 | 3.05 | 0.45 |
| 1:CA:971:G:OP1 | 1:CA:972:C:H5'' | 2.16 | 0.45 |
| 2:CB:167:ASP:OD2 | 2:CB:191:SER:HA | 2.17 | 0.45 |
| 8:CH:89:LYS:HG3 | 8:CH:90:ASP:N | 2.32 | 0.45 |
| 9:CI:46:MET:O | 9:CI:49:ARG:HB3 | 2.16 | 0.45 |
| 10:CJ:15:HIS:HB3 | 10:CJ:70:HIS:CD2 | 2.52 | 0.45 |
| 12:CL:12:ARG:HG2 | 12:CL:12:ARG:HH11 | 1.81 | 0.45 |
| 14:CN:23:LYS:HG3 | 14:CN:24:ARG:N | 2.31 | 0.45 |
| 16:CP:38:PHE:O | 16:CP:38:PHE:CD1 | 2.69 | 0.45 |
| 17:CQ:81:LYS:N | 17:CQ:81:LYS:HD2 | 2.32 | 0.45 |
| 21:CU:14:VAL:O | 21:CU:16:LEU:HG | 2.17 | 0.45 |
| 21:CU:39:GLU:HA | 21:CU:42:THR:OG1 | 2.16 | 0.45 |
| 22:DA:137:U:H2' | 22:DA:140:C:C2 | 2.52 | 0.45 |
| 22:DA:192:C:H2' | 22:DA:193:U:H5' | 1.99 | 0.45 |
| 22:DA:220:G:H5'' | 22:DA:221:A:P | 2.57 | 0.45 |
| 22:DA:282:A:N1 | 22:DA:359:G:C6 | 2.84 | 0.45 |
| 22:DA:600:G:H1' | 26:DE:100:MET:CG | 2.46 | 0.45 |
| 22:DA:727:A:H2' | 22:DA:728:G:C8 | 2.51 | 0.45 |
| 22:DA:836:G:C5 | 22:DA:837:C:C4 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:965:C:H4' | 22:DA:2273:A:H1' | 1.99 | 0.45 |
| 22:DA:1059:G:H1' | 30:DI:117:MET:HE1 | 1.97 | 0.45 |
| 22:DA:1203:U:O4 | 22:DA:1204:A:C6 | 2.70 | 0.45 |
| 22:DA:1246:A:OP2 | 33:DL:13:LYS:NZ | 2.49 | 0.45 |
| 22:DA:1332:G:C6 | 22:DA:1609:A:N7 | 2.85 | 0.45 |
| 22:DA:1565:C:O2' | 22:DA:1566:A:OP2 | 2.28 | 0.45 |
| 22:DA:1598:A:H2' | 22:DA:1599:U:O4' | 2.17 | 0.45 |
| 22:DA:1799:G:N1 | 22:DA:1819:A:OP2 | 2.46 | 0.45 |
| 22:DA:2215:C:O2' | 22:DA:2216:G:H5' | 2.17 | 0.45 |
| 22:DA:2221:G:C6 | 22:DA:2222:C:C5 | 3.04 | 0.45 |
| 22:DA:2283:C:C4 | 22:DA:2389:G:C4 | 3.04 | 0.45 |
| 22:DA:2712:C:C2 | 22:DA:2715:C:OP1 | 2.70 | 0.45 |
| 22:DA:2756:U:C4 | 22:DA:2759:G:O6 | 2.70 | 0.45 |
| 22:DA:2898:U:H2' | 22:DA:2899:A:C8 | 2.52 | 0.45 |
| 25:DD:101:PHE:O | 25:DD:103:ASP:N | 2.50 | 0.45 |
| 29:DH:34:GLY:O | 29:DH:35:LYS:CD | 2.65 | 0.45 |
| 42:DU:39:ILE:HG22 | 42:DU:39:ILE:O | 2.16 | 0.45 |
| 1:AA:66:A:H4' | 1:AA:173:U:C5 | 2.52 | 0.45 |
| 1:AA:69:G:H5' | 1:AA:70:U:P | 2.57 | 0.45 |
| 1:AA:346:G:P | 32:BK:105:ARG:NH1 | 2.89 | 0.45 |
| 1:AA:767:A:H2' | 1:AA:768:A:O4' | 2.17 | 0.45 |
| 1:AA:1010:U:O2 | 1:AA:1019:A:N1 | 2.50 | 0.45 |
| 1:AA:1033:G:O2' | 1:AA:1034:G:H5' | 2.16 | 0.45 |
| 1:AA:1237:C:C4 | 1:AA:1336:C:N3 | 2.84 | 0.45 |
| 2:AB:119:THR:O | 2:AB:120:GLN:HB2 | 2.17 | 0.45 |
| 4:AD:15:GLU:OE2 | 4:AD:56:ARG:NH2 | 2.49 | 0.45 |
| 7:AG:145:ALA:C | 7:AG:147:ALA:H | 2.20 | 0.45 |
| 9:AI:127:PHE:O | 9:AI:127:PHE:CD2 | 2.70 | 0.45 |
| 10:AJ:86:ALA:O | 10:AJ:90:LEU:HB2 | 2.16 | 0.45 |
| 12:AL:86:ARG:HA | 12:AL:94:ARG:HA | 1.98 | 0.45 |
| 16:AP:19:VAL:HG13 | 16:AP:37:GLY:C | 2.36 | 0.45 |
| 20:AT:44:LYS:HD3 | 20:AT:87:ALA:HA | 1.98 | 0.45 |
| 20:AT:54:MET:HA | 20:AT:57:ILE:HG22 | 1.98 | 0.45 |
| 22:BA:55:G:N2 | 22:BA:56:A:C4 | 2.85 | 0.45 |
| 22:BA:404:A:C8 | 22:BA:406:G:C6 | 3.04 | 0.45 |
| 22:BA:1026:G:H2' | 22:BA:1027:A:C8 | 2.51 | 0.45 |
| 22:BA:1131:G:C6 | 31:BJ:77:HIS:CD2 | 3.05 | 0.45 |
| 22:BA:1775:U:H2' | 22:BA:1776:G:O5' | 2.17 | 0.45 |
| 22:BA:1911:U:H2' | 22:BA:1918:A:N1 | 2.31 | 0.45 |
| 22:BA:2154:A:H2' | 22:BA:2155:U:C6 | 2.51 | 0.45 |
| 27:BF:108:VAL:HG12 | 27:BF:109:PRO:HD3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BF:121:SER:HB3 | 27:BF:129:SER:O | 2.16 | 0.45 |
| 28:BG:69:ARG:C | 28:BG:69:ARG:HD3 | 2.36 | 0.45 |
| 30:BI:58:VAL:HG12 | 30:BI:59:ILE:H | 1.81 | 0.45 |
| 31:BJ:17:VAL:HG23 | 31:BJ:137:PRO:HB2 | 1.98 | 0.45 |
| 31:BJ:73:VAL:HG11 | 31:BJ:75:TYR:CZ | 2.52 | 0.45 |
| 31:BJ:77:HIS:HA | 31:BJ:83:GLY:O | 2.17 | 0.45 |
| 36:BO:31:THR:HG22 | 36:BO:34:HIS:N | 2.32 | 0.45 |
| 42:BU:72:ILE:HD12 | 42:BU:72:ILE:N | 2.32 | 0.45 |
| 42:BU:99:ASN:O | 42:BU:100:SER:C | 2.54 | 0.45 |
| 53:B5:214:TYR:O | 53:B5:215:VAL:CB | 2.64 | 0.45 |
| 1:CA:162:A:H2' | 1:CA:163:C:O4' | 2.17 | 0.45 |
| 1:CA:1272:G:H2' | 1:CA:1273:C:O4' | 2.16 | 0.45 |
| 1:CA:1317:C:C4 | 14:CN:53:ARG:HD2 | 2.51 | 0.45 |
| 2:CB:71:GLY:CA | 2:CB:164:ILE:CG2 | 2.95 | 0.45 |
| 2:CB:131:LYS:HE2 | 2:CB:131:LYS:HA | 1.98 | 0.45 |
| 2:CB:135:LEU:O | 2:CB:139:ARG:HG3 | 2.17 | 0.45 |
| 2:CB:139:ARG:HD2 | 2:CB:140:GLU:N | 2.31 | 0.45 |
| 2:CB:148:LEU:HD12 | 2:CB:148:LEU:N | 2.32 | 0.45 |
| 12:CL:24:LEU:HD22 | 12:CL:59:ASN:OD1 | 2.17 | 0.45 |
| 21:CU:24:GLU:OE1 | 21:CU:24:GLU:N | 2.50 | 0.45 |
| 22:DA:36:G:N1 | 22:DA:445:C:C4 | 2.85 | 0.45 |
| 22:DA:78:U:OP2 | 46:DY:2:LYS:HD2 | 2.16 | 0.45 |
| 22:DA:515:A:C8 | 22:DA:516:C:C6 | 3.04 | 0.45 |
| 22:DA:606:U:O2' | 26:DE:95:LYS:NZ | 2.46 | 0.45 |
| 22:DA:613:A:OP2 | 22:DA:614:A:N7 | 2.50 | 0.45 |
| 22:DA:656:G:O2' | 22:DA:657:U:H5' | 2.17 | 0.45 |
| 22:DA:1292:G:C6 | 22:DA:1293:C:N4 | 2.84 | 0.45 |
| 22:DA:1357:C:H2' | 22:DA:1358:G:C5' | 2.47 | 0.45 |
| 22:DA:1435:G:O2' | 22:DA:1436:G:H5' | 2.16 | 0.45 |
| 22:DA:1663:G:C6 | 22:DA:1992:G:N7 | 2.85 | 0.45 |
| 22:DA:2371:G:C2 | 22:DA:2372:U:C6 | 3.04 | 0.45 |
| 22:DA:2848:G:C8 | 37:DP:95:ALA:HB2 | 2.51 | 0.45 |
| 29:DH:147:VAL:HG12 | 29:DH:148:ALA:N | 2.32 | 0.45 |
| 40:DS:61:ASN:O | 40:DS:62:ASP:CB | 2.63 | 0.45 |
| 1:AA:731:G:OP1 | 1:AA:766:A:H1' | 2.17 | 0.45 |
| 1:AA:771:G:C5 | 1:AA:772:U:C5 | 3.05 | 0.45 |
| 1:AA:900:A:N1 | 1:AA:901:A:C2 | 2.85 | 0.45 |
| 1:AA:999:C:H2' | 1:AA:1000:A:C8 | 2.51 | 0.45 |
| 1:AA:1012:A:N1 | 1:AA:1018:G:N7 | 2.64 | 0.45 |
| 1:AA:1309:G:C6 | 1:AA:1310:G:C5 | 3.04 | 0.45 |
| 2:AB:104:TRP:CZ3 | 2:AB:158:PRO:HD3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:125:THR:O | 2:AB:126:PHE:HB3 | 2.16 | 0.45 |
| 2:AB:132:LYS:HG3 | 2:AB:133:GLU:N | 2.32 | 0.45 |
| 4:AD:76:TYR:CD1 | 4:AD:76:TYR:C | 2.89 | 0.45 |
| 4:AD:107:PHE:CG | 4:AD:145:ILE:HD11 | 2.50 | 0.45 |
| 7:AG:99:LEU:O | 7:AG:100:ALA:C | 2.55 | 0.45 |
| 8:AH:11:LEU:HD11 | 8:AH:127:CYS:CB | 2.47 | 0.45 |
| 11:AK:108:THR:HG22 | 11:AK:109:ASN:ND2 | 2.31 | 0.45 |
| 12:AL:21:VAL:HG22 | 12:AL:21:VAL:O | 2.17 | 0.45 |
| 20:AT:44:LYS:HB3 | 20:AT:87:ALA:HB1 | 1.99 | 0.45 |
| 22:BA:669:G:C5 | 22:BA:801:G:C6 | 3.04 | 0.45 |
| 22:BA:749:A:H4' | 22:BA:1271:G:N3 | 2.32 | 0.45 |
| 22:BA:909:A:H2' | 22:BA:912:C:C5 | 2.51 | 0.45 |
| 22:BA:1056:G:N1 | 22:BA:1102:C:C5 | 2.84 | 0.45 |
| 22:BA:1456:G:C5 | 22:BA:1457:U:C5 | 3.04 | 0.45 |
| 22:BA:1469:A:C2 | 22:BA:1470:A:C4 | 3.04 | 0.45 |
| 22:BA:1503:A:N6 | 22:BA:1504:A:N6 | 2.65 | 0.45 |
| 22:BA:1586:A:N7 | 22:BA:1587:G:N7 | 2.65 | 0.45 |
| 22:BA:1683:U:O2' | 22:BA:1684:G:H5' | 2.16 | 0.45 |
| 22:BA:2185:U:C2' | 22:BA:2186:G:H5' | 2.47 | 0.45 |
| 22:BA:2488:G:C2' | 22:BA:2489:U:H5' | 2.47 | 0.45 |
| 28:BG:118:PRO:O | 28:BG:119:ALA:C | 2.55 | 0.45 |
| 28:BG:126:PRO:HG2 | 28:BG:130:GLU:HB3 | 1.98 | 0.45 |
| 31:BJ:7:LYS:HA | 31:BJ:8:PRO:HD3 | 1.85 | 0.45 |
| 39:BR:74:ILE:O | 39:BR:86:GLN:HA | 2.16 | 0.45 |
| 41:BT:34:VAL:HG21 | 41:BT:43:ILE:HD11 | 1.99 | 0.45 |
| 42:BU:49:VAL:O | 42:BU:49:VAL:HG23 | 2.17 | 0.45 |
| 45:BX:3:ARG:CD | 45:BX:30:LEU:HD13 | 2.47 | 0.45 |
| 1:CA:109:A:N1 | 1:CA:327:A:C6 | 2.84 | 0.45 |
| 1:CA:862:C:C4 | 1:CA:863:U:C5 | 3.05 | 0.45 |
| 1:CA:926:G:C6 | 1:CA:1505:G:C6 | 3.04 | 0.45 |
| 1:CA:951:G:N3 | 1:CA:970:C:O2' | 2.39 | 0.45 |
| 1:CA:992:U:C2 | 1:CA:1043:G:N7 | 2.85 | 0.45 |
| 1:CA:1053:G:C4 | 1:CA:1199:U:C5 | 3.05 | 0.45 |
| 1:CA:1181:G:O2' | 1:CA:1182:G:C8 | 2.64 | 0.45 |
| 1:CA:1513:A:H2' | 1:CA:1514:G:C8 | 2.52 | 0.45 |
| 4:CD:14:ARG:HG2 | 4:CD:56:ARG:NH2 | 2.31 | 0.45 |
| 14:CN:54:ASP:HA | 14:CN:59:ARG:CD | 2.46 | 0.45 |
| 15:CO:62:GLN:O | 15:CO:66:LEU:HD23 | 2.17 | 0.45 |
| 21:CU:29:LEU:C | 21:CU:29:LEU:HD23 | 2.37 | 0.45 |
| 22:DA:2:G:O6 | 22:DA:2900:A:N6 | 2.50 | 0.45 |
| 22:DA:82:U:O2 | 22:DA:83:A:C8 | 2.68 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 22:DA:515:A:H2' | 22:DA:516:C:H5' | 1.98 | 0.45 |
| 22:DA:571:U:C4 | 22:DA:2030:A:C6 | 3.05 | 0.45 |
| 22:DA:641:U:C5 | 22:DA:642:U:O4 | 2.69 | 0.45 |
| 22:DA:645:C:H2' | 22:DA:647:G:C5 | 2.52 | 0.45 |
| 22:DA:681:G:C2 | 22:DA:797:G:C2 | 3.04 | 0.45 |
| 22:DA:1090:A:C2 | 22:DA:1091:G:N7 | 2.85 | 0.45 |
| 22:DA:1208:C:C4 | 22:DA:1209:U:C5 | 3.05 | 0.45 |
| 22:DA:1264:A:N7 | 22:DA:1265:A:C5 | 2.85 | 0.45 |
| 22:DA:1275:A:C5 | 35:DN:16:HIS:CD2 | 3.04 | 0.45 |
| 22:DA:1277:G:H5' | 35:DN:20:MET:HE1 | 1.98 | 0.45 |
| 22:DA:1347:A:C5 | 22:DA:1348:C:C5 | 3.04 | 0.45 |
| 22:DA:1413:A:H2' | 22:DA:1414:C:C6 | 2.51 | 0.45 |
| 22:DA:1838:C:C5 | 22:DA:1899:A:C5 | 3.05 | 0.45 |
| 22:DA:2044:C:C2 | 22:DA:2625:G:N2 | 2.84 | 0.45 |
| 22:DA:2066:C:H5'' | 58:DA:3504:HOH:O | 2.17 | 0.45 |
| 22:DA:2074:U:C2 | 22:DA:2436:G:C2 | 3.05 | 0.45 |
| 22:DA:2193:G:C4 | 22:DA:2194:U:C5 | 3.04 | 0.45 |
| 22:DA:2311:A:H3' | 22:DA:2312:U:C6 | 2.52 | 0.45 |
| 22:DA:2345:G:N3 | 22:DA:2381:A:H2' | 2.31 | 0.45 |
| 25:DD:13:ARG:HD3 | 25:DD:21:SER:OG | 2.16 | 0.45 |
| 30:DI:47:ASP:HA | 30:DI:51:LYS:HD2 | 1.99 | 0.45 |
| 32:DK:34:GLY:O | 32:DK:35:VAL:C | 2.53 | 0.45 |
| 36:DO:7:ARG:CD | 36:DO:97:PHE:CE1 | 2.99 | 0.45 |
| 37:DP:39:ARG:HG3 | 37:DP:40:LEU:N | 2.31 | 0.45 |
| 41:DT:7:LEU:HD22 | 41:DT:46:ALA:CA | 2.47 | 0.45 |
| 1:AA:207:C:H2' | 1:AA:208:U:O2 | 2.17 | 0.45 |
| 1:AA:374:A:N1 | 1:AA:390:U:O2' | 2.45 | 0.45 |
| 1:AA:542:G:OP1 | 4:AD:10:LYS:CE | 2.65 | 0.45 |
| 1:AA:575:G:O2' | 1:AA:821:G:H5' | 2.17 | 0.45 |
| 1:AA:587:G:N2 | 1:AA:755:G:C5 | 2.85 | 0.45 |
| 1:AA:638:U:H2' | 1:AA:639:G:O4' | 2.16 | 0.45 |
| 1:AA:820:U:H4' | 1:AA:821:G:OP2 | 2.16 | 0.45 |
| 1:AA:994:A:N1 | 1:AA:1047:G:H4' | 2.31 | 0.45 |
| 1:AA:1064:G:O2' | 1:AA:1190:G:N2 | 2.49 | 0.45 |
| 2:AB:47:VAL:C | 2:AB:49:MET:H | 2.19 | 0.45 |
| 2:AB:67:ILE:O | 2:AB:68:LEU:HB3 | 2.16 | 0.45 |
| 2:AB:82:ASP:OD1 | 2:AB:84:ALA:HB3 | 2.16 | 0.45 |
| 7:AG:14:PRO:O | 7:AG:15:ASP:O | 2.35 | 0.45 |
| 11:AK:102:ALA:O | 11:AK:103:ALA:C | 2.55 | 0.45 |
| 19:AS:50:ALA:HB1 | 19:AS:57:HIS:CB | 2.45 | 0.45 |
| 22:BA:231:A:C6 | 22:BA:232:G:C2 | 3.05 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:245:G:N7 | 51:B3:8:ARG:NH1 | 2.64 | 0.45 |
| 22:BA:595:C:H2' | 22:BA:596:U:C6 | 2.51 | 0.45 |
| 22:BA:783:A:H8 | 22:BA:784:G:H4' | 1.80 | 0.45 |
| 22:BA:876:C:H2' | 22:BA:877:A:O4' | 2.16 | 0.45 |
| 22:BA:998:C:C2' | 22:BA:999:U:O5' | 2.65 | 0.45 |
| 22:BA:1360:G:C6 | 22:BA:1372:U:C2 | 3.05 | 0.45 |
| 22:BA:1717:A:H2' | 22:BA:1718:G:O4' | 2.17 | 0.45 |
| 22:BA:1917:U:O4 | 22:BA:1918:A:C6 | 2.68 | 0.45 |
| 22:BA:2032:G:C8 | 58:BA:3534:HOH:O | 2.70 | 0.45 |
| 22:BA:2780:G:OP2 | 31:BJ:120:ARG:HD3 | 2.17 | 0.45 |
| 30:BI:103:ARG:HE | 30:BI:104:ALA:N | 2.15 | 0.45 |
| 34:BM:41:LEU:HD22 | 34:BM:124:LEU:HD22 | 1.99 | 0.45 |
| 38:BQ:76:TYR:C | 38:BQ:76:TYR:CD2 | 2.89 | 0.45 |
| 38:BQ:76:TYR:CZ | 38:BQ:80:ILE:HG13 | 2.52 | 0.45 |
| 38:BQ:89:GLU:H | 39:BR:49:ILE:HD12 | 1.81 | 0.45 |
| 44:BW:41:ARG:HH11 | 44:BW:41:ARG:CG | 2.30 | 0.45 |
| 46:BY:14:LEU:HA | 46:BY:17:GLU:HB3 | 1.99 | 0.45 |
| 1:CA:792:A:H1' | 1:CA:794:A:N7 | 2.32 | 0.45 |
| 1:CA:976:G:H1' | 1:CA:1363:A:N6 | 2.32 | 0.45 |
| 1:CA:1053:G:N7 | 1:CA:1200:C:H5' | 2.32 | 0.45 |
| 1:CA:1293:C:H2' | 1:CA:1294:G:O4' | 2.17 | 0.45 |
| 2:CB:62:SER:C | 2:CB:64:LYS:N | 2.70 | 0.45 |
| 2:CB:165:ASP:O | 2:CB:166:ALA:C | 2.54 | 0.45 |
| 4:CD:90:LEU:HD21 | 4:CD:200:ILE:HD11 | 1.98 | 0.45 |
| 6:CF:59:TYR:HE2 | 18:CR:67:LEU:CD2 | 2.30 | 0.45 |
| 7:CG:53:ARG:NH2 | 7:CG:125:SER:OG | 2.49 | 0.45 |
| 10:CJ:40:ILE:HG22 | 10:CJ:42:LEU:HG | 1.97 | 0.45 |
| 22:DA:7:G:H2' | 22:DA:8:C:O4' | 2.17 | 0.45 |
| 22:DA:17:G:H4' | 38:DQ:25:TYR:CE1 | 2.51 | 0.45 |
| 22:DA:87:U:O2 | 46:DY:44:LYS:NZ | 2.49 | 0.45 |
| 22:DA:211:C:OP1 | 50:D2:25:LYS:NZ | 2.37 | 0.45 |
| 22:DA:303:G:C6 | 22:DA:304:U:N3 | 2.85 | 0.45 |
| 22:DA:572:A:H5'' | 22:DA:573:U:OP2 | 2.17 | 0.45 |
| 22:DA:966:G:H4' | 22:DA:2272:U:O2 | 2.16 | 0.45 |
| 22:DA:994:C:O2' | 39:DR:10:LYS:HE3 | 2.16 | 0.45 |
| 22:DA:1040:A:C2 | 22:DA:1041:G:C4 | 3.05 | 0.45 |
| 22:DA:1351:C:H2' | 22:DA:1352:U:H1' | 1.99 | 0.45 |
| 22:DA:1358:G:N2 | 22:DA:1374:G:C6 | 2.85 | 0.45 |
| 22:DA:1452:G:C8 | 22:DA:1457:U:N3 | 2.85 | 0.45 |
| 22:DA:1651:G:C6 | 22:DA:1652:A:C5 | 3.05 | 0.45 |
| 22:DA:1813:G:H2' | 22:DA:1814:G:O4' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2037:A:C6 | 22:DA:2038:G:C6 | 3.04 | 0.45 |
| 22:DA:2170:A:C2 | 22:DA:2171:A:C6 | 3.04 | 0.45 |
| 22:DA:2370:G:O2' | 49:D1:44:ARG:NH1 | 2.50 | 0.45 |
| 22:DA:2446:G:C6 | 22:DA:2501:C:H2' | 2.51 | 0.45 |
| 22:DA:2499:C:C4 | 22:DA:2500:U:C4 | 3.05 | 0.45 |
| 22:DA:2880:C:C2 | 22:DA:2881:U:C6 | 3.05 | 0.45 |
| 24:DC:69:ARG:NH2 | 24:DC:116:ILE:CD1 | 2.80 | 0.45 |
| 25:DD:108:ASP:N | 25:DD:204:LYS:O | 2.50 | 0.45 |
| 25:DD:187:LEU:HD21 | 25:DD:203:VAL:HG11 | 1.99 | 0.45 |
| 27:DF:40:VAL:HG13 | 27:DF:41:GLY:N | 2.31 | 0.45 |
| 29:DH:31:VAL:CG1 | 29:DH:32:PRO:HD3 | 2.47 | 0.45 |
| 29:DH:83:LYS:HG3 | 29:DH:149:GLU:HG3 | 1.94 | 0.45 |
| 29:DH:93:SER:HB3 | 29:DH:123:ARG:HG3 | 1.99 | 0.45 |
| 33:DL:135:ILE:HG22 | 33:DL:140:GLY:HA2 | 1.98 | 0.45 |
| 40:DS:39:THR:O | 40:DS:41:LYS:N | 2.50 | 0.45 |
| 44:DW:70:GLU:O | 44:DW:79:PHE:N | 2.49 | 0.45 |
| 48:D0:20:ASP:N | 48:D0:20:ASP:OD2 | 2.49 | 0.45 |
| 54:D6:4:PRO:CB | 54:D6:5:MHU:HM1 | 2.46 | 0.45 |
| 1:AA:351:G:H1' | 1:AA:352:C:OP1 | 2.17 | 0.45 |
| 1:AA:792:A:H1' | 1:AA:794:A:N7 | 2.31 | 0.45 |
| 1:AA:980:C:C5 | 1:AA:981:U:C4 | 3.04 | 0.45 |
| 1:AA:1343:G:H2' | 1:AA:1344:C:C6 | 2.51 | 0.45 |
| 3:AC:84:VAL:HG13 | 3:AC:101:ILE:HG21 | 1.99 | 0.45 |
| 5:AE:94:VAL:CG2 | 5:AE:111:MET:SD | 3.05 | 0.45 |
| 6:AF:45:ARG:O | 6:AF:56:LYS:HA | 2.17 | 0.45 |
| 11:AK:69:ARG:HD2 | 22:BA:2146:C:C4 | 2.52 | 0.45 |
| 21:AU:35:ARG:O | 21:AU:36:GLU:C | 2.55 | 0.45 |
| 22:BA:38:A:H5' | 26:BE:45:ALA:HB3 | 1.99 | 0.45 |
| 22:BA:211:C:O2' | 22:BA:212:G:H5' | 2.17 | 0.45 |
| 22:BA:528:A:H3' | 22:BA:528:A:H8 | 1.80 | 0.45 |
| 22:BA:1167:C:H2' | 22:BA:1168:G:H5'' | 1.99 | 0.45 |
| 22:BA:1381:G:H1' | 22:BA:1571:A:N1 | 2.32 | 0.45 |
| 22:BA:1585:C:H2' | 22:BA:1586:A:H5' | 1.99 | 0.45 |
| 22:BA:1816:C:C6 | 24:BC:62:TYR:CE1 | 3.04 | 0.45 |
| 22:BA:2681:C:C2 | 22:BA:2724:U:O4 | 2.69 | 0.45 |
| 22:BA:2810:A:H2' | 22:BA:2811:G:O4' | 2.16 | 0.45 |
| 26:BE:111:GLU:CG | 26:BE:114:ARG:NH1 | 2.80 | 0.45 |
| 26:BE:145:ASP:HA | 26:BE:166:LYS:O | 2.16 | 0.45 |
| 29:BH:40:THR:O | 29:BH:42:LYS:N | 2.48 | 0.45 |
| 29:BH:72:ILE:HG23 | 29:BH:142:VAL:HG22 | 1.99 | 0.45 |
| 30:BI:39:CYS:HA | 30:BI:42:PHE:HB2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BK:23:LYS:HB3 | 32:BK:40:LYS:HB3 | 1.99 | 0.45 |
| 33:BL:91:ASP:O | 33:BL:92:LEU:C | 2.55 | 0.45 |
| 33:BL:111:ILE:N | 33:BL:111:ILE:CD1 | 2.80 | 0.45 |
| 43:BV:14:LYS:CD | 43:BV:18:ARG:HH11 | 2.30 | 0.45 |
| 46:BY:7:ARG:O | 46:BY:8:GLU:HG3 | 2.17 | 0.45 |
| 1:CA:101:A:C5 | 1:CA:102:G:N7 | 2.85 | 0.45 |
| 1:CA:263:A:OP2 | 20:CT:74:ARG:NH1 | 2.50 | 0.45 |
| 1:CA:1117:A:H5' | 9:CI:110:GLN:NE2 | 2.32 | 0.45 |
| 1:CA:1124:G:N2 | 1:CA:1127:G:N2 | 2.65 | 0.45 |
| 3:CC:101:ILE:HG23 | 3:CC:101:ILE:O | 2.16 | 0.45 |
| 4:CD:22:LYS:C | 4:CD:24:GLY:N | 2.68 | 0.45 |
| 5:CE:19:ASN:O | 5:CE:33:PHE:HA | 2.17 | 0.45 |
| 8:CH:78:VAL:HG12 | 8:CH:79:SER:N | 2.32 | 0.45 |
| 10:CJ:17:LEU:HD23 | 10:CJ:18:ILE:N | 2.31 | 0.45 |
| 18:CR:46:GLY:C | 18:CR:47:THR:HG23 | 2.37 | 0.45 |
| 21:CU:37:PHE:O | 21:CU:39:GLU:N | 2.44 | 0.45 |
| 22:DA:55:G:H2' | 22:DA:55:G:N3 | 2.32 | 0.45 |
| 22:DA:259:G:C4 | 22:DA:260:G:C8 | 3.04 | 0.45 |
| 22:DA:453:A:O3' | 22:DA:472:A:N6 | 2.49 | 0.45 |
| 22:DA:686:U:H6 | 22:DA:788:A:N1 | 2.15 | 0.45 |
| 22:DA:779:U:H5'' | 24:DC:49:ILE:HD11 | 1.98 | 0.45 |
| 22:DA:1312:U:C2 | 22:DA:1603:A:C2 | 3.05 | 0.45 |
| 22:DA:1464:G:N1 | 22:DA:1465:G:C5 | 2.84 | 0.45 |
| 22:DA:1476:U:O2' | 22:DA:1477:A:H5' | 2.17 | 0.45 |
| 22:DA:1949:G:C6 | 22:DA:1950:G:C6 | 3.05 | 0.45 |
| 22:DA:2135:A:C2 | 22:DA:2136:G:H1' | 2.51 | 0.45 |
| 23:DB:17:C:H2' | 23:DB:18:G:H5' | 1.98 | 0.45 |
| 23:DB:59:A:H2' | 23:DB:60:C:O4' | 2.17 | 0.45 |
| 33:DL:20:GLY:HA2 | 33:DL:28:GLY:HA2 | 1.98 | 0.45 |
| 37:DP:70:VAL:HG12 | 37:DP:71:GLU:N | 2.32 | 0.45 |
| 44:DW:34:GLY:N | 44:DW:61:ALA:O | 2.40 | 0.45 |
| 1:AA:316:C:C5 | 1:AA:351:G:C2 | 3.04 | 0.45 |
| 1:AA:927:G:H4' | 1:AA:1503:A:N7 | 2.32 | 0.45 |
| 1:AA:947:G:C6 | 1:AA:948:C:C4 | 3.04 | 0.45 |
| 1:AA:1048:G:C2 | 1:AA:1050:G:C5 | 3.05 | 0.45 |
| 1:AA:1134:G:N2 | 1:AA:1135:U:C2 | 2.84 | 0.45 |
| 1:AA:1140:C:O2' | 1:AA:1141:C:P | 2.75 | 0.45 |
| 1:AA:1144:G:N1 | 1:AA:1145:A:C2 | 2.85 | 0.45 |
| 1:AA:1387:G:C6 | 1:AA:1388:C:N4 | 2.85 | 0.45 |
| 1:AA:1425:U:O2' | 1:AA:1426:G:H5' | 2.17 | 0.45 |
| 5:AE:46:VAL:HG22 | 5:AE:118:ALA:HA | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:AG:69:VAL:HG21 | 7:AG:104:ILE:HG13 | 1.99 | 0.45 |
| 10:AJ:52:LEU:HB2 | 14:AN:81:ARG:CD | 2.47 | 0.45 |
| 22:BA:5:A:H2' | 22:BA:6:A:C8 | 2.52 | 0.45 |
| 22:BA:674:G:H1' | 26:BE:69:ARG:HD3 | 1.99 | 0.45 |
| 22:BA:674:G:H5'' | 26:BE:71:GLY:N | 2.32 | 0.45 |
| 22:BA:695:G:C2 | 22:BA:696:G:C8 | 3.05 | 0.45 |
| 22:BA:1056:G:H5'' | 22:BA:1057:A:C4' | 2.47 | 0.45 |
| 22:BA:1486:U:O2' | 22:BA:1487:U:H5' | 2.17 | 0.45 |
| 22:BA:1832:C:C4 | 22:BA:1833:C:C5 | 3.05 | 0.45 |
| 22:BA:1916:A:OP2 | 22:BA:1916:A:H3' | 2.17 | 0.45 |
| 22:BA:2020:A:H5' | 48:B0:9:THR:HG22 | 1.98 | 0.45 |
| 22:BA:2052:A:H4' | 25:BD:148:GLN:O | 2.16 | 0.45 |
| 22:BA:2502:G:H5' | 22:BA:2503:A:C5' | 2.47 | 0.45 |
| 22:BA:2515:C:O2 | 22:BA:2570:G:C2 | 2.70 | 0.45 |
| 27:BF:14:LYS:O | 27:BF:18:THR:CG2 | 2.65 | 0.45 |
| 27:BF:143:TYR:O | 27:BF:146:VAL:HG22 | 2.17 | 0.45 |
| 30:BI:97:LYS:HG2 | 30:BI:139:VAL:HG22 | 1.99 | 0.45 |
| 36:BO:36:TYR:N | 36:BO:36:TYR:CD2 | 2.84 | 0.45 |
| 42:BU:26:LYS:HD2 | 42:BU:26:LYS:HA | 1.89 | 0.45 |
| 42:BU:52:LEU:HA | 42:BU:54:GLN:OE1 | 2.17 | 0.45 |
| 46:BY:15:ASN:O | 46:BY:19:LEU:HG | 2.16 | 0.45 |
| 53:B5:64:SER:O | 53:B5:65:LEU:HB3 | 2.17 | 0.45 |
| 1:CA:9:G:OP2 | 5:CE:126:LYS:NZ | 2.47 | 0.45 |
| 1:CA:206:C:H2' | 1:CA:207:C:C5' | 2.45 | 0.45 |
| 1:CA:669:G:N2 | 1:CA:738:C:O2 | 2.50 | 0.45 |
| 1:CA:756:C:C4 | 1:CA:757:U:C5 | 3.05 | 0.45 |
| 1:CA:1004:A:C2 | 1:CA:1026:G:N3 | 2.84 | 0.45 |
| 1:CA:1315:U:O4 | 1:CA:1316:G:C6 | 2.70 | 0.45 |
| 2:CB:16:PHE:CZ | 2:CB:18:HIS:CE1 | 3.05 | 0.45 |
| 2:CB:85:LEU:O | 2:CB:85:LEU:HD12 | 2.17 | 0.45 |
| 9:CI:12:ARG:CD | 9:CI:107:ASP:HB3 | 2.47 | 0.45 |
| 10:CJ:91:ASP:O | 10:CJ:92:LEU:CB | 2.64 | 0.45 |
| 11:CK:100:LEU:O | 11:CK:103:ALA:N | 2.49 | 0.45 |
| 13:CM:22:ILE:HD12 | 13:CM:22:ILE:N | 2.32 | 0.45 |
| 14:CN:67:THR:HG23 | 14:CN:83:LYS:HD2 | 1.98 | 0.45 |
| 15:CO:45:GLU:O | 15:CO:46:HIS:CB | 2.65 | 0.45 |
| 19:CS:22:ALA:CB | 19:CS:47:LEU:HD13 | 2.46 | 0.45 |
| 22:DA:30:G:C5 | 22:DA:31:C:N3 | 2.85 | 0.45 |
| 22:DA:45:G:H2' | 22:DA:215:G:N7 | 2.32 | 0.45 |
| 22:DA:143:C:H2' | 22:DA:144:A:H5' | 1.98 | 0.45 |
| 22:DA:292:U:C5 | 22:DA:293:U:C5 | 3.05 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:377:G:C6 | 22:DA:378:C:N4 | 2.85 | 0.45 |
| 22:DA:599:A:C2 | 22:DA:659:G:C6 | 3.04 | 0.45 |
| 22:DA:663:G:O6 | 22:DA:664:G:C6 | 2.70 | 0.45 |
| 22:DA:669:G:N2 | 22:DA:670:A:N1 | 2.65 | 0.45 |
| 22:DA:708:G:N2 | 22:DA:724:U:H1' | 2.31 | 0.45 |
| 22:DA:745:G:O2' | 22:DA:748:G:H1' | 2.17 | 0.45 |
| 22:DA:794:A:C6 | 22:DA:795:C:N3 | 2.85 | 0.45 |
| 22:DA:1222:U:H1' | 22:DA:1228:G:N2 | 2.32 | 0.45 |
| 22:DA:1231:U:H2' | 22:DA:1232:G:C8 | 2.52 | 0.45 |
| 22:DA:1358:G:C2' | 22:DA:1359:A:OP2 | 2.65 | 0.45 |
| 22:DA:1425:G:H2' | 22:DA:1426:G:O4' | 2.17 | 0.45 |
| 22:DA:1662:U:O2 | 22:DA:2687:U:H4' | 2.16 | 0.45 |
| 22:DA:1724:G:O6 | 22:DA:1736:U:C2 | 2.70 | 0.45 |
| 22:DA:2331:G:C5 | 22:DA:2332:C:C4 | 3.05 | 0.45 |
| 22:DA:2345:G:H5' | 22:DA:2347:C:O4' | 2.16 | 0.45 |
| 22:DA:2504:U:C5 | 56:DA:3001:DOL:C16 | 2.98 | 0.45 |
| 22:DA:2543:G:N3 | 22:DA:2765:A:H2' | 2.32 | 0.45 |
| 22:DA:2740:A:C6 | 22:DA:2764:A:C8 | 3.05 | 0.45 |
| 23:DB:25:U:C4 | 23:DB:26:C:C4 | 3.04 | 0.45 |
| 24:DC:246:THR:C | 24:DC:248:TRP:H | 2.20 | 0.45 |
| 27:DF:128:TYR:CB | 27:DF:170:LEU:CD1 | 2.95 | 0.45 |
| 29:DH:86:ASP:C | 29:DH:88:GLY:H | 2.19 | 0.45 |
| 30:DI:91:GLY:O | 30:DI:93:PRO:HD3 | 2.17 | 0.45 |
| 33:DL:56:PRO:O | 33:DL:60:ARG:CB | 2.64 | 0.45 |
| 33:DL:58:TYR:O | 51:D3:13:ARG:HD3 | 2.17 | 0.45 |
| 35:DN:114:GLU:OE2 | 35:DN:118:ARG:HD2 | 2.17 | 0.45 |
| 41:DT:38:ALA:O | 41:DT:39:THR:CB | 2.65 | 0.45 |
| 41:DT:73:ARG:HA | 41:DT:73:ARG:CZ | 2.47 | 0.45 |
| 47:DZ:13:ALA:HB2 | 47:DZ:24:LEU:HD12 | 1.98 | 0.45 |
| 49:D1:9:ILE:HG23 | 49:D1:25:LYS:HB3 | 1.99 | 0.45 |
| 1:AA:85:U:O2 | 1:AA:85:U:O4' | 2.35 | 0.45 |
| 1:AA:105:G:N2 | 1:AA:379:C:O3' | 2.50 | 0.45 |
| 1:AA:500:G:C6 | 1:AA:546:A:C2 | 3.05 | 0.45 |
| 1:AA:832:G:C4 | 1:AA:833:G:C8 | 3.05 | 0.45 |
| 1:AA:933:G:OP2 | 7:AG:3:ARG:CB | 2.65 | 0.45 |
| 2:AB:77:SER:O | 2:AB:80:VAL:HB | 2.17 | 0.45 |
| 4:AD:91:LEU:HD11 | 4:AD:195:ILE:HD11 | 1.99 | 0.45 |
| 8:AH:80:ARG:HB2 | 8:AH:81:PRO:HD2 | 1.99 | 0.45 |
| 9:AI:44:ALA:H | 9:AI:46:MET:HE1 | 1.82 | 0.45 |
| 14:AN:93:ILE:HD12 | 14:AN:96:LEU:HD23 | 1.99 | 0.45 |
| 17:AQ:17:MET:CG | 17:AQ:20:SER:HB3 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AS:11:ILE:HG13 | 19:AS:15:LEU:HD23 | 1.99 | 0.45 |
| 22:BA:18:U:O3' | 38:BQ:23:GLY:HA2 | 2.16 | 0.45 |
| 22:BA:83:A:N6 | 22:BA:101:A:C4 | 2.85 | 0.45 |
| 22:BA:136:G:C6 | 22:BA:137:U:O4 | 2.70 | 0.45 |
| 22:BA:503:A:H4' | 22:BA:504:A:O5' | 2.17 | 0.45 |
| 22:BA:780:G:H2' | 22:BA:782:A:N7 | 2.32 | 0.45 |
| 22:BA:832:U:H2' | 22:BA:833:A:C8 | 2.51 | 0.45 |
| 22:BA:1064:C:O2 | 22:BA:1064:C:H2' | 2.16 | 0.45 |
| 22:BA:1283:G:N2 | 22:BA:1285:A:H3' | 2.32 | 0.45 |
| 22:BA:1501:G:C2 | 22:BA:1502:A:C8 | 3.04 | 0.45 |
| 22:BA:1838:C:C6 | 22:BA:1899:A:C6 | 3.05 | 0.45 |
| 22:BA:1885:A:C2' | 22:BA:1886:U:H5' | 2.47 | 0.45 |
| 22:BA:1993:U:C2' | 22:BA:1994:C:H5' | 2.47 | 0.45 |
| 22:BA:2273:A:H2' | 22:BA:2274:A:C8 | 2.52 | 0.45 |
| 22:BA:2345:G:H4' | 22:BA:2346:A:H5'' | 1.98 | 0.45 |
| 22:BA:2451:A:C2 | 56:BA:3001:DOL:C12 | 2.99 | 0.45 |
| 23:BB:42:C:OP1 | 27:BF:64:LYS:HE2 | 2.16 | 0.45 |
| 27:BF:2:ALA:O | 27:BF:5:HIS:N | 2.50 | 0.45 |
| 29:BH:12:LEU:HG | 29:BH:13:GLY:N | 2.31 | 0.45 |
| 29:BH:76:GLU:HA | 29:BH:142:VAL:CG1 | 2.46 | 0.45 |
| 42:BU:34:VAL:HG23 | 42:BU:65:ILE:HG22 | 1.99 | 0.45 |
| 1:CA:115:G:C2 | 1:CA:289:G:N7 | 2.84 | 0.45 |
| 1:CA:803:G:C6 | 1:CA:804:U:C4 | 3.05 | 0.45 |
| 1:CA:842:U:O2' | 1:CA:846:G:C6 | 2.70 | 0.45 |
| 1:CA:878:A:C6 | 1:CA:879:C:C4 | 3.05 | 0.45 |
| 1:CA:1080:A:C8 | 1:CA:1081:A:H1' | 2.52 | 0.45 |
| 1:CA:1179:A:H2' | 1:CA:1180:A:O4' | 2.17 | 0.45 |
| 1:CA:1227:A:OP2 | 13:CM:110:LYS:HD2 | 2.17 | 0.45 |
| 1:CA:1386:G:C2 | 1:CA:1387:G:C8 | 3.05 | 0.45 |
| 1:CA:1410:A:H2' | 1:CA:1411:C:C6 | 2.52 | 0.45 |
| 1:CA:1422:G:O3' | 32:DK:49:ARG:NH2 | 2.49 | 0.45 |
| 12:CL:90:LEU:HB2 | 12:CL:93:VAL:HG21 | 1.98 | 0.45 |
| 14:CN:65:ARG:HB2 | 14:CN:78:GLY:O | 2.17 | 0.45 |
| 16:CP:6:LEU:CD1 | 16:CP:71:VAL:HG23 | 2.47 | 0.45 |
| 21:CU:34:ARG:HE | 21:CU:35:ARG:HB2 | 1.82 | 0.45 |
| 22:DA:8:C:O2' | 22:DA:9:G:H5' | 2.16 | 0.45 |
| 22:DA:158:U:C2' | 22:DA:159:G:H5' | 2.45 | 0.45 |
| 22:DA:204:A:H5' | 22:DA:206:U:O4' | 2.17 | 0.45 |
| 22:DA:249:C:O5' | 22:DA:2394:C:O2' | 2.35 | 0.45 |
| 22:DA:415:A:C2 | 22:DA:2409:G:N1 | 2.84 | 0.45 |
| 22:DA:515:A:C2' | 22:DA:516:C:H5' | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:581:C:H2' | 22:DA:582:A:C8 | 2.52 | 0.45 |
| 22:DA:630:G:H3' | 22:DA:631:A:H5'' | 1.99 | 0.45 |
| 22:DA:683:U:OP1 | 50:D2:26:ASN:CB | 2.65 | 0.45 |
| 22:DA:1006:C:P | 58:DA:3779:HOH:O | 2.74 | 0.45 |
| 22:DA:1262:A:N3 | 22:DA:1262:A:H2' | 2.32 | 0.45 |
| 22:DA:1358:G:H2' | 22:DA:1359:A:OP2 | 2.17 | 0.45 |
| 22:DA:1388:G:N2 | 22:DA:1400:U:C2 | 2.85 | 0.45 |
| 22:DA:1614:A:H2' | 22:DA:1615:C:H5' | 1.99 | 0.45 |
| 22:DA:1649:G:N1 | 22:DA:2009:A:C6 | 2.85 | 0.45 |
| 22:DA:1651:G:H4' | 35:DN:39:PRO:HG2 | 1.99 | 0.45 |
| 22:DA:1829:A:H2' | 24:DC:15:HIS:NE2 | 2.32 | 0.45 |
| 22:DA:2063:C:O2 | 22:DA:2063:C:H2' | 2.17 | 0.45 |
| 22:DA:2111:U:O2 | 22:DA:2111:U:O4' | 2.34 | 0.45 |
| 22:DA:2193:G:H2' | 22:DA:2194:U:C6 | 2.52 | 0.45 |
| 22:DA:2211:A:C4' | 22:DA:2212:A:OP1 | 2.65 | 0.45 |
| 22:DA:2221:G:C2' | 22:DA:2222:C:H5' | 2.47 | 0.45 |
| 22:DA:2308:G:H4' | 22:DA:2309:A:OP2 | 2.15 | 0.45 |
| 22:DA:2451:A:C2 | 56:DA:3001:DOL:HC12 | 2.52 | 0.45 |
| 22:DA:2821:A:OP2 | 25:DD:115:GLY:N | 2.50 | 0.45 |
| 22:DA:2868:A:C6 | 22:DA:2869:G:C6 | 3.05 | 0.45 |
| 27:DF:111:ILE:HB | 27:DF:114:PHE:CB | 2.47 | 0.45 |
| 29:DH:15:LEU:HD22 | 29:DH:15:LEU:N | 2.32 | 0.45 |
| 30:DI:24:VAL:HB | 30:DI:28:LEU:HD23 | 1.99 | 0.45 |
| 32:DK:73:ASP:OD2 | 32:DK:75:SER:OG | 2.28 | 0.45 |
| 33:DL:29:LYS:HG3 | 33:DL:30:THR:HG23 | 1.98 | 0.45 |
| 34:DM:67:VAL:HG11 | 34:DM:96:ILE:HD12 | 1.99 | 0.45 |
| 34:DM:124:LEU:N | 34:DM:124:LEU:HD23 | 2.32 | 0.45 |
| 43:DV:48:MET:SD | 43:DV:86:LEU:HG | 2.56 | 0.45 |
| 50:D2:34:ARG:HB2 | 50:D2:42:LEU:HD12 | 1.99 | 0.45 |
| 1:AA:9:G:C6 | 1:AA:26:A:N6 | 2.85 | 0.44 |
| 1:AA:192:A:C2 | 1:AA:193:C:C2 | 3.05 | 0.44 |
| 1:AA:320:A:H2' | 1:AA:321:A:C1' | 2.48 | 0.44 |
| 1:AA:531:U:H5'' | 3:AC:161:GLU:OE2 | 2.16 | 0.44 |
| 1:AA:855:U:N3 | 1:AA:856:C:C5 | 2.86 | 0.44 |
| 2:AB:79:ALA:O | 2:AB:214:LEU:HD21 | 2.18 | 0.44 |
| 2:AB:84:ALA:O | 2:AB:89:GLN:CB | 2.65 | 0.44 |
| 3:AC:7:PRO:HD2 | 3:AC:184:TYR:CD2 | 2.52 | 0.44 |
| 4:AD:126:ASN:HA | 4:AD:142:VAL:HG23 | 1.99 | 0.44 |
| 5:AE:35:ALA:CB | 5:AE:60:ILE:HA | 2.47 | 0.44 |
| 5:AE:50:TYR:O | 5:AE:63:ALA:HB2 | 2.17 | 0.44 |
| 10:AJ:66:GLU:HB3 | 14:AN:99:ALA:CB | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:80:THR:C | 10:AJ:82:LYS:N | 2.71 | 0.44 |
| 14:AN:64:CYS:HB2 | 14:AN:80:SER:HB2 | 1.99 | 0.44 |
| 14:AN:93:ILE:HG21 | 14:AN:96:LEU:HD22 | 2.00 | 0.44 |
| 15:AO:61:SER:O | 15:AO:65:LYS:HG3 | 2.18 | 0.44 |
| 16:AP:46:LYS:HD3 | 16:AP:47:GLU:H | 1.80 | 0.44 |
| 20:AT:3:ASN:O | 20:AT:4:ILE:C | 2.55 | 0.44 |
| 20:AT:7:ALA:HB1 | 20:AT:10:ARG:HB2 | 1.99 | 0.44 |
| 22:BA:250:G:H2' | 22:BA:251:A:C8 | 2.52 | 0.44 |
| 22:BA:301:G:HO2' | 22:BA:302:C:H6 | 1.61 | 0.44 |
| 22:BA:613:A:H2' | 22:BA:614:A:H5' | 1.98 | 0.44 |
| 22:BA:1098:A:H5' | 22:BA:1099:G:OP2 | 2.17 | 0.44 |
| 24:BC:162:VAL:HG13 | 24:BC:176:LEU:HD23 | 1.97 | 0.44 |
| 25:BD:61:THR:HB | 25:BD:63:PRO:HD2 | 1.99 | 0.44 |
| 29:BH:93:SER:O | 1:CA:368:U:C6 | 2.71 | 0.44 |
| 30:BI:108:GLU:HA | 30:BI:111:GLN:HB3 | 1.99 | 0.44 |
| 34:BM:57:VAL:O | 34:BM:60:GLN:HB2 | 2.16 | 0.44 |
| 40:BS:36:LEU:HD13 | 40:BS:48:LYS:HA | 1.99 | 0.44 |
| 41:BT:29:THR:OG1 | 41:BT:86:THR:HG22 | 2.17 | 0.44 |
| 42:BU:61:LYS:HE3 | 42:BU:62:GLU:O | 2.17 | 0.44 |
| 43:BV:26:PHE:CE1 | 43:BV:42:LEU:HD12 | 2.52 | 0.44 |
| 43:BV:80:HIS:ND1 | 43:BV:83:LYS:CG | 2.80 | 0.44 |
| 1:CA:186:C:O2 | 1:CA:186:C:H2' | 2.17 | 0.44 |
| 1:CA:484:G:N7 | 1:CA:486:U:C1' | 2.80 | 0.44 |
| 1:CA:519:C:N4 | 1:CA:520:A:N1 | 2.65 | 0.44 |
| 1:CA:609:A:C5 | 1:CA:610:U:C6 | 3.05 | 0.44 |
| 1:CA:714:G:H2' | 1:CA:715:A:C8 | 2.53 | 0.44 |
| 1:CA:992:U:O4' | 1:CA:993:G:C2 | 2.70 | 0.44 |
| 1:CA:1000:A:H3' | 1:CA:1001:C:C6 | 2.53 | 0.44 |
| 1:CA:1306:A:H1' | 1:CA:1332:A:N7 | 2.32 | 0.44 |
| 5:CE:38:VAL:HG11 | 5:CE:114:VAL:HA | 1.99 | 0.44 |
| 9:CI:35:LEU:HD21 | 9:CI:48:VAL:HG21 | 1.97 | 0.44 |
| 10:CJ:15:HIS:HA | 10:CJ:18:ILE:HG22 | 1.98 | 0.44 |
| 20:CT:58:VAL:CG1 | 20:CT:72:ALA:HB1 | 2.47 | 0.44 |
| 22:DA:185:G:C5 | 22:DA:212:G:N2 | 2.84 | 0.44 |
| 22:DA:294:A:C6 | 22:DA:345:A:N3 | 2.85 | 0.44 |
| 22:DA:846:U:H1' | 22:DA:847:U:C5 | 2.51 | 0.44 |
| 22:DA:993:G:N2 | 39:DR:23:GLU:OE1 | 2.50 | 0.44 |
| 22:DA:1153:C:H2' | 22:DA:1154:G:O4' | 2.17 | 0.44 |
| 22:DA:1211:C:H3' | 22:DA:1212:G:H5' | 1.99 | 0.44 |
| 22:DA:1476:U:H1' | 22:DA:1732:C:O2 | 2.17 | 0.44 |
| 22:DA:1731:G:C6 | 22:DA:1733:G:C8 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1783:A:C6 | 22:DA:2587:A:C2 | 3.05 | 0.44 |
| 22:DA:1906:G:OP1 | 22:DA:1930:G:C8 | 2.69 | 0.44 |
| 22:DA:2043:C:H2' | 22:DA:2043:C:O2 | 2.16 | 0.44 |
| 22:DA:2634:A:C2 | 22:DA:2635:A:C4 | 3.05 | 0.44 |
| 24:DC:87:ARG:HB3 | 24:DC:87:ARG:CZ | 2.46 | 0.44 |
| 27:DF:85:ILE:HG13 | 27:DF:85:ILE:O | 2.17 | 0.44 |
| 29:DH:5:LEU:CD1 | 29:DH:13:GLY:CA | 2.95 | 0.44 |
| 30:DI:33:VAL:O | 30:DI:33:VAL:HG12 | 2.16 | 0.44 |
| 31:DJ:9:GLU:O | 31:DJ:10:THR:HG23 | 2.18 | 0.44 |
| 33:DL:55:MET:SD | 33:DL:59:ARG:CB | 3.06 | 0.44 |
| 36:DO:51:ALA:HB1 | 36:DO:77:ALA:CB | 2.46 | 0.44 |
| 36:DO:51:ALA:HB1 | 36:DO:77:ALA:HB1 | 1.99 | 0.44 |
| 1:AA:131:A:C2 | 1:AA:132:C:C4 | 3.05 | 0.44 |
| 1:AA:172:A:N7 | 1:AA:174:A:N7 | 2.65 | 0.44 |
| 1:AA:603:U:H2' | 1:AA:604:G:C8 | 2.52 | 0.44 |
| 1:AA:874:G:C6 | 1:AA:875:U:C4 | 3.06 | 0.44 |
| 1:AA:908:A:O2' | 1:AA:909:A:H5' | 2.17 | 0.44 |
| 1:AA:1419:G:C5 | 1:AA:1420:U:C5 | 3.06 | 0.44 |
| 1:AA:1535:C:OP2 | 1:AA:1535:C:C6 | 2.71 | 0.44 |
| 3:AC:21:THR:HG23 | 3:AC:58:GLU:HB3 | 1.99 | 0.44 |
| 8:AH:10:MET:HE1 | 8:AH:33:LYS:CB | 2.46 | 0.44 |
| 9:AI:25:ASN:HB2 | 9:AI:27:LYS:HG2 | 1.99 | 0.44 |
| 11:AK:63:ALA:CB | 11:AK:92:GLY:HA3 | 2.48 | 0.44 |
| 13:AM:14:HIS:HB2 | 13:AM:17:ILE:HD13 | 1.99 | 0.44 |
| 17:AQ:16:LYS:CA | 17:AQ:17:MET:SD | 3.05 | 0.44 |
| 17:AQ:30:LYS:HG2 | 17:AQ:37:PHE:CZ | 2.52 | 0.44 |
| 21:AU:34:ARG:NH2 | 21:AU:35:ARG:HD2 | 2.32 | 0.44 |
| 22:BA:111:A:C2 | 22:BA:112:U:C2 | 3.06 | 0.44 |
| 22:BA:465:G:H2' | 22:BA:466:A:C8 | 2.52 | 0.44 |
| 22:BA:846:U:O2' | 22:BA:847:U:OP2 | 2.34 | 0.44 |
| 22:BA:954:G:C5 | 22:BA:955:U:C5 | 3.05 | 0.44 |
| 22:BA:1768:C:C2 | 22:BA:1769:U:C6 | 3.05 | 0.44 |
| 22:BA:1935:G:O2' | 22:BA:1936:A:H5' | 2.18 | 0.44 |
| 22:BA:2128:G:OP2 | 53:B5:37:LYS:HB2 | 2.17 | 0.44 |
| 22:BA:2554:U:C4 | 22:BA:2555:U:O4 | 2.70 | 0.44 |
| 23:BB:24:G:N2 | 23:BB:28:C:O2 | 2.50 | 0.44 |
| 25:BD:13:ARG:HD3 | 25:BD:21:SER:OG | 2.17 | 0.44 |
| 26:BE:197:GLU:O | 26:BE:201:ALA:N | 2.50 | 0.44 |
| 28:BG:153:ARG:O | 28:BG:154:PRO:C | 2.55 | 0.44 |
| 30:BI:73:THR:HG21 | 30:BI:116:ASP:HB3 | 1.98 | 0.44 |
| 31:BJ:98:GLU:OE2 | 31:BJ:126:ALA:HB2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:BP:73:VAL:HG23 | 37:BP:73:VAL:O | 2.15 | 0.44 |
| 41:BT:29:THR:HG23 | 41:BT:86:THR:N | 2.31 | 0.44 |
| 41:BT:47:VAL:HG12 | 41:BT:55:VAL:CG2 | 2.47 | 0.44 |
| 1:CA:829:G:C5 | 1:CA:858:G:N2 | 2.85 | 0.44 |
| 1:CA:1345:U:H4' | 1:CA:1346:A:H5' | 1.97 | 0.44 |
| 1:CA:1434:A:N6 | 1:CA:1435:G:C6 | 2.85 | 0.44 |
| 2:CB:35:ARG:O | 2:CB:38:VAL:N | 2.45 | 0.44 |
| 2:CB:117:LEU:HB3 | 2:CB:141:LEU:HG | 1.98 | 0.44 |
| 3:CC:65:ARG:O | 3:CC:66:VAL:C | 2.55 | 0.44 |
| 17:CQ:14:SER:HB3 | 17:CQ:22:VAL:HG12 | 1.99 | 0.44 |
| 22:DA:590:A:C5 | 22:DA:591:U:C5 | 3.05 | 0.44 |
| 22:DA:626:A:C2 | 33:DL:78:ARG:HD3 | 2.52 | 0.44 |
| 22:DA:877:A:H2' | 22:DA:878:A:OP2 | 2.17 | 0.44 |
| 22:DA:1343:G:C5 | 22:DA:1344:U:C4 | 3.04 | 0.44 |
| 22:DA:1483:G:C4 | 22:DA:1484:U:C5 | 3.05 | 0.44 |
| 22:DA:1688:U:C4 | 22:DA:1698:A:C2 | 3.06 | 0.44 |
| 22:DA:1965:C:OP1 | 22:DA:1966:A:H2' | 2.17 | 0.44 |
| 22:DA:2286:G:C4' | 22:DA:2287:A:O5' | 2.60 | 0.44 |
| 22:DA:2502:G:H5' | 22:DA:2503:A:C5' | 2.46 | 0.44 |
| 22:DA:2526:G:C5 | 22:DA:2527:C:C5 | 3.05 | 0.44 |
| 22:DA:2582:G:C2 | 22:DA:2583:G:C8 | 3.05 | 0.44 |
| 22:DA:2683:C:H4' | 25:DD:13:ARG:NH1 | 2.31 | 0.44 |
| 22:DA:2853:C:H2' | 22:DA:2854:G:C8 | 2.53 | 0.44 |
| 25:DD:32:ASN:HB3 | 25:DD:50:VAL:HB | 1.99 | 0.44 |
| 27:DF:122:PHE:O | 27:DF:123:ASP:C | 2.56 | 0.44 |
| 28:DG:70:ALA:O | 28:DG:74:SER:OG | 2.34 | 0.44 |
| 29:DH:1:MET:CE | 29:DH:27:ARG:NH1 | 2.80 | 0.44 |
| 31:DJ:24:THR:O | 31:DJ:25:LEU:C | 2.56 | 0.44 |
| 33:DL:110:VAL:O | 33:DL:111:ILE:O | 2.35 | 0.44 |
| 35:DN:2:ARG:O | 35:DN:2:ARG:CD | 2.65 | 0.44 |
| 35:DN:65:LEU:HD11 | 35:DN:69:ARG:NH2 | 2.33 | 0.44 |
| 41:DT:74:ILE:HD12 | 41:DT:75:GLY:N | 2.32 | 0.44 |
| 44:DW:45:PHE:HB3 | 44:DW:80:ILE:CD1 | 2.47 | 0.44 |
| 46:DY:46:VAL:O | 46:DY:46:VAL:HG12 | 2.18 | 0.44 |
| 1:AA:587:G:N2 | 1:AA:755:G:C8 | 2.85 | 0.44 |
| 1:AA:960:U:O2' | 1:AA:1223:C:C5' | 2.65 | 0.44 |
| 1:AA:1493:A:HO2' | 1:AA:1494:G:P | 2.39 | 0.44 |
| 2:AB:24:ASN:O | 2:AB:27:MET:N | 2.47 | 0.44 |
| 2:AB:208:ARG:O | 2:AB:210:VAL:N | 2.50 | 0.44 |
| 4:AD:26:ARG:HD3 | 4:AD:31:LYS:HD2 | 1.99 | 0.44 |
| 6:AF:80:PHE:C | 6:AF:80:PHE:CD2 | 2.90 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AF:91:ARG:CG | 6:AF:92:THR:N | 2.81 | 0.44 |
| 9:AI:63:LEU:N | 9:AI:63:LEU:CD2 | 2.79 | 0.44 |
| 10:AJ:35:GLN:O | 10:AJ:36:VAL:O | 2.35 | 0.44 |
| 11:AK:71:ALA:O | 11:AK:73:ALA:N | 2.49 | 0.44 |
| 13:AM:16:VAL:HG22 | 13:AM:41:GLU:HB2 | 1.98 | 0.44 |
| 19:AS:15:LEU:CD1 | 19:AS:33:THR:HG21 | 2.48 | 0.44 |
| 22:BA:829:A:N7 | 22:BA:2247:A:O2' | 2.49 | 0.44 |
| 22:BA:1177:G:O2' | 22:BA:1178:C:O5' | 2.30 | 0.44 |
| 22:BA:1190:G:OP1 | 33:BL:32:GLY:HA2 | 2.17 | 0.44 |
| 22:BA:1392:A:C6 | 22:BA:1393:A:C6 | 3.06 | 0.44 |
| 22:BA:1536:C:O4' | 22:BA:1537:G:C2 | 2.70 | 0.44 |
| 22:BA:1735:A:C2' | 22:BA:1736:U:H5' | 2.47 | 0.44 |
| 22:BA:2488:G:O2' | 22:BA:2489:U:H5' | 2.17 | 0.44 |
| 22:BA:2885:G:H2' | 22:BA:2886:A:C4' | 2.47 | 0.44 |
| 23:BB:15:A:O2' | 23:BB:16:G:H5' | 2.16 | 0.44 |
| 26:BE:29:HIS:NE2 | 33:BL:8:PRO:HD3 | 2.32 | 0.44 |
| 29:BH:57:LYS:CG | 29:BH:58:LEU:N | 2.81 | 0.44 |
| 30:BI:105:GLN:O | 30:BI:106:LEU:CB | 2.65 | 0.44 |
| 31:BJ:75:TYR:CD1 | 31:BJ:86:GLN:HB3 | 2.52 | 0.44 |
| 36:BO:30:ARG:HG2 | 36:BO:31:THR:N | 2.33 | 0.44 |
| 41:BT:61:LEU:C | 41:BT:61:LEU:HD12 | 2.37 | 0.44 |
| 43:BV:51:GLN:HB2 | 43:BV:57:TYR:OH | 2.17 | 0.44 |
| 46:BY:61:ALA:O | 46:BY:62:GLY:C | 2.55 | 0.44 |
| 53:B5:133:GLY:O | 53:B5:134:PRO:CB | 2.64 | 0.44 |
| 1:CA:39:G:C2 | 1:CA:40:C:C2 | 3.05 | 0.44 |
| 1:CA:218:U:C2' | 1:CA:219:U:H5' | 2.47 | 0.44 |
| 1:CA:327:A:C2 | 1:CA:329:A:C4 | 3.04 | 0.44 |
| 1:CA:407:U:OP1 | 4:CD:3:ARG:NH2 | 2.50 | 0.44 |
| 1:CA:689:C:H2' | 1:CA:690:G:O4' | 2.16 | 0.44 |
| 1:CA:775:G:C2' | 1:CA:776:G:H5' | 2.48 | 0.44 |
| 1:CA:836:G:C6 | 1:CA:837:U:C2 | 3.05 | 0.44 |
| 1:CA:1007:U:C2' | 1:CA:1008:U:H5' | 2.46 | 0.44 |
| 1:CA:1206:G:C6 | 1:CA:1207:G:C5 | 3.05 | 0.44 |
| 1:CA:1265:C:C2 | 1:CA:1266:G:N7 | 2.85 | 0.44 |
| 3:CC:141:ALA:O | 3:CC:146:ALA:HB3 | 2.16 | 0.44 |
| 7:CG:136:LYS:O | 7:CG:136:LYS:HD2 | 2.17 | 0.44 |
| 10:CJ:52:LEU:HD23 | 10:CJ:62:ARG:HG2 | 1.98 | 0.44 |
| 10:CJ:52:LEU:HD23 | 10:CJ:62:ARG:CG | 2.47 | 0.44 |
| 11:CK:112:ASP:HB3 | 21:CU:20:LYS:HE3 | 2.00 | 0.44 |
| 12:CL:114:ARG:CZ | 12:CL:121:ARG:HA | 2.47 | 0.44 |
| 14:CN:58:SER:O | 14:CN:59:ARG:HG3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:92:U:H2' | 22:DA:93:G:O4' | 2.15 | 0.44 |
| 22:DA:121:G:H1' | 22:DA:131:A:N1 | 2.32 | 0.44 |
| 22:DA:200:U:C6 | 22:DA:201:C:C5 | 3.05 | 0.44 |
| 22:DA:253:C:H2' | 22:DA:254:G:H5' | 1.98 | 0.44 |
| 22:DA:419:U:C4 | 22:DA:420:C:C5 | 3.06 | 0.44 |
| 22:DA:600:G:H1' | 26:DE:100:MET:HG2 | 2.00 | 0.44 |
| 22:DA:681:G:C4 | 22:DA:682:G:C8 | 3.06 | 0.44 |
| 22:DA:730:A:OP1 | 22:DA:1775:U:O2' | 2.24 | 0.44 |
| 22:DA:769:U:N3 | 22:DA:770:G:N7 | 2.65 | 0.44 |
| 22:DA:1439:A:C2 | 22:DA:1553:A:C4 | 3.05 | 0.44 |
| 22:DA:2234:G:C6 | 22:DA:2235:G:C5 | 3.05 | 0.44 |
| 22:DA:2518:A:N3 | 22:DA:2518:A:H2' | 2.32 | 0.44 |
| 22:DA:2800:A:H3' | 22:DA:2801:G:H5' | 1.99 | 0.44 |
| 24:DC:18:LYS:O | 24:DC:19:VAL:CB | 2.65 | 0.44 |
| 24:DC:221:ARG:NH2 | 58:DC:306:HOH:O | 2.50 | 0.44 |
| 25:DD:18:ASP:OD2 | 25:DD:18:ASP:N | 2.51 | 0.44 |
| 27:DF:136:ILE:HA | 27:DF:141:ILE:HG21 | 1.98 | 0.44 |
| 28:DG:91:GLY:HA3 | 28:DG:160:LYS:HG3 | 1.99 | 0.44 |
| 29:DH:25:TYR:O | 29:DH:29:PHE:HB3 | 2.18 | 0.44 |
| 29:DH:37:VAL:HG22 | 29:DH:38:PRO:HD2 | 1.98 | 0.44 |
| 30:DI:20:PRO:CG | 30:DI:23:PRO:HG2 | 2.47 | 0.44 |
| 33:DL:50:PHE:CZ | 33:DL:52:GLY:O | 2.70 | 0.44 |
| 33:DL:91:ASP:HB3 | 33:DL:94:THR:HB | 2.00 | 0.44 |
| 35:DN:34:ILE:HD11 | 35:DN:44:LEU:CD2 | 2.48 | 0.44 |
| 35:DN:87:PHE:CZ | 35:DN:94:TYR:HB3 | 2.52 | 0.44 |
| 38:DQ:93:LYS:O | 38:DQ:97:ASP:HB2 | 2.17 | 0.44 |
| 41:DT:72:GLN:O | 41:DT:74:ILE:HG23 | 2.18 | 0.44 |
| 44:DW:45:PHE:CG | 44:DW:80:ILE:HD11 | 2.52 | 0.44 |
| 44:DW:46:HIS:CD2 | 44:DW:77:ARG:HD3 | 2.52 | 0.44 |
| 1:AA:600:A:C2 | 1:AA:601:G:C4 | 3.05 | 0.44 |
| 1:AA:636:U:H5'' | 17:AQ:6:ARG:HG2 | 1.99 | 0.44 |
| 1:AA:727:G:N2 | 1:AA:731:G:C4 | 2.85 | 0.44 |
| 1:AA:803:G:C5 | 1:AA:804:U:C4 | 3.06 | 0.44 |
| 1:AA:945:G:C2 | 1:AA:946:A:C8 | 3.05 | 0.44 |
| 1:AA:1182:G:C4' | 1:AA:1183:U:H5' | 2.48 | 0.44 |
| 1:AA:1317:C:O2' | 14:AN:49:GLN:HG2 | 2.17 | 0.44 |
| 4:AD:4:TYR:O | 4:AD:5:LEU:HB3 | 2.18 | 0.44 |
| 4:AD:90:LEU:C | 4:AD:90:LEU:HD12 | 2.38 | 0.44 |
| 5:AE:83:HIS:HB2 | 5:AE:84:PRO:CD | 2.48 | 0.44 |
| 5:AE:101:GLU:CB | 5:AE:122:ASN:CB | 2.94 | 0.44 |
| 8:AH:30:SER:O | 8:AH:31:LYS:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:AI:13:LYS:O | 9:AI:15:SER:N | 2.47 | 0.44 |
| 9:AI:84:THR:HG21 | 9:AI:103:PHE:CB | 2.47 | 0.44 |
| 13:AM:16:VAL:CG2 | 13:AM:41:GLU:HB2 | 2.47 | 0.44 |
| 22:BA:428:A:H2' | 22:BA:429:A:C8 | 2.52 | 0.44 |
| 22:BA:668:A:H2' | 22:BA:669:G:OP1 | 2.17 | 0.44 |
| 22:BA:1059:G:O2' | 30:BI:129:ILE:HA | 2.17 | 0.44 |
| 22:BA:1071:G:P | 22:BA:1071:G:H8 | 2.39 | 0.44 |
| 22:BA:1794:A:C2' | 22:BA:1795:C:O5' | 2.66 | 0.44 |
| 22:BA:1850:G:C2 | 22:BA:1893:C:O2 | 2.71 | 0.44 |
| 22:BA:1875:G:C2' | 22:BA:1876:A:OP2 | 2.65 | 0.44 |
| 22:BA:2218:G:O2' | 22:BA:2219:U:H5' | 2.17 | 0.44 |
| 22:BA:2280:G:C2 | 22:BA:2281:A:C8 | 3.05 | 0.44 |
| 22:BA:2716:C:C2' | 22:BA:2717:C:H5' | 2.48 | 0.44 |
| 24:BC:195:VAL:CG1 | 24:BC:196:GLY:N | 2.80 | 0.44 |
| 26:BE:32:VAL:HG23 | 26:BE:33:VAL:N | 2.32 | 0.44 |
| 27:BF:5:HIS:CE1 | 27:BF:9:LYS:HE3 | 2.53 | 0.44 |
| 29:BH:62:LEU:HD12 | 29:BH:62:LEU:O | 2.17 | 0.44 |
| 32:BK:66:LYS:HB3 | 32:BK:66:LYS:HE2 | 1.84 | 0.44 |
| 33:BL:62:PRO:CG | 51:B3:25:LYS:HD3 | 2.47 | 0.44 |
| 34:BM:78:LEU:N | 34:BM:78:LEU:HD12 | 2.32 | 0.44 |
| 44:BW:56:ASP:O | 44:BW:57:HIS:CB | 2.65 | 0.44 |
| 1:CA:142:G:C2 | 1:CA:143:A:H1' | 2.52 | 0.44 |
| 1:CA:374:A:N3 | 1:CA:375:U:C6 | 2.86 | 0.44 |
| 1:CA:743:A:C5 | 1:CA:744:C:C5 | 3.06 | 0.44 |
| 1:CA:1071:C:H2' | 1:CA:1072:G:H8 | 1.82 | 0.44 |
| 2:CB:71:GLY:HA2 | 2:CB:164:ILE:CG2 | 2.47 | 0.44 |
| 14:CN:87:ALA:HB1 | 14:CN:92:GLU:HB2 | 2.00 | 0.44 |
| 15:CO:13:SER:O | 15:CO:14:GLU:HG3 | 2.18 | 0.44 |
| 17:CQ:51:ASN:ND2 | 17:CQ:51:ASN:O | 2.51 | 0.44 |
| 22:DA:84:A:N6 | 22:DA:99:U:H4' | 2.32 | 0.44 |
| 22:DA:188:G:C6 | 22:DA:189:G:C4 | 3.05 | 0.44 |
| 22:DA:207:A:C4 | 22:DA:208:C:C6 | 3.06 | 0.44 |
| 22:DA:449:A:N7 | 22:DA:450:G:N7 | 2.65 | 0.44 |
| 22:DA:1179:G:C6 | 22:DA:1180:U:H1' | 2.52 | 0.44 |
| 22:DA:1275:A:H4' | 22:DA:1276:A:OP1 | 2.16 | 0.44 |
| 22:DA:1286:A:C6 | 22:DA:1329:U:C4 | 3.04 | 0.44 |
| 22:DA:1310:G:H2' | 22:DA:1311:G:H5' | 1.99 | 0.44 |
| 22:DA:1312:U:O2 | 22:DA:1603:A:C2 | 2.71 | 0.44 |
| 22:DA:1345:C:H5' | 22:DA:1396:U:O4 | 2.17 | 0.44 |
| 22:DA:1409:U:H2' | 22:DA:1410:G:O4' | 2.17 | 0.44 |
| 22:DA:1726:C:H2' | 22:DA:1727:C:H6 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2032:G:H1' | 25:DD:150:GLN:HE22 | 1.79 | 0.44 |
| 22:DA:2308:G:C4' | 22:DA:2309:A:OP2 | 2.65 | 0.44 |
| 23:DB:76:G:H2' | 23:DB:77:U:O4' | 2.18 | 0.44 |
| 24:DC:178:SER:O | 24:DC:271:ARG:HB2 | 2.17 | 0.44 |
| 26:DE:108:ILE:HD13 | 26:DE:181:ILE:HG13 | 1.98 | 0.44 |
| 27:DF:117:LEU:CD2 | 27:DF:176:PRO:HG2 | 2.47 | 0.44 |
| 30:DI:28:LEU:HD11 | 30:DI:35:ILE:CD1 | 2.47 | 0.44 |
| 1:AA:8:A:H5' | 5:AE:125:ALA:O | 2.17 | 0.44 |
| 1:AA:721:G:C6 | 1:AA:733:G:C2 | 3.05 | 0.44 |
| 1:AA:723:U:O5' | 21:AU:49:LYS:HG2 | 2.17 | 0.44 |
| 1:AA:926:G:C6 | 1:AA:1505:G:C5 | 3.05 | 0.44 |
| 1:AA:937:A:N6 | 1:AA:1345:U:O4 | 2.50 | 0.44 |
| 1:AA:949:A:C5 | 1:AA:950:U:C5 | 3.05 | 0.44 |
| 1:AA:1504:G:OP2 | 1:AA:1507:A:O2' | 2.26 | 0.44 |
| 2:AB:15:HIS:O | 2:AB:16:PHE:C | 2.55 | 0.44 |
| 2:AB:33:GLY:O | 2:AB:34:ALA:HB2 | 2.18 | 0.44 |
| 2:AB:87:CYS:C | 2:AB:89:GLN:N | 2.71 | 0.44 |
| 3:AC:159:GLY:O | 3:AC:160:ALA:C | 2.55 | 0.44 |
| 5:AE:56:VAL:N | 5:AE:57:PRO:HD2 | 2.33 | 0.44 |
| 6:AF:45:ARG:HG2 | 6:AF:46:GLN:N | 2.32 | 0.44 |
| 6:AF:90:MET:O | 6:AF:91:ARG:O | 2.36 | 0.44 |
| 8:AH:111:MET:CE | 8:AH:116:ALA:HA | 2.46 | 0.44 |
| 11:AK:16:VAL:HG13 | 11:AK:17:SER:H | 1.82 | 0.44 |
| 14:AN:87:ALA:O | 14:AN:92:GLU:HB2 | 2.18 | 0.44 |
| 22:BA:414:C:H2' | 22:BA:415:A:C8 | 2.52 | 0.44 |
| 22:BA:685:A:H1' | 22:BA:688:U:O4 | 2.18 | 0.44 |
| 22:BA:1100:C:H2' | 22:BA:1101:U:C6 | 2.52 | 0.44 |
| 22:BA:1359:A:N7 | 22:BA:1373:A:C2 | 2.85 | 0.44 |
| 22:BA:1441:G:H2' | 22:BA:1442:U:C6 | 2.52 | 0.44 |
| 22:BA:1442:U:H2' | 22:BA:1443:U:C6 | 2.52 | 0.44 |
| 22:BA:1635:A:C2 | 22:BA:1636:U:H1' | 2.52 | 0.44 |
| 22:BA:1688:U:C4 | 22:BA:1698:A:C2 | 3.06 | 0.44 |
| 22:BA:1917:U:N3 | 22:BA:1918:A:C4 | 2.85 | 0.44 |
| 22:BA:2352:A:C2' | 22:BA:2353:G:H5' | 2.48 | 0.44 |
| 22:BA:2511:U:O4 | 22:BA:2575:C:N3 | 2.50 | 0.44 |
| 22:BA:2623:G:H4' | 22:BA:2825:G:C8 | 2.53 | 0.44 |
| 23:BB:54:G:H21 | 27:BF:26:MET:CE | 2.30 | 0.44 |
| 24:BC:195:VAL:O | 24:BC:196:GLY:O | 2.35 | 0.44 |
| 29:BH:31:VAL:N | 29:BH:32:PRO:CD | 2.80 | 0.44 |
| 30:BI:67:PHE:CD2 | 30:BI:67:PHE:N | 2.85 | 0.44 |
| 30:BI:74:PRO:O | 30:BI:75:PRO:O | 2.36 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BN:69:ARG:C | 35:BN:70:THR:HG23 | 2.37 | 0.44 |
| 35:BN:106:ASP:C | 35:BN:106:ASP:OD1 | 2.55 | 0.44 |
| 38:BQ:58:ARG:O | 38:BQ:62:ILE:HG13 | 2.18 | 0.44 |
| 39:BR:49:ILE:HG22 | 39:BR:52:PRO:C | 2.38 | 0.44 |
| 48:B0:25:VAL:C | 48:B0:26:THR:HG23 | 2.38 | 0.44 |
| 1:CA:68:G:N2 | 1:CA:152:A:H1' | 2.33 | 0.44 |
| 1:CA:178:C:H2' | 1:CA:179:A:O4' | 2.18 | 0.44 |
| 1:CA:302:G:C6 | 1:CA:303:A:C5 | 3.05 | 0.44 |
| 1:CA:330:C:O2 | 1:CA:330:C:H2' | 2.15 | 0.44 |
| 1:CA:577:G:O2' | 1:CA:578:C:H5' | 2.17 | 0.44 |
| 1:CA:1068:G:H2' | 1:CA:1069:C:H5' | 2.00 | 0.44 |
| 2:CB:56:GLU:HG2 | 2:CB:198:PHE:CZ | 2.53 | 0.44 |
| 2:CB:82:ASP:N | 2:CB:85:LEU:HB3 | 2.33 | 0.44 |
| 2:CB:99:GLY:C | 2:CB:101:LEU:H | 2.21 | 0.44 |
| 2:CB:186:ILE:HA | 2:CB:200:ILE:HB | 1.98 | 0.44 |
| 2:CB:206:ALA:O | 2:CB:207:ILE:C | 2.55 | 0.44 |
| 4:CD:11:LEU:HD13 | 4:CD:63:ARG:HD3 | 2.00 | 0.44 |
| 5:CE:103:THR:O | 5:CE:122:ASN:HA | 2.18 | 0.44 |
| 9:CI:130:ARG:HD2 | 9:CI:130:ARG:HA | 1.81 | 0.44 |
| 10:CJ:7:ARG:HD2 | 10:CJ:73:LEU:HD21 | 1.99 | 0.44 |
| 14:CN:48:LEU:O | 14:CN:48:LEU:HD23 | 2.17 | 0.44 |
| 16:CP:67:ILE:HG22 | 16:CP:68:SER:O | 2.17 | 0.44 |
| 17:CQ:28:PHE:CE1 | 17:CQ:37:PHE:HB3 | 2.53 | 0.44 |
| 18:CR:33:ILE:CA | 18:CR:40:VAL:HG23 | 2.45 | 0.44 |
| 19:CS:74:PHE:CD1 | 19:CS:74:PHE:N | 2.84 | 0.44 |
| 22:DA:39:G:C5 | 22:DA:40:U:C5 | 3.05 | 0.44 |
| 22:DA:118:A:N3 | 22:DA:178:G:H1' | 2.32 | 0.44 |
| 22:DA:207:A:C2 | 22:DA:208:C:H1' | 2.52 | 0.44 |
| 22:DA:469:G:O6 | 50:D2:37:LYS:NZ | 2.43 | 0.44 |
| 22:DA:699:A:C2' | 22:DA:700:G:H5' | 2.48 | 0.44 |
| 22:DA:1090:A:N1 | 22:DA:1091:G:N7 | 2.66 | 0.44 |
| 22:DA:1369:G:N3 | 22:DA:1370:C:C6 | 2.84 | 0.44 |
| 22:DA:1497:U:O2' | 22:DA:1577:C:H5'' | 2.18 | 0.44 |
| 22:DA:1524:G:C2 | 22:DA:1525:A:C8 | 3.05 | 0.44 |
| 22:DA:1604:C:H5'' | 58:DA:3406:HOH:O | 2.17 | 0.44 |
| 22:DA:1867:G:O6 | 22:DA:1875:G:C2 | 2.70 | 0.44 |
| 22:DA:2436:G:C2 | 22:DA:2437:G:C8 | 3.05 | 0.44 |
| 23:DB:58:A:H2' | 23:DB:59:A:O4' | 2.18 | 0.44 |
| 24:DC:124:ILE:O | 24:DC:124:ILE:HG22 | 2.16 | 0.44 |
| 27:DF:57:LEU:HB2 | 27:DF:65:PRO:HG2 | 2.00 | 0.44 |
| 30:DI:65:ARG:HG3 | 30:DI:66:SER:N | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:DO:67:ASN:O | 36:DO:70:ALA:N | 2.51 | 0.44 |
| 37:DP:103:ARG:HD3 | 37:DP:108:ALA:HB2 | 1.98 | 0.44 |
| 39:DR:27:ILE:HG13 | 39:DR:33:VAL:HG11 | 2.00 | 0.44 |
| 42:DU:83:VAL:HG11 | 42:DU:94:ARG:HB3 | 1.99 | 0.44 |
| 46:DY:1:MET:HA | 46:DY:4:LYS:HB2 | 1.99 | 0.44 |
| 1:AA:417:G:C2 | 1:AA:418:C:C2 | 3.06 | 0.44 |
| 1:AA:452:A:H2' | 1:AA:453:G:H5' | 2.00 | 0.44 |
| 1:AA:663:A:N1 | 1:AA:743:A:C2 | 2.85 | 0.44 |
| 1:AA:771:G:O2' | 1:AA:772:U:H5' | 2.16 | 0.44 |
| 1:AA:781:A:H4' | 1:AA:1522:U:O2' | 2.17 | 0.44 |
| 1:AA:1014:A:C4 | 19:AS:34:TRP:CZ3 | 3.06 | 0.44 |
| 1:AA:1068:G:O2' | 1:AA:1191:A:N1 | 2.38 | 0.44 |
| 1:AA:1538:C:O2' | 1:AA:1539:C:H5' | 2.17 | 0.44 |
| 2:AB:117:LEU:O | 2:AB:120:GLN:HB3 | 2.18 | 0.44 |
| 2:AB:144:LEU:N | 2:AB:144:LEU:HD23 | 2.32 | 0.44 |
| 3:AC:14:ILE:O | 3:AC:15:VAL:HG22 | 2.18 | 0.44 |
| 3:AC:191:THR:HB | 3:AC:193:TYR:CE2 | 2.52 | 0.44 |
| 5:AE:45:ARG:HA | 5:AE:72:ILE:O | 2.18 | 0.44 |
| 18:AR:70:TYR:HB2 | 18:AR:71:THR:HG22 | 2.00 | 0.44 |
| 20:AT:55:GLN:N | 20:AT:56:PRO:HD2 | 2.33 | 0.44 |
| 22:BA:26:G:H1' | 22:BA:514:A:H61 | 1.83 | 0.44 |
| 22:BA:297:G:OP1 | 42:BU:92:LYS:NZ | 2.49 | 0.44 |
| 22:BA:662:G:O3' | 33:BL:16:GLY:HA2 | 2.17 | 0.44 |
| 22:BA:880:G:C4 | 22:BA:881:G:C8 | 3.06 | 0.44 |
| 22:BA:1014:A:C6 | 22:BA:1015:U:C4 | 3.05 | 0.44 |
| 22:BA:1179:G:C5 | 22:BA:1180:U:N1 | 2.86 | 0.44 |
| 22:BA:2563:U:H1' | 22:BA:2566:A:N6 | 2.33 | 0.44 |
| 22:BA:2824:C:C4 | 22:BA:2825:G:C5 | 3.05 | 0.44 |
| 23:BB:94:A:H2' | 23:BB:95:U:C6 | 2.53 | 0.44 |
| 24:BC:123:ALA:O | 24:BC:125:LYS:N | 2.51 | 0.44 |
| 25:BD:9:VAL:O | 25:BD:197:THR:OG1 | 2.35 | 0.44 |
| 29:BH:89:LYS:CE | 29:BH:124:THR:HG22 | 2.48 | 0.44 |
| 31:BJ:114:LEU:CG | 31:BJ:118:MET:HE3 | 2.39 | 0.44 |
| 41:BT:67:VAL:C | 41:BT:68:LYS:HG2 | 2.38 | 0.44 |
| 46:BY:9:LYS:HB3 | 46:BY:12:GLU:CG | 2.48 | 0.44 |
| 46:BY:32:ALA:HB2 | 46:BY:37:LEU:CD2 | 2.48 | 0.44 |
| 48:B0:41:HIS:HA | 48:B0:49:TYR:OH | 2.17 | 0.44 |
| 53:B5:65:LEU:HD21 | 53:B5:195:ARG:CB | 2.47 | 0.44 |
| 1:CA:57:G:C6 | 1:CA:58:C:C4 | 3.06 | 0.44 |
| 1:CA:121:U:H3' | 1:CA:122:G:C5' | 2.48 | 0.44 |
| 1:CA:183:C:H2' | 1:CA:183:C:O2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:427:U:O2' | 1:CA:541:G:OP1 | 2.29 | 0.44 |
| 1:CA:528:C:O2 | 1:CA:528:C:H2' | 2.16 | 0.44 |
| 1:CA:570:G:H1' | 1:CA:820:U:C4 | 2.52 | 0.44 |
| 1:CA:676:A:H2' | 1:CA:677:U:C6 | 2.52 | 0.44 |
| 3:CC:23:PHE:CG | 3:CC:24:ALA:N | 2.85 | 0.44 |
| 3:CC:172:ARG:C | 3:CC:174:PRO:HD3 | 2.37 | 0.44 |
| 3:CC:184:TYR:CD1 | 3:CC:201:TRP:CD1 | 3.06 | 0.44 |
| 7:CG:42:ILE:CG2 | 7:CG:116:MET:HG3 | 2.48 | 0.44 |
| 10:CJ:22:THR:HA | 10:CJ:25:ILE:HG22 | 1.98 | 0.44 |
| 10:CJ:81:GLU:HA | 10:CJ:84:VAL:HG12 | 2.00 | 0.44 |
| 12:CL:44:LYS:HB3 | 12:CL:45:PRO:HD3 | 1.99 | 0.44 |
| 14:CN:31:ILE:N | 14:CN:31:ILE:HD12 | 2.32 | 0.44 |
| 20:CT:36:TYR:CD1 | 20:CT:37:ALA:N | 2.85 | 0.44 |
| 22:DA:108:G:H1' | 22:DA:347:A:N3 | 2.33 | 0.44 |
| 22:DA:453:A:H4' | 22:DA:472:A:H62 | 1.82 | 0.44 |
| 22:DA:693:A:C5 | 22:DA:694:U:C4 | 3.06 | 0.44 |
| 22:DA:920:A:OP1 | 47:DZ:19:LYS:HE3 | 2.18 | 0.44 |
| 22:DA:1066:U:C2' | 22:DA:1067:A:OP1 | 2.66 | 0.44 |
| 22:DA:1190:G:OP1 | 33:DL:32:GLY:CA | 2.66 | 0.44 |
| 22:DA:1364:G:H2' | 22:DA:1365:A:C5' | 2.44 | 0.44 |
| 22:DA:1645:G:H4' | 22:DA:1646:C:C5 | 2.52 | 0.44 |
| 22:DA:2128:G:H1' | 22:DA:2173:A:O2' | 2.17 | 0.44 |
| 22:DA:2513:A:C5 | 22:DA:2514:U:C4 | 3.06 | 0.44 |
| 22:DA:2540:C:C2 | 22:DA:2541:A:C8 | 3.05 | 0.44 |
| 22:DA:2699:C:H2' | 22:DA:2700:A:O4' | 2.17 | 0.44 |
| 23:DB:68:C:H2' | 23:DB:69:G:O4' | 2.16 | 0.44 |
| 24:DC:174:LEU:O | 24:DC:181:MET:HA | 2.17 | 0.44 |
| 27:DF:2:ALA:N | 27:DF:94:GLU:OE2 | 2.50 | 0.44 |
| 30:DI:28:LEU:HD11 | 30:DI:35:ILE:HD12 | 1.99 | 0.44 |
| 34:DM:70:ASP:C | 34:DM:70:ASP:OD1 | 2.56 | 0.44 |
| 1:AA:77:A:H2' | 1:AA:78:A:C8 | 2.53 | 0.44 |
| 1:AA:268:U:H2' | 1:AA:269:C:C6 | 2.52 | 0.44 |
| 1:AA:276:G:P | 17:AQ:17:MET:HE2 | 2.57 | 0.44 |
| 1:AA:427:U:C4 | 1:AA:428:G:C6 | 3.06 | 0.44 |
| 1:AA:828:U:C5 | 1:AA:859:G:C4 | 3.06 | 0.44 |
| 1:AA:957:U:H1' | 1:AA:960:U:N3 | 2.33 | 0.44 |
| 1:AA:1024:G:C2' | 1:AA:1025:U:O5' | 2.66 | 0.44 |
| 1:AA:1027:C:C2 | 1:AA:1034:G:O6 | 2.70 | 0.44 |
| 2:AB:132:LYS:O | 2:AB:136:MET:HB2 | 2.17 | 0.44 |
| 10:AJ:18:ILE:CG2 | 10:AJ:19:ASP:N | 2.80 | 0.44 |
| 10:AJ:23:ALA:O | 10:AJ:27:GLU:HB2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:AJ:71:LEU:O | 10:AJ:72:ARG:HD3 | 2.17 | 0.44 |
| 11:AK:91:PRO:C | 11:AK:93:ARG:H | 2.20 | 0.44 |
| 16:AP:6:LEU:HD13 | 16:AP:71:VAL:HG23 | 1.99 | 0.44 |
| 16:AP:43:ALA:O | 16:AP:46:LYS:HD2 | 2.17 | 0.44 |
| 20:AT:54:MET:CE | 20:AT:58:VAL:HG21 | 2.47 | 0.44 |
| 21:AU:19:PHE:O | 21:AU:22:SER:HB3 | 2.18 | 0.44 |
| 22:BA:57:C:H2' | 22:BA:58:G:O4' | 2.18 | 0.44 |
| 22:BA:197:A:C6 | 22:BA:198:C:C2 | 3.06 | 0.44 |
| 22:BA:481:G:C2 | 22:BA:507:A:C4 | 3.06 | 0.44 |
| 22:BA:1103:A:OP2 | 22:BA:1104:C:C5 | 2.71 | 0.44 |
| 22:BA:1185:G:H5'' | 22:BA:1186:G:P | 2.58 | 0.44 |
| 22:BA:1366:A:C2 | 22:BA:1367:A:H1' | 2.52 | 0.44 |
| 22:BA:2502:G:C5' | 22:BA:2503:A:H5'' | 2.46 | 0.44 |
| 26:BE:31:VAL:HG21 | 26:BE:104:ALA:HB2 | 1.99 | 0.44 |
| 29:BH:97:ARG:O | 29:BH:101:ASP:HB2 | 2.17 | 0.44 |
| 29:BH:100:ALA:HB2 | 29:BH:115:VAL:HG21 | 1.98 | 0.44 |
| 30:BI:72:LYS:CD | 30:BI:72:LYS:N | 2.80 | 0.44 |
| 30:BI:97:LYS:HB3 | 30:BI:139:VAL:CG2 | 2.48 | 0.44 |
| 33:BL:77:ILE:HD11 | 33:BL:101:ILE:HG21 | 2.00 | 0.44 |
| 33:BL:89:VAL:O | 33:BL:94:THR:HG21 | 2.18 | 0.44 |
| 37:BP:34:GLU:N | 37:BP:37:LYS:O | 2.46 | 0.44 |
| 1:CA:78:A:C2 | 1:CA:92:U:O2 | 2.71 | 0.44 |
| 1:CA:128:G:C2 | 1:CA:234:C:C2 | 3.05 | 0.44 |
| 1:CA:462:G:O6 | 1:CA:469:C:N4 | 2.50 | 0.44 |
| 1:CA:635:A:C6 | 1:CA:636:U:C4 | 3.05 | 0.44 |
| 1:CA:756:C:H2' | 1:CA:757:U:O5' | 2.18 | 0.44 |
| 1:CA:1002:G:C2 | 1:CA:1003:G:H1' | 2.53 | 0.44 |
| 1:CA:1007:U:C2' | 1:CA:1008:U:C5' | 2.95 | 0.44 |
| 1:CA:1015:G:H2' | 1:CA:1016:A:O4' | 2.18 | 0.44 |
| 1:CA:1092:A:N1 | 1:CA:1183:U:O2 | 2.51 | 0.44 |
| 1:CA:1265:C:N3 | 1:CA:1266:G:N7 | 2.65 | 0.44 |
| 1:CA:1291:U:H4' | 9:CI:42:GLU:HG2 | 2.00 | 0.44 |
| 1:CA:1537:U:C4 | 1:CA:1538:C:C4 | 3.06 | 0.44 |
| 2:CB:21:ARG:HA | 2:CB:21:ARG:NE | 2.30 | 0.44 |
| 4:CD:24:GLY:O | 4:CD:161:LEU:HD11 | 2.17 | 0.44 |
| 4:CD:195:ILE:O | 4:CD:195:ILE:CG1 | 2.66 | 0.44 |
| 5:CE:83:HIS:HB2 | 5:CE:84:PRO:HD2 | 1.98 | 0.44 |
| 5:CE:105:ILE:HG13 | 5:CE:105:ILE:O | 2.17 | 0.44 |
| 16:CP:67:ILE:HG23 | 16:CP:71:VAL:CG1 | 2.48 | 0.44 |
| 19:CS:58:VAL:HA | 19:CS:59:PRO:HD3 | 1.89 | 0.44 |
| 22:DA:40:U:C5 | 22:DA:41:C:N4 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:54:G:N1 | 22:DA:55:G:N7 | 2.65 | 0.44 |
| 22:DA:187:G:N1 | 22:DA:210:C:C2 | 2.85 | 0.44 |
| 22:DA:406:G:H2' | 22:DA:407:G:C8 | 2.52 | 0.44 |
| 22:DA:422:A:C2 | 22:DA:423:A:C4 | 3.05 | 0.44 |
| 22:DA:426:C:C4 | 22:DA:427:U:C5 | 3.06 | 0.44 |
| 22:DA:465:G:N2 | 22:DA:684:G:H1' | 2.33 | 0.44 |
| 22:DA:517:C:C2' | 22:DA:518:G:O5' | 2.66 | 0.44 |
| 22:DA:599:A:C2 | 22:DA:659:G:C5 | 3.05 | 0.44 |
| 22:DA:1193:G:C2 | 22:DA:1194:A:C5 | 3.06 | 0.44 |
| 22:DA:1248:G:C5 | 26:DE:46:GLN:NE2 | 2.86 | 0.44 |
| 22:DA:1403:A:C2 | 22:DA:1404:C:C2 | 3.06 | 0.44 |
| 22:DA:1999:C:H5'' | 22:DA:2723:C:O2' | 2.18 | 0.44 |
| 22:DA:2134:A:C2 | 22:DA:2159:G:H1' | 2.53 | 0.44 |
| 22:DA:2166:U:H2' | 22:DA:2167:U:H5' | 2.00 | 0.44 |
| 22:DA:2350:C:H2' | 22:DA:2351:G:O4' | 2.17 | 0.44 |
| 22:DA:2410:G:H2' | 22:DA:2411:A:O4' | 2.17 | 0.44 |
| 24:DC:158:ALA:HA | 24:DC:195:VAL:HG22 | 2.00 | 0.44 |
| 25:DD:4:LEU:HD22 | 25:DD:101:PHE:CE2 | 2.52 | 0.44 |
| 25:DD:125:TRP:O | 25:DD:126:ASN:CB | 2.66 | 0.44 |
| 26:DE:131:THR:HB | 26:DE:164:LEU:HD22 | 1.99 | 0.44 |
| 29:DH:31:VAL:CB | 29:DH:32:PRO:HD3 | 2.47 | 0.44 |
| 32:DK:111:LYS:HG3 | 32:DK:112:PHE:CE1 | 2.52 | 0.44 |
| 33:DL:55:MET:SD | 33:DL:59:ARG:CZ | 3.06 | 0.44 |
| 40:DS:30:SER:HA | 40:DS:33:LEU:HD12 | 1.99 | 0.44 |
| 41:DT:24:MET:HG2 | 41:DT:29:THR:O | 2.18 | 0.44 |
| 45:DX:39:TRP:HB2 | 45:DX:46:PHE:CE2 | 2.53 | 0.44 |
| 45:DX:47:VAL:O | 45:DX:47:VAL:CG1 | 2.65 | 0.44 |
| 45:DX:52:SER:O | 45:DX:55:GLY:N | 2.51 | 0.44 |
| 48:D0:40:ARG:O | 48:D0:41:HIS:HB2 | 2.18 | 0.44 |
| 1:AA:197:A:N3 | 1:AA:198:G:H1' | 2.33 | 0.44 |
| 1:AA:200:G:N2 | 1:AA:218:U:O2 | 2.51 | 0.44 |
| 1:AA:264:C:H2' | 1:AA:265:G:O4' | 2.18 | 0.44 |
| 1:AA:397:A:N7 | 1:AA:548:G:C8 | 2.85 | 0.44 |
| 1:AA:723:U:H2' | 1:AA:855:U:H4' | 1.99 | 0.44 |
| 1:AA:1028:C:C5 | 1:AA:1029:U:C5 | 3.05 | 0.44 |
| 1:AA:1220:G:H2' | 1:AA:1221:G:O4' | 2.18 | 0.44 |
| 1:AA:1317:C:H2' | 1:AA:1318:A:H5' | 1.99 | 0.44 |
| 1:AA:1399:C:C4 | 1:AA:1502:A:N1 | 2.86 | 0.44 |
| 2:AB:81:LYS:HG3 | 2:AB:91:PHE:CZ | 2.53 | 0.44 |
| 2:AB:94:HIS:ND1 | 2:AB:146:ASN:HB2 | 2.32 | 0.44 |
| 4:AD:152:GLN:O | 4:AD:155:VAL:HG12 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AN:26:GLU:HG2 | 14:AN:27:LEU:N | 2.33 | 0.44 |
| 16:AP:5:ARG:HA | 16:AP:68:SER:OG | 2.18 | 0.44 |
| 17:AQ:79:VAL:O | 17:AQ:80:GLU:HB2 | 2.18 | 0.44 |
| 22:BA:18:U:O2' | 22:BA:19:A:H5' | 2.17 | 0.44 |
| 22:BA:590:A:H2' | 22:BA:591:U:C6 | 2.53 | 0.44 |
| 22:BA:900:A:C5 | 22:BA:901:C:C6 | 3.06 | 0.44 |
| 22:BA:910:A:H2' | 22:BA:911:A:C8 | 2.53 | 0.44 |
| 22:BA:1087:G:N2 | 22:BA:1090:A:C8 | 2.86 | 0.44 |
| 22:BA:1091:G:H2' | 22:BA:1092:C:C5 | 2.52 | 0.44 |
| 22:BA:1408:G:C6 | 22:BA:1409:U:C4 | 3.06 | 0.44 |
| 22:BA:2232:C:C4 | 22:BA:2233:U:C4 | 3.05 | 0.44 |
| 22:BA:2533:U:H2' | 22:BA:2534:A:H5' | 1.99 | 0.44 |
| 27:BF:132:VAL:O | 27:BF:132:VAL:CG2 | 2.66 | 0.44 |
| 29:BH:57:LYS:HG3 | 29:BH:58:LEU:N | 2.33 | 0.44 |
| 33:BL:26:GLY:C | 33:BL:27:LEU:HD23 | 2.38 | 0.44 |
| 34:BM:45:GLN:HG2 | 34:BM:125:PRO:HD3 | 1.99 | 0.44 |
| 39:BR:34:GLU:HG3 | 39:BR:60:LYS:HE2 | 1.99 | 0.44 |
| 45:BX:4:VAL:N | 45:BX:33:LEU:HD11 | 2.33 | 0.44 |
| 1:CA:120:A:H2' | 1:CA:120:A:OP2 | 2.18 | 0.44 |
| 1:CA:237:G:C4 | 1:CA:238:A:C8 | 3.06 | 0.44 |
| 1:CA:685:G:C2 | 1:CA:686:U:C4 | 3.06 | 0.44 |
| 1:CA:1361:G:C4 | 1:CA:1362:A:C8 | 3.06 | 0.44 |
| 9:CI:88:MET:HB2 | 9:CI:92:GLU:OE2 | 2.17 | 0.44 |
| 11:CK:35:THR:OG1 | 11:CK:40:ASN:N | 2.51 | 0.44 |
| 21:CU:14:VAL:C | 21:CU:16:LEU:HG | 2.38 | 0.44 |
| 22:DA:82:U:N3 | 22:DA:83:A:N7 | 2.66 | 0.44 |
| 22:DA:281:C:H2' | 22:DA:282:A:C8 | 2.53 | 0.44 |
| 22:DA:601:C:H2' | 22:DA:602:A:O4' | 2.18 | 0.44 |
| 22:DA:687:C:N3 | 22:DA:788:A:H5' | 2.33 | 0.44 |
| 22:DA:770:G:O4' | 22:DA:1379:U:C5 | 2.71 | 0.44 |
| 22:DA:835:C:C4 | 22:DA:836:G:N7 | 2.85 | 0.44 |
| 22:DA:1222:U:H2' | 22:DA:1223:G:C8 | 2.53 | 0.44 |
| 22:DA:1362:C:N3 | 22:DA:1363:C:C2 | 2.86 | 0.44 |
| 22:DA:1804:C:N4 | 22:DA:1814:G:N2 | 2.66 | 0.44 |
| 22:DA:1936:A:C8 | 22:DA:1945:G:C6 | 3.06 | 0.44 |
| 24:DC:69:ARG:NH2 | 24:DC:116:ILE:HD11 | 2.32 | 0.44 |
| 27:DF:4:LEU:O | 27:DF:8:TYR:N | 2.51 | 0.44 |
| 27:DF:33:LYS:HD3 | 27:DF:92:ARG:NH1 | 2.33 | 0.44 |
| 33:DL:116:VAL:HG21 | 33:DL:135:ILE:HA | 1.99 | 0.44 |
| 36:DO:53:THR:HB | 36:DO:65:THR:CG2 | 2.48 | 0.44 |
| 42:DU:12:ILE:CG2 | 42:DU:80:ALA:HB2 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DU:18:ASP:HB3 | 42:DU:21:LYS:HG3 | 1.99 | 0.44 |
| 47:DZ:2:ALA:CB | 47:DZ:39:GLU:HB2 | 2.48 | 0.44 |
| 50:D2:9:VAL:O | 50:D2:10:LEU:C | 2.56 | 0.44 |
| 1:AA:43:C:H2' | 1:AA:44:A:O4' | 2.18 | 0.44 |
| 1:AA:283:U:C5 | 1:AA:284:C:C5 | 3.06 | 0.44 |
| 1:AA:557:G:C6 | 1:AA:558:G:N1 | 2.86 | 0.44 |
| 1:AA:602:A:C2 | 1:AA:603:U:O2 | 2.71 | 0.44 |
| 1:AA:722:G:C2' | 1:AA:723:U:OP2 | 2.65 | 0.44 |
| 1:AA:1149:C:O2' | 1:AA:1150:A:H5' | 2.18 | 0.44 |
| 1:AA:1211:U:H1' | 1:AA:1213:A:C2 | 2.53 | 0.44 |
| 1:AA:1296:C:H5'' | 1:AA:1297:G:OP2 | 2.18 | 0.44 |
| 2:AB:66:LYS:N | 2:AB:66:LYS:HD3 | 2.33 | 0.44 |
| 7:AG:139:GLU:OE1 | 7:AG:139:GLU:HA | 2.18 | 0.44 |
| 9:AI:20:PHE:O | 9:AI:63:LEU:HA | 2.17 | 0.44 |
| 9:AI:36:GLU:HA | 9:AI:40:GLY:HA3 | 2.00 | 0.44 |
| 10:AJ:27:GLU:C | 10:AJ:29:ALA:H | 2.22 | 0.44 |
| 11:AK:86:VAL:HG12 | 11:AK:93:ARG:NH1 | 2.33 | 0.44 |
| 12:AL:56:ARG:NH1 | 12:AL:62:GLU:HG3 | 2.33 | 0.44 |
| 14:AN:53:ARG:HG3 | 14:AN:59:ARG:CZ | 2.48 | 0.44 |
| 16:AP:2:VAL:HG22 | 16:AP:65:ALA:HB2 | 1.99 | 0.44 |
| 16:AP:77:GLU:C | 16:AP:79:ASN:N | 2.71 | 0.44 |
| 17:AQ:12:VAL:O | 17:AQ:13:VAL:CG1 | 2.66 | 0.44 |
| 22:BA:142:A:C8 | 22:BA:143:C:C5 | 3.06 | 0.44 |
| 22:BA:273:G:N2 | 22:BA:365:U:O2 | 2.51 | 0.44 |
| 22:BA:301:G:H4' | 22:BA:301:G:OP1 | 2.18 | 0.44 |
| 22:BA:713:G:C6 | 22:BA:714:U:C4 | 3.06 | 0.44 |
| 22:BA:1722:A:N6 | 22:BA:1738:G:H1' | 2.33 | 0.44 |
| 22:BA:1996:C:H4' | 22:BA:1997:C:OP1 | 2.18 | 0.44 |
| 22:BA:2018:G:C2 | 22:BA:2019:A:C4 | 3.06 | 0.44 |
| 29:BH:4:ILE:HG23 | 29:BH:17:ASP:O | 2.17 | 0.44 |
| 29:BH:99:ILE:CD1 | 29:BH:117:LEU:HD13 | 2.48 | 0.44 |
| 31:BJ:30:THR:CG2 | 31:BJ:31:GLU:N | 2.81 | 0.44 |
| 32:BK:103:VAL:O | 32:BK:122:VAL:HB | 2.18 | 0.44 |
| 35:BN:8:ARG:NH2 | 35:BN:39:PRO:HA | 2.33 | 0.44 |
| 35:BN:84:GLY:N | 35:BN:85:PRO:HD2 | 2.33 | 0.44 |
| 39:BR:48:LYS:O | 39:BR:48:LYS:CG | 2.66 | 0.44 |
| 52:B4:25:VAL:HB | 52:B4:35:GLN:HB2 | 1.99 | 0.44 |
| 53:B5:65:LEU:CD2 | 53:B5:195:ARG:CB | 2.95 | 0.44 |
| 53:B5:84:ILE:O | 53:B5:84:ILE:HG22 | 2.17 | 0.44 |
| 1:CA:9:G:H5' | 5:CE:108:GLY:HA3 | 2.00 | 0.44 |
| 1:CA:39:G:N2 | 1:CA:40:C:C2 | 2.86 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:539:A:H2' | 1:CA:540:G:C8 | 2.53 | 0.44 |
| 1:CA:844:G:C8 | 1:CA:844:G:OP2 | 2.71 | 0.44 |
| 1:CA:974:A:C8 | 14:CN:71:HIS:CD2 | 3.06 | 0.44 |
| 1:CA:1004:A:C5 | 1:CA:1005:A:C6 | 3.05 | 0.44 |
| 1:CA:1317:C:H2' | 1:CA:1318:A:O5' | 2.18 | 0.44 |
| 1:CA:1417:G:N2 | 1:CA:1484:C:C4 | 2.86 | 0.44 |
| 2:CB:186:ILE:HA | 2:CB:200:ILE:O | 2.18 | 0.44 |
| 3:CC:111:LEU:HD22 | 3:CC:111:LEU:N | 2.33 | 0.44 |
| 11:CK:40:ASN:O | 11:CK:41:ALA:HB3 | 2.18 | 0.44 |
| 11:CK:77:TYR:CD1 | 11:CK:77:TYR:N | 2.86 | 0.44 |
| 14:CN:41:ARG:HG2 | 14:CN:42:TRP:N | 2.32 | 0.44 |
| 17:CQ:25:ILE:HG12 | 17:CQ:42:THR:O | 2.18 | 0.44 |
| 17:CQ:25:ILE:O | 17:CQ:41:THR:HA | 2.18 | 0.44 |
| 22:DA:738:G:N1 | 22:DA:739:A:C2 | 2.86 | 0.44 |
| 22:DA:856:G:C2 | 22:DA:922:C:C2 | 3.06 | 0.44 |
| 22:DA:972:A:N1 | 22:DA:973:A:N6 | 2.65 | 0.44 |
| 22:DA:983:A:N6 | 22:DA:984:A:C2 | 2.86 | 0.44 |
| 22:DA:1109:C:C4 | 22:DA:1110:G:O6 | 2.71 | 0.44 |
| 22:DA:1139:G:N2 | 22:DA:1140:C:C2 | 2.86 | 0.44 |
| 22:DA:1330:C:H2' | 22:DA:1331:G:O5' | 2.17 | 0.44 |
| 22:DA:1332:G:O6 | 22:DA:1609:A:C8 | 2.71 | 0.44 |
| 22:DA:1355:G:H2' | 22:DA:1356:G:C5' | 2.48 | 0.44 |
| 22:DA:1362:C:C2' | 22:DA:1363:C:H5' | 2.48 | 0.44 |
| 22:DA:1810:A:H2' | 22:DA:1811:G:O4' | 2.18 | 0.44 |
| 22:DA:2018:G:H2' | 22:DA:2019:A:O4' | 2.18 | 0.44 |
| 22:DA:2064:C:H2' | 22:DA:2065:C:C6 | 2.53 | 0.44 |
| 22:DA:2104:C:N3 | 22:DA:2186:G:N2 | 2.66 | 0.44 |
| 22:DA:2179:C:H2' | 22:DA:2180:U:C6 | 2.52 | 0.44 |
| 22:DA:2252:G:H2' | 22:DA:2253:G:O4' | 2.17 | 0.44 |
| 22:DA:2409:G:C6 | 22:DA:2410:G:C6 | 3.06 | 0.44 |
| 24:DC:104:ILE:HD12 | 24:DC:104:ILE:O | 2.18 | 0.44 |
| 24:DC:176:LEU:HD12 | 24:DC:180:GLU:HB3 | 1.99 | 0.44 |
| 24:DC:251:GLN:HG2 | 24:DC:255:LYS:HB2 | 2.00 | 0.44 |
| 26:DE:130:LYS:HB2 | 26:DE:133:LEU:HB2 | 2.00 | 0.44 |
| 31:DJ:39:LYS:HZ3 | 31:DJ:39:LYS:CB | 2.31 | 0.44 |
| 31:DJ:40:HIS:CG | 31:DJ:40:HIS:O | 2.69 | 0.44 |
| 33:DL:30:THR:OG1 | 33:DL:31:GLY:N | 2.51 | 0.44 |
| 39:DR:78:ARG:CB | 39:DR:83:TYR:CD1 | 3.00 | 0.44 |
| 42:DU:96:PHE:CZ | 42:DU:103:ILE:HG13 | 2.53 | 0.44 |
| 43:DV:80:HIS:CG | 43:DV:81:PRO:HD2 | 2.53 | 0.44 |
| 50:D2:12:ARG:NH2 | 50:D2:44:VAL:CG1 | 2.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:AA:184:G:C6 | 1:AA:185:U:C4 | 3.06 | 0.43 |
| 1:AA:192:A:H2' | 1:AA:193:C:C6 | 2.53 | 0.43 |
| 1:AA:554:A:H5' | 12:AL:26:ALA:HB1 | 2.00 | 0.43 |
| 1:AA:651:C:H2' | 1:AA:652:U:O5' | 2.18 | 0.43 |
| 1:AA:654:G:C2' | 1:AA:655:A:H5' | 2.48 | 0.43 |
| 1:AA:862:C:H2' | 1:AA:863:U:H5' | 2.00 | 0.43 |
| 1:AA:935:A:C2 | 1:AA:936:C:C2 | 3.05 | 0.43 |
| 1:AA:1005:A:N6 | 1:AA:1006:G:C2 | 2.87 | 0.43 |
| 1:AA:1130:A:C1' | 1:AA:1146:A:C2 | 3.01 | 0.43 |
| 1:AA:1154:G:H2' | 1:AA:1155:A:C8 | 2.53 | 0.43 |
| 4:AD:58:LYS:HE2 | 4:AD:69:GLU:OE2 | 2.18 | 0.43 |
| 9:AI:30:ILE:CG2 | 9:AI:65:ILE:HD11 | 2.48 | 0.43 |
| 18:AR:32:TYR:CG | 18:AR:55:LEU:HD11 | 2.53 | 0.43 |
| 22:BA:141:G:C6 | 41:BT:1:MET:HE1 | 2.53 | 0.43 |
| 22:BA:143:C:O2 | 41:BT:1:MET:N | 2.44 | 0.43 |
| 22:BA:464:U:C6 | 22:BA:788:A:C2 | 3.06 | 0.43 |
| 22:BA:1073:A:C2' | 22:BA:1074:G:H5'' | 2.48 | 0.43 |
| 22:BA:1098:A:N7 | 22:BA:1099:G:C6 | 2.86 | 0.43 |
| 22:BA:1125:G:C6 | 22:BA:1126:A:N6 | 2.86 | 0.43 |
| 22:BA:1199:U:H2' | 22:BA:1200:C:C6 | 2.53 | 0.43 |
| 22:BA:1479:G:H2' | 22:BA:1480:C:O4' | 2.18 | 0.43 |
| 22:BA:1839:G:C2' | 22:BA:1840:G:O5' | 2.66 | 0.43 |
| 22:BA:1880:U:H2' | 22:BA:1881:C:C6 | 2.53 | 0.43 |
| 22:BA:2298:A:C2 | 22:BA:2321:U:C5 | 3.06 | 0.43 |
| 22:BA:2315:G:H2' | 22:BA:2316:G:C8 | 2.52 | 0.43 |
| 22:BA:2808:G:C2 | 22:BA:2891:U:C5 | 3.06 | 0.43 |
| 26:BE:157:LEU:HG | 26:BE:169:VAL:HG21 | 2.00 | 0.43 |
| 29:BH:89:LYS:HE3 | 29:BH:124:THR:HG22 | 1.99 | 0.43 |
| 31:BJ:52:ASP:O | 31:BJ:121:LYS:HE2 | 2.18 | 0.43 |
| 1:CA:198:G:O2' | 1:CA:199:A:H5' | 2.18 | 0.43 |
| 1:CA:229:U:H2' | 1:CA:230:G:C8 | 2.53 | 0.43 |
| 1:CA:747:A:N6 | 1:CA:748:G:C6 | 2.86 | 0.43 |
| 1:CA:980:C:O3' | 14:CN:13:ARG:NH2 | 2.51 | 0.43 |
| 1:CA:1018:G:O6 | 1:CA:1019:A:N6 | 2.51 | 0.43 |
| 1:CA:1052:U:C5' | 1:CA:1053:G:OP2 | 2.66 | 0.43 |
| 1:CA:1361:G:C4 | 1:CA:1362:A:N7 | 2.86 | 0.43 |
| 2:CB:26:LYS:HB2 | 2:CB:193:PRO:HD2 | 2.00 | 0.43 |
| 2:CB:164:ILE:O | 2:CB:186:ILE:O | 2.36 | 0.43 |
| 4:CD:62:ARG:NH1 | 4:CD:69:GLU:OE1 | 2.51 | 0.43 |
| 4:CD:153:SER:O | 4:CD:154:ARG:C | 2.56 | 0.43 |
| 5:CE:83:HIS:NE2 | 8:CH:96:MET:CE | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:CQ:10:GLY:HA3 | 17:CQ:25:ILE:HD13 | 2.00 | 0.43 |
| 17:CQ:14:SER:HB3 | 17:CQ:22:VAL:CG1 | 2.48 | 0.43 |
| 22:DA:104:A:C5 | 22:DA:105:C:N3 | 2.86 | 0.43 |
| 22:DA:528:A:C2 | 22:DA:2043:C:H4' | 2.53 | 0.43 |
| 22:DA:936:A:C2 | 22:DA:937:C:C2 | 3.06 | 0.43 |
| 22:DA:1448:G:C4 | 22:DA:1449:G:C8 | 3.06 | 0.43 |
| 22:DA:1744:A:C5 | 22:DA:1745:A:C5 | 3.05 | 0.43 |
| 22:DA:1757:A:N1 | 22:DA:1762:A:C2 | 2.86 | 0.43 |
| 22:DA:2061:G:C8 | 22:DA:2501:C:H4' | 2.53 | 0.43 |
| 22:DA:2141:G:N2 | 22:DA:2151:U:O2 | 2.51 | 0.43 |
| 22:DA:2513:A:C6 | 22:DA:2514:U:C4 | 3.06 | 0.43 |
| 22:DA:2720:U:C6 | 22:DA:2872:A:N1 | 2.86 | 0.43 |
| 22:DA:2843:G:N2 | 22:DA:2875:C:N3 | 2.66 | 0.43 |
| 26:DE:45:ALA:HA | 26:DE:87:ALA:O | 2.18 | 0.43 |
| 27:DF:5:HIS:O | 27:DF:9:LYS:HG3 | 2.18 | 0.43 |
| 27:DF:163:ASP:N | 27:DF:163:ASP:OD1 | 2.51 | 0.43 |
| 30:DI:33:VAL:HA | 30:DI:67:PHE:CE2 | 2.53 | 0.43 |
| 31:DJ:10:THR:O | 31:DJ:11:VAL:O | 2.35 | 0.43 |
| 37:DP:53:ARG:N | 37:DP:57:SER:OG | 2.50 | 0.43 |
| 42:DU:82:ARG:HB2 | 42:DU:82:ARG:CZ | 2.47 | 0.43 |
| 48:D0:44:THR:OG1 | 48:D0:48:TYR:N | 2.51 | 0.43 |
| 51:D3:7:VAL:O | 51:D3:10:ALA:HB3 | 2.18 | 0.43 |
| 1:AA:300:A:H2' | 1:AA:301:G:O4' | 2.18 | 0.43 |
| 1:AA:690:G:C6 | 1:AA:691:G:C6 | 3.07 | 0.43 |
| 1:AA:998:C:H2' | 1:AA:999:C:C6 | 2.54 | 0.43 |
| 1:AA:1227:A:O2' | 13:AM:115:PRO:HD2 | 2.18 | 0.43 |
| 1:AA:1250:A:O3' | 9:AI:69:GLY:HA2 | 2.18 | 0.43 |
| 1:AA:1322:C:O2' | 1:AA:1323:G:OP2 | 2.29 | 0.43 |
| 4:AD:30:THR:O | 4:AD:31:LYS:C | 2.55 | 0.43 |
| 7:AG:42:ILE:HG21 | 7:AG:116:MET:CG | 2.48 | 0.43 |
| 8:AH:29:SER:OG | 8:AH:30:SER:N | 2.50 | 0.43 |
| 9:AI:36:GLU:HA | 9:AI:40:GLY:CA | 2.49 | 0.43 |
| 10:AJ:54:SER:OG | 10:AJ:55:PRO:HD2 | 2.18 | 0.43 |
| 17:AQ:4:LYS:HD2 | 17:AQ:4:LYS:C | 2.39 | 0.43 |
| 22:BA:255:A:H2' | 22:BA:256:A:O4' | 2.19 | 0.43 |
| 22:BA:976:G:C2 | 22:BA:977:G:C8 | 3.06 | 0.43 |
| 22:BA:1003:G:C2 | 22:BA:1004:U:C5 | 3.06 | 0.43 |
| 22:BA:1439:A:C2 | 22:BA:1553:A:C5 | 3.06 | 0.43 |
| 22:BA:1665:A:H2' | 22:BA:1666:G:O4' | 2.18 | 0.43 |
| 22:BA:1754:A:N6 | 22:BA:1755:A:C6 | 2.86 | 0.43 |
| 22:BA:1844:C:O3' | 24:BC:256:LYS:NZ | 2.50 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1963:U:H6 | 22:BA:1963:U:O5' | 2.01 | 0.43 |
| 22:BA:2248:C:OP2 | 22:BA:2249:U:C5 | 2.70 | 0.43 |
| 22:BA:2267:A:H2 | 58:BA:3511:HOH:O | 2.00 | 0.43 |
| 26:BE:46:GLN:O | 26:BE:88:ARG:NH1 | 2.51 | 0.43 |
| 37:BP:106:LYS:O | 37:BP:109:ARG:HD3 | 2.19 | 0.43 |
| 43:BV:72:VAL:HG12 | 43:BV:93:ARG:HA | 2.00 | 0.43 |
| 1:CA:421:U:C4' | 1:CA:421:U:OP1 | 2.67 | 0.43 |
| 1:CA:1068:G:C2' | 1:CA:1069:C:H5' | 2.47 | 0.43 |
| 1:CA:1151:A:C2 | 1:CA:1152:A:C4 | 3.06 | 0.43 |
| 1:CA:1225:A:C2' | 1:CA:1225:A:N3 | 2.81 | 0.43 |
| 1:CA:1457:G:H2' | 1:CA:1458:G:O4' | 2.18 | 0.43 |
| 2:CB:115:LYS:O | 2:CB:119:THR:HB | 2.18 | 0.43 |
| 6:CF:38:ARG:HG3 | 6:CF:63:ASN:HB2 | 1.98 | 0.43 |
| 9:CI:116:VAL:HG23 | 10:CJ:62:ARG:HD3 | 2.00 | 0.43 |
| 12:CL:25:GLU:HB3 | 12:CL:27:CYS:SG | 2.58 | 0.43 |
| 22:DA:35:G:N2 | 22:DA:450:G:H1' | 2.33 | 0.43 |
| 22:DA:54:G:C6 | 22:DA:55:G:N7 | 2.86 | 0.43 |
| 22:DA:185:G:C6 | 22:DA:212:G:N2 | 2.86 | 0.43 |
| 22:DA:192:C:O2' | 22:DA:802:A:N3 | 2.51 | 0.43 |
| 22:DA:483:A:O2' | 42:DU:56:GLY:HA3 | 2.18 | 0.43 |
| 22:DA:603:A:N3 | 22:DA:604:G:H1' | 2.34 | 0.43 |
| 22:DA:633:A:H5'' | 33:DL:70:LYS:CD | 2.48 | 0.43 |
| 22:DA:969:G:H2' | 22:DA:970:U:C6 | 2.54 | 0.43 |
| 22:DA:1341:G:C2 | 41:DT:84:TYR:CD2 | 3.06 | 0.43 |
| 22:DA:1351:C:O3' | 22:DA:1571:A:O2' | 2.36 | 0.43 |
| 22:DA:1362:C:H2' | 22:DA:1363:C:H5' | 2.00 | 0.43 |
| 22:DA:1477:A:N6 | 22:DA:1514:G:H1' | 2.33 | 0.43 |
| 22:DA:1568:G:H5'' | 24:DC:61:ALA:N | 2.33 | 0.43 |
| 22:DA:1670:C:C5 | 22:DA:1671:U:C4 | 3.06 | 0.43 |
| 22:DA:2232:C:OP1 | 45:DX:27:ARG:NH1 | 2.50 | 0.43 |
| 22:DA:2280:G:O2' | 22:DA:2388:A:N1 | 2.46 | 0.43 |
| 22:DA:2331:G:N2 | 22:DA:2385:C:C2 | 2.86 | 0.43 |
| 22:DA:2464:G:H2' | 22:DA:2465:C:O4' | 2.17 | 0.43 |
| 22:DA:2897:U:H2' | 22:DA:2898:U:C6 | 2.53 | 0.43 |
| 24:DC:9:THR:O | 24:DC:10:SER:HB3 | 2.15 | 0.43 |
| 25:DD:148:GLN:N | 25:DD:148:GLN:CD | 2.72 | 0.43 |
| 29:DH:127:GLU:CG | 29:DH:144:VAL:O | 2.65 | 0.43 |
| 33:DL:62:PRO:HG3 | 51:D3:26:HIS:O | 2.18 | 0.43 |
| 35:DN:108:ALA:HB3 | 35:DN:110:MET:CE | 2.49 | 0.43 |
| 37:DP:65:SER:O | 37:DP:66:ASN:C | 2.57 | 0.43 |
| 44:DW:36:ILE:HG23 | 44:DW:58:THR:CG2 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:D0:44:THR:O | 48:D0:47:GLY:N | 2.52 | 0.43 |
| 49:D1:9:ILE:HB | 49:D1:52:ALA:HA | 2.00 | 0.43 |
| 49:D1:19:HIS:CD2 | 49:D1:19:HIS:C | 2.91 | 0.43 |
| 50:D2:43:THR:O | 50:D2:44:VAL:HB | 2.17 | 0.43 |
| 1:AA:167:A:H2' | 1:AA:168:G:O4' | 2.18 | 0.43 |
| 1:AA:500:G:C2' | 1:AA:501:C:O5' | 2.66 | 0.43 |
| 1:AA:558:G:C5 | 1:AA:559:A:C2 | 3.07 | 0.43 |
| 1:AA:681:A:C6 | 1:AA:710:G:C6 | 3.07 | 0.43 |
| 1:AA:1069:C:H4' | 1:AA:1192:C:O2 | 2.19 | 0.43 |
| 1:AA:1126:U:O4' | 1:AA:1281:C:C2 | 2.71 | 0.43 |
| 1:AA:1442:G:H2' | 1:AA:1443:C:H6 | 1.83 | 0.43 |
| 2:AB:75:ALA:O | 2:AB:76:ALA:CB | 2.65 | 0.43 |
| 3:AC:141:ALA:O | 3:AC:146:ALA:HB3 | 2.18 | 0.43 |
| 4:AD:174:ASP:O | 4:AD:175:ALA:CB | 2.66 | 0.43 |
| 6:AF:42:TRP:HB2 | 6:AF:59:TYR:HB2 | 2.01 | 0.43 |
| 8:AH:115:ALA:O | 8:AH:118:GLN:N | 2.51 | 0.43 |
| 14:AN:90:ARG:HB2 | 14:AN:92:GLU:HG2 | 2.00 | 0.43 |
| 14:AN:100:SER:O | 14:AN:101:TRP:HB3 | 2.18 | 0.43 |
| 17:AQ:81:LYS:C | 17:AQ:83:VAL:N | 2.72 | 0.43 |
| 19:AS:58:VAL:CG1 | 19:AS:75:ALA:HB1 | 2.49 | 0.43 |
| 20:AT:72:ALA:O | 20:AT:73:ALA:C | 2.56 | 0.43 |
| 22:BA:45:G:H5'' | 22:BA:46:G:OP1 | 2.18 | 0.43 |
| 22:BA:587:C:C5 | 22:BA:671:C:H1' | 2.53 | 0.43 |
| 22:BA:784:G:C5' | 24:BC:226:ASN:OD1 | 2.66 | 0.43 |
| 22:BA:927:A:H2' | 22:BA:928:A:O4' | 2.19 | 0.43 |
| 22:BA:1087:G:C2' | 22:BA:1089:A:H1' | 2.48 | 0.43 |
| 22:BA:1607:C:N4 | 22:BA:1622:G:C8 | 2.86 | 0.43 |
| 22:BA:2308:G:O6 | 22:BA:2311:A:C8 | 2.71 | 0.43 |
| 22:BA:2517:C:C5 | 22:BA:2542:A:C4 | 3.06 | 0.43 |
| 23:BB:22:U:H2' | 23:BB:23:G:C8 | 2.52 | 0.43 |
| 27:BF:171:ALA:O | 27:BF:173:PHE:N | 2.51 | 0.43 |
| 28:BG:10:VAL:HG13 | 28:BG:10:VAL:O | 2.18 | 0.43 |
| 29:BH:80:ILE:HG21 | 29:BH:94:ILE:HG13 | 2.00 | 0.43 |
| 31:BJ:53:TYR:CD1 | 31:BJ:121:LYS:HB3 | 2.53 | 0.43 |
| 1:CA:97:G:C6 | 1:CA:98:A:H1' | 2.53 | 0.43 |
| 1:CA:256:U:OP1 | 17:CQ:19:LYS:NZ | 2.40 | 0.43 |
| 1:CA:404:G:O6 | 4:CD:2:ALA:N | 2.51 | 0.43 |
| 1:CA:411:A:H4' | 1:CA:412:A:O5' | 2.17 | 0.43 |
| 1:CA:459:A:C8 | 1:CA:459:A:OP2 | 2.72 | 0.43 |
| 1:CA:577:G:N3 | 1:CA:578:C:C6 | 2.86 | 0.43 |
| 1:CA:1027:C:N4 | 1:CA:1034:G:O6 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1244:G:C2 | 1:CA:1294:G:C2 | 3.07 | 0.43 |
| 1:CA:1319:A:H5' | 19:CS:5:LEU:HD11 | 1.99 | 0.43 |
| 1:CA:1385:G:H2' | 1:CA:1386:G:O4' | 2.19 | 0.43 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:C6 | 2.53 | 0.43 |
| 2:CB:20:THR:OG1 | 2:CB:21:ARG:N | 2.51 | 0.43 |
| 2:CB:68:LEU:HG | 2:CB:154:MET:HE1 | 2.00 | 0.43 |
| 4:CD:34:ILE:O | 4:CD:34:ILE:CG2 | 2.66 | 0.43 |
| 5:CE:38:VAL:HG12 | 5:CE:39:VAL:N | 2.34 | 0.43 |
| 9:CI:63:LEU:HG | 9:CI:63:LEU:O | 2.18 | 0.43 |
| 11:CK:60:PRO:N | 11:CK:91:PRO:HB2 | 2.34 | 0.43 |
| 12:CL:9:ARG:HB2 | 12:CL:9:ARG:CZ | 2.48 | 0.43 |
| 13:CM:50:GLU:HA | 13:CM:50:GLU:OE2 | 2.19 | 0.43 |
| 15:CO:53:ARG:O | 15:CO:54:ARG:C | 2.57 | 0.43 |
| 19:CS:40:ILE:HD13 | 19:CS:66:MET:HB3 | 1.98 | 0.43 |
| 22:DA:498:G:C4 | 22:DA:499:U:C5 | 3.07 | 0.43 |
| 22:DA:513:A:C2 | 22:DA:514:A:N7 | 2.86 | 0.43 |
| 22:DA:683:U:H2' | 22:DA:684:G:O5' | 2.18 | 0.43 |
| 22:DA:694:U:C3' | 22:DA:695:G:C5' | 2.95 | 0.43 |
| 22:DA:1357:C:N4 | 22:DA:1358:G:N1 | 2.66 | 0.43 |
| 22:DA:1519:G:H3' | 22:DA:1520:U:C6 | 2.53 | 0.43 |
| 22:DA:1563:U:H2' | 22:DA:1564:C:C6 | 2.52 | 0.43 |
| 22:DA:1622:G:H2' | 22:DA:1623:G:O4' | 2.18 | 0.43 |
| 22:DA:1638:C:O3' | 22:DA:2709:G:N2 | 2.51 | 0.43 |
| 22:DA:1754:A:C6 | 22:DA:1755:A:C5 | 3.06 | 0.43 |
| 22:DA:1796:U:H2' | 22:DA:1797:G:C8 | 2.53 | 0.43 |
| 22:DA:1881:C:H2' | 22:DA:1882:U:O4' | 2.17 | 0.43 |
| 22:DA:2502:G:H5' | 22:DA:2503:A:O5' | 2.19 | 0.43 |
| 22:DA:2711:A:N6 | 22:DA:2714:G:C5 | 2.86 | 0.43 |
| 25:DD:3:GLY:O | 25:DD:82:PHE:CE1 | 2.72 | 0.43 |
| 31:DJ:31:GLU:HB3 | 31:DJ:142:ILE:CG1 | 2.48 | 0.43 |
| 37:DP:75:GLN:HB2 | 37:DP:78:SER:HB2 | 2.00 | 0.43 |
| 40:DS:15:GLN:O | 40:DS:19:LEU:HD22 | 2.18 | 0.43 |
| 42:DU:57:GLY:O | 42:DU:59:VAL:HG23 | 2.18 | 0.43 |
| 42:DU:72:ILE:HD13 | 42:DU:83:VAL:HB | 2.00 | 0.43 |
| 43:DV:28:ALA:O | 43:DV:40:ILE:HB | 2.18 | 0.43 |
| 43:DV:75:GLN:HB3 | 43:DV:90:ASP:O | 2.17 | 0.43 |
| 48:D0:54:VAL:O | 48:D0:55:ILE:HB | 2.18 | 0.43 |
| 1:AA:116:A:C4 | 1:AA:117:G:C8 | 3.07 | 0.43 |
| 1:AA:157:U:O2' | 1:AA:158:G:H5' | 2.18 | 0.43 |
| 1:AA:266:G:H4' | 1:AA:267:C:OP1 | 2.17 | 0.43 |
| 1:AA:389:A:C6 | 1:AA:390:U:H1' | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:867:G:N2 | 1:AA:868:C:C2 | 2.86 | 0.43 |
| 1:AA:963:G:H2' | 1:AA:963:G:N3 | 2.33 | 0.43 |
| 2:AB:93:ASN:OD1 | 2:AB:94:HIS:ND1 | 2.52 | 0.43 |
| 4:AD:23:SER:O | 4:AD:24:GLY:O | 2.37 | 0.43 |
| 5:AE:30:ILE:HD11 | 5:AE:54:ARG:NH1 | 2.34 | 0.43 |
| 6:AF:67:PRO:O | 6:AF:69:GLU:N | 2.52 | 0.43 |
| 7:AG:27:VAL:O | 7:AG:31:MET:N | 2.50 | 0.43 |
| 7:AG:49:THR:O | 7:AG:53:ARG:HB2 | 2.18 | 0.43 |
| 7:AG:69:VAL:HG12 | 7:AG:135:VAL:HA | 2.01 | 0.43 |
| 9:AI:6:TYR:CD1 | 9:AI:89:GLU:OE2 | 2.71 | 0.43 |
| 14:AN:21:PHE:HE1 | 14:AN:55:SER:HG | 1.62 | 0.43 |
| 14:AN:43:ASN:C | 14:AN:45:VAL:H | 2.20 | 0.43 |
| 19:AS:51:VAL:CG2 | 19:AS:71:LEU:HB3 | 2.48 | 0.43 |
| 20:AT:58:VAL:HG12 | 20:AT:72:ALA:HB1 | 2.00 | 0.43 |
| 22:BA:24:G:O2' | 40:BS:77:ASP:HB3 | 2.18 | 0.43 |
| 22:BA:103:A:H2' | 22:BA:104:A:O4' | 2.18 | 0.43 |
| 22:BA:362:A:C4 | 22:BA:363:G:C8 | 3.07 | 0.43 |
| 22:BA:744:U:H2' | 22:BA:745:G:O4' | 2.19 | 0.43 |
| 22:BA:975:A:C4 | 22:BA:990:A:C5 | 3.06 | 0.43 |
| 22:BA:1153:C:N4 | 22:BA:1154:G:C6 | 2.86 | 0.43 |
| 22:BA:1253:A:C8 | 58:BA:3335:HOH:O | 2.66 | 0.43 |
| 22:BA:1494:A:C2 | 22:BA:1495:A:N9 | 2.87 | 0.43 |
| 22:BA:1840:G:C2 | 22:BA:1841:U:C2 | 3.06 | 0.43 |
| 22:BA:2622:U:O2' | 22:BA:2825:G:N7 | 2.50 | 0.43 |
| 22:BA:2680:U:O2' | 22:BA:2681:C:H5' | 2.18 | 0.43 |
| 23:BB:2:G:C2 | 23:BB:119:A:N3 | 2.87 | 0.43 |
| 26:BE:48:THR:O | 26:BE:49:ARG:C | 2.55 | 0.43 |
| 27:BF:17:MET:CE | 27:BF:22:TYR:HB2 | 2.49 | 0.43 |
| 29:BH:27:ARG:O | 29:BH:28:ASN:CB | 2.66 | 0.43 |
| 29:BH:76:GLU:HA | 29:BH:142:VAL:HG12 | 2.00 | 0.43 |
| 30:BI:77:ALA:HB2 | 30:BI:132:THR:CG2 | 2.48 | 0.43 |
| 30:BI:124:ALA:O | 30:BI:127:ARG:HG2 | 2.17 | 0.43 |
| 31:BJ:35:ARG:HG2 | 31:BJ:40:HIS:CD2 | 2.52 | 0.43 |
| 1:CA:86:G:O2' | 1:CA:87:C:P | 2.76 | 0.43 |
| 1:CA:160:A:C5 | 1:CA:346:G:O6 | 2.72 | 0.43 |
| 1:CA:216:U:H5'' | 1:CA:464:U:H4' | 2.00 | 0.43 |
| 1:CA:451:A:OP2 | 16:CP:70:ARG:NH2 | 2.47 | 0.43 |
| 1:CA:652:U:C2 | 1:CA:752:G:N2 | 2.86 | 0.43 |
| 1:CA:683:G:O2' | 1:CA:684:U:H5' | 2.19 | 0.43 |
| 1:CA:706:A:O2' | 11:CK:31:ILE:CD1 | 2.66 | 0.43 |
| 1:CA:1014:A:C2 | 19:CS:34:TRP:CZ2 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:81:LYS:CG | 2:CB:85:LEU:HD22 | 2.48 | 0.43 |
| 3:CC:182:ILE:HD13 | 3:CC:203:PHE:HA | 2.00 | 0.43 |
| 5:CE:96:MET:CE | 5:CE:111:MET:CE | 2.95 | 0.43 |
| 6:CF:70:VAL:HG23 | 6:CF:71:ILE:HD12 | 1.99 | 0.43 |
| 8:CH:74:SER:O | 8:CH:130:ALA:N | 2.50 | 0.43 |
| 12:CL:43:LYS:N | 12:CL:89:ASP:O | 2.44 | 0.43 |
| 15:CO:27:VAL:O | 15:CO:31:LEU:CD1 | 2.67 | 0.43 |
| 16:CP:5:ARG:O | 16:CP:19:VAL:HA | 2.19 | 0.43 |
| 17:CQ:14:SER:CB | 17:CQ:22:VAL:HG12 | 2.49 | 0.43 |
| 17:CQ:75:LEU:CD1 | 17:CQ:75:LEU:C | 2.87 | 0.43 |
| 22:DA:40:U:C4 | 22:DA:41:C:N4 | 2.86 | 0.43 |
| 22:DA:301:G:H5' | 22:DA:334:C:O2 | 2.18 | 0.43 |
| 22:DA:672:C:C2 | 22:DA:809:G:N2 | 2.86 | 0.43 |
| 22:DA:772:C:H2' | 22:DA:773:U:O4' | 2.18 | 0.43 |
| 22:DA:892:A:H3' | 22:DA:892:A:N3 | 2.34 | 0.43 |
| 22:DA:972:A:C6 | 22:DA:973:A:C6 | 3.06 | 0.43 |
| 22:DA:1045:C:H4' | 22:DA:1046:A:H5' | 2.00 | 0.43 |
| 22:DA:1120:G:C6 | 22:DA:1121:C:N4 | 2.86 | 0.43 |
| 22:DA:1287:A:H2' | 22:DA:1288:G:H5' | 2.01 | 0.43 |
| 22:DA:1378:A:C4' | 22:DA:1379:U:OP1 | 2.66 | 0.43 |
| 22:DA:1567:G:H2' | 24:DC:85:PRO:HG3 | 2.00 | 0.43 |
| 22:DA:1829:A:OP2 | 22:DA:1829:A:O4' | 2.36 | 0.43 |
| 22:DA:2112:G:H5' | 22:DA:2113:U:OP2 | 2.19 | 0.43 |
| 22:DA:2167:U:O2 | 22:DA:2170:A:OP2 | 2.37 | 0.43 |
| 22:DA:2333:A:N7 | 22:DA:2335:A:C4 | 2.86 | 0.43 |
| 22:DA:2489:U:HO2' | 22:DA:2491:U:H5 | 1.64 | 0.43 |
| 22:DA:2756:U:H4' | 22:DA:2757:A:OP1 | 2.19 | 0.43 |
| 24:DC:2:ALA:N | 24:DC:199:GLU:OE1 | 2.51 | 0.43 |
| 25:DD:186:LEU:CD1 | 37:DP:8:LEU:CD1 | 2.97 | 0.43 |
| 26:DE:22:ASP:OD2 | 26:DE:22:ASP:N | 2.51 | 0.43 |
| 27:DF:12:VAL:O | 27:DF:12:VAL:HG12 | 2.19 | 0.43 |
| 27:DF:114:PHE:O | 27:DF:114:PHE:CG | 2.71 | 0.43 |
| 30:DI:15:ALA:HB3 | 30:DI:52:GLY:N | 2.32 | 0.43 |
| 32:DK:23:LYS:HB3 | 32:DK:40:LYS:HB3 | 1.99 | 0.43 |
| 33:DL:29:LYS:O | 33:DL:29:LYS:CG | 2.66 | 0.43 |
| 41:DT:8:LEU:CD2 | 41:DT:50:LEU:HD21 | 2.47 | 0.43 |
| 41:DT:61:LEU:HD12 | 41:DT:61:LEU:C | 2.38 | 0.43 |
| 1:AA:219:U:H2' | 1:AA:220:G:C8 | 2.53 | 0.43 |
| 1:AA:404:G:N7 | 4:AD:2:ALA:HB3 | 2.32 | 0.43 |
| 1:AA:557:G:C6 | 1:AA:558:G:C6 | 3.07 | 0.43 |
| 1:AA:803:G:C6 | 1:AA:804:U:C4 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1319:A:C5 | 1:AA:1323:G:C4 | 3.07 | 0.43 |
| 2:AB:15:HIS:O | 2:AB:16:PHE:O | 2.36 | 0.43 |
| 4:AD:107:PHE:CD1 | 4:AD:145:ILE:CD1 | 3.02 | 0.43 |
| 7:AG:49:THR:O | 7:AG:53:ARG:HB3 | 2.19 | 0.43 |
| 12:AL:87:VAL:CG2 | 12:AL:96:HIS:CE1 | 3.01 | 0.43 |
| 18:AR:25:ASP:C | 18:AR:27:ALA:N | 2.71 | 0.43 |
| 22:BA:71:A:H5'' | 22:BA:72:U:H3' | 2.01 | 0.43 |
| 22:BA:275:C:H3' | 22:BA:276:U:H5'' | 1.99 | 0.43 |
| 22:BA:612:G:H2' | 22:BA:614:A:C8 | 2.52 | 0.43 |
| 22:BA:1739:A:H2' | 22:BA:1740:G:O4' | 2.18 | 0.43 |
| 22:BA:1922:G:C2 | 22:BA:1923:U:C1' | 3.02 | 0.43 |
| 22:BA:2480:C:C2' | 22:BA:2481:G:H5' | 2.48 | 0.43 |
| 22:BA:2495:G:C2' | 22:BA:2496:C:H5' | 2.49 | 0.43 |
| 22:BA:2620:C:H2' | 22:BA:2621:G:O4' | 2.18 | 0.43 |
| 25:BD:104:VAL:HG23 | 25:BD:105:LYS:N | 2.33 | 0.43 |
| 26:BE:48:THR:C | 26:BE:50:ALA:H | 2.22 | 0.43 |
| 27:BF:108:VAL:CG2 | 27:BF:117:LEU:HD21 | 2.49 | 0.43 |
| 28:BG:74:SER:HA | 28:BG:77:ILE:CG1 | 2.49 | 0.43 |
| 28:BG:83:PHE:CE2 | 28:BG:138:LYS:HB2 | 2.54 | 0.43 |
| 29:BH:9:VAL:O | 29:BH:10:ALA:O | 2.36 | 0.43 |
| 29:BH:96:THR:O | 29:BH:100:ALA:N | 2.50 | 0.43 |
| 34:BM:24:THR:HG23 | 34:BM:24:THR:O | 2.18 | 0.43 |
| 37:BP:96:LYS:HB3 | 37:BP:98:TYR:CE1 | 2.52 | 0.43 |
| 43:BV:26:PHE:HB2 | 43:BV:27:PRO:HD2 | 2.00 | 0.43 |
| 1:CA:211:G:O2' | 1:CA:212:G:C4' | 2.67 | 0.43 |
| 1:CA:369:G:OP2 | 1:CA:388:G:N2 | 2.51 | 0.43 |
| 1:CA:635:A:C5 | 1:CA:636:U:C5 | 3.07 | 0.43 |
| 1:CA:800:G:N2 | 1:CA:801:U:O4 | 2.51 | 0.43 |
| 1:CA:1319:A:OP2 | 19:CS:5:LEU:HD21 | 2.18 | 0.43 |
| 1:CA:1483:A:N1 | 22:DA:1959:G:O2' | 2.43 | 0.43 |
| 2:CB:86:SER:O | 2:CB:87:CYS:O | 2.36 | 0.43 |
| 3:CC:25:ASN:O | 3:CC:29:PHE:HB2 | 2.19 | 0.43 |
| 3:CC:147:LYS:HB2 | 3:CC:203:PHE:CD2 | 2.54 | 0.43 |
| 5:CE:105:ILE:H | 5:CE:122:ASN:C | 2.22 | 0.43 |
| 6:CF:25:TYR:N | 6:CF:25:TYR:CD2 | 2.84 | 0.43 |
| 13:CM:14:HIS:HB2 | 13:CM:17:ILE:HD12 | 1.99 | 0.43 |
| 13:CM:83:LEU:N | 13:CM:83:LEU:HD23 | 2.33 | 0.43 |
| 16:CP:3:THR:HG22 | 16:CP:4:ILE:N | 2.34 | 0.43 |
| 22:DA:39:G:C6 | 22:DA:40:U:O4 | 2.72 | 0.43 |
| 22:DA:45:G:O3' | 22:DA:46:G:O4' | 2.36 | 0.43 |
| 22:DA:49:A:N6 | 22:DA:177:G:C4 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:64:A:H2' | 22:DA:65:U:C6 | 2.53 | 0.43 |
| 22:DA:380:G:O3' | 45:DX:16:ASN:HB2 | 2.18 | 0.43 |
| 22:DA:607:U:H5 | 22:DA:619:G:C5 | 2.37 | 0.43 |
| 22:DA:874:G:C2 | 22:DA:904:G:C2 | 3.06 | 0.43 |
| 22:DA:922:C:H2' | 22:DA:923:G:C8 | 2.54 | 0.43 |
| 22:DA:1272:A:C2 | 22:DA:1618:A:N3 | 2.86 | 0.43 |
| 22:DA:1364:G:C5 | 22:DA:1368:G:N1 | 2.86 | 0.43 |
| 22:DA:1760:C:H3' | 22:DA:1761:C:C6 | 2.53 | 0.43 |
| 22:DA:1791:A:C8 | 22:DA:1792:G:C8 | 3.06 | 0.43 |
| 22:DA:1896:G:H2' | 22:DA:1897:G:O4' | 2.19 | 0.43 |
| 22:DA:1965:C:H3' | 22:DA:1966:A:C8 | 2.54 | 0.43 |
| 22:DA:2038:G:N7 | 22:DA:2039:U:C5 | 2.87 | 0.43 |
| 22:DA:2061:G:C5 | 56:DA:3001:DOL:HC19 | 2.53 | 0.43 |
| 22:DA:2092:U:H4' | 22:DA:2093:G:H5'' | 2.00 | 0.43 |
| 22:DA:2283:C:N4 | 22:DA:2389:G:C5 | 2.86 | 0.43 |
| 22:DA:2515:C:O2' | 22:DA:2516:A:H5' | 2.19 | 0.43 |
| 22:DA:2641:G:H5'' | 31:DJ:78:THR:HB | 2.01 | 0.43 |
| 22:DA:2676:C:O2 | 22:DA:2732:G:N2 | 2.51 | 0.43 |
| 22:DA:2684:U:C4' | 32:DK:70:ARG:NH1 | 2.81 | 0.43 |
| 30:DI:67:PHE:N | 30:DI:67:PHE:CD2 | 2.86 | 0.43 |
| 38:DQ:25:TYR:CD2 | 38:DQ:25:TYR:C | 2.92 | 0.43 |
| 41:DT:48:GLN:HB2 | 41:DT:49:LYS:CE | 2.49 | 0.43 |
| 50:D2:6:GLN:OE1 | 50:D2:6:GLN:HA | 2.18 | 0.43 |
| 52:D4:7:VAL:HG13 | 52:D4:38:GLY:CA | 2.49 | 0.43 |
| 1:AA:242:G:C2 | 1:AA:245:U:C4 | 3.07 | 0.43 |
| 1:AA:244:U:O4 | 1:AA:906:A:H1' | 2.18 | 0.43 |
| 1:AA:590:U:N3 | 1:AA:591:U:C4 | 2.87 | 0.43 |
| 1:AA:730:G:H2' | 1:AA:730:G:N3 | 2.33 | 0.43 |
| 1:AA:810:C:O2 | 1:AA:810:C:H2' | 2.17 | 0.43 |
| 1:AA:840:C:N3 | 1:AA:846:G:O6 | 2.52 | 0.43 |
| 1:AA:1108:G:N3 | 1:AA:1108:G:H2' | 2.34 | 0.43 |
| 1:AA:1264:U:O2 | 1:AA:1272:G:C2 | 2.71 | 0.43 |
| 10:AJ:28:THR:HG22 | 10:AJ:86:ALA:HB1 | 2.01 | 0.43 |
| 11:AK:26:SER:O | 11:AK:27:PHE:C | 2.57 | 0.43 |
| 14:AN:43:ASN:O | 14:AN:45:VAL:N | 2.51 | 0.43 |
| 15:AO:46:HIS:C | 15:AO:48:LYS:H | 2.22 | 0.43 |
| 16:AP:12:LYS:O | 16:AP:13:LYS:HB2 | 2.18 | 0.43 |
| 20:AT:33:LYS:O | 20:AT:34:LYS:C | 2.57 | 0.43 |
| 22:BA:25:U:C2' | 22:BA:26:G:H5' | 2.49 | 0.43 |
| 22:BA:90:U:C4 | 22:BA:91:A:C5 | 3.07 | 0.43 |
| 22:BA:332:A:C2 | 22:BA:335:C:C5 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:569:U:H1' | 22:BA:947:A:O4' | 2.18 | 0.43 |
| 22:BA:1081:U:O2 | 22:BA:1081:U:H2' | 2.19 | 0.43 |
| 22:BA:1374:G:H2' | 22:BA:1375:U:O4' | 2.19 | 0.43 |
| 22:BA:1910:G:N1 | 22:BA:1921:G:C5 | 2.87 | 0.43 |
| 22:BA:2311:A:O2' | 27:BF:85:ILE:HD11 | 2.18 | 0.43 |
| 22:BA:2507:C:H5'' | 22:BA:2573:C:N4 | 2.33 | 0.43 |
| 24:BC:207:LYS:O | 24:BC:210:ALA:HB3 | 2.19 | 0.43 |
| 25:BD:37:VAL:HG12 | 25:BD:38:LYS:N | 2.33 | 0.43 |
| 27:BF:41:GLY:C | 27:BF:43:ALA:H | 2.21 | 0.43 |
| 28:BG:2:SER:C | 28:BG:4:VAL:N | 2.71 | 0.43 |
| 29:BH:41:LYS:HA | 29:BH:44:ILE:HG12 | 2.01 | 0.43 |
| 29:BH:94:ILE:CD1 | 29:BH:98:ASP:HB3 | 2.48 | 0.43 |
| 29:BH:103:VAL:O | 29:BH:108:VAL:O | 2.37 | 0.43 |
| 30:BI:132:THR:O | 30:BI:132:THR:HG22 | 2.18 | 0.43 |
| 31:BJ:7:LYS:O | 31:BJ:11:VAL:HG23 | 2.19 | 0.43 |
| 31:BJ:84:ILE:HG23 | 31:BJ:84:ILE:O | 2.18 | 0.43 |
| 32:BK:109:SER:O | 32:BK:110:GLU:C | 2.56 | 0.43 |
| 33:BL:81:ASP:HB3 | 33:BL:100:ILE:CD1 | 2.49 | 0.43 |
| 34:BM:11:LYS:CE | 34:BM:87:GLY:O | 2.67 | 0.43 |
| 39:BR:49:ILE:O | 39:BR:49:ILE:HG13 | 2.19 | 0.43 |
| 39:BR:79:ARG:O | 39:BR:81:LYS:HG2 | 2.19 | 0.43 |
| 42:BU:54:GLN:N | 42:BU:55:PRO:CD | 2.82 | 0.43 |
| 1:CA:51:A:H4' | 1:CA:52:C:C5' | 2.48 | 0.43 |
| 1:CA:130:A:OP1 | 17:CQ:65:ARG:HD2 | 2.18 | 0.43 |
| 1:CA:135:C:C2 | 16:CP:1:MET:HB2 | 2.53 | 0.43 |
| 1:CA:161:A:C2 | 1:CA:162:A:C4 | 3.07 | 0.43 |
| 1:CA:185:U:H2' | 1:CA:186:C:C6 | 2.54 | 0.43 |
| 1:CA:577:G:C8 | 1:CA:816:A:N1 | 2.86 | 0.43 |
| 1:CA:767:A:H2' | 1:CA:768:A:O4' | 2.19 | 0.43 |
| 1:CA:793:U:O2' | 1:CA:1516:G:H1' | 2.18 | 0.43 |
| 1:CA:1107:C:C2 | 1:CA:1108:G:C8 | 3.06 | 0.43 |
| 1:CA:1125:U:O2' | 1:CA:1126:U:H2' | 2.18 | 0.43 |
| 1:CA:1323:G:O2' | 1:CA:1362:A:N3 | 2.40 | 0.43 |
| 1:CA:1409:C:N4 | 1:CA:1410:A:N6 | 2.67 | 0.43 |
| 3:CC:102:ASN:C | 3:CC:103:ILE:HG13 | 2.38 | 0.43 |
| 4:CD:53:VAL:HG23 | 4:CD:54:GLN:N | 2.34 | 0.43 |
| 5:CE:122:ASN:O | 5:CE:123:VAL:O | 2.36 | 0.43 |
| 8:CH:6:PRO:O | 8:CH:9:ASP:HB3 | 2.18 | 0.43 |
| 12:CL:29:GLN:HB2 | 12:CL:82:ILE:O | 2.17 | 0.43 |
| 14:CN:17:ALA:HA | 14:CN:55:SER:O | 2.19 | 0.43 |
| 21:CU:18:ARG:O | 21:CU:19:PHE:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:38:A:C2 | 22:DA:442:G:C6 | 3.07 | 0.43 |
| 22:DA:55:G:C2 | 22:DA:116:C:C2 | 3.06 | 0.43 |
| 22:DA:193:U:C4 | 22:DA:194:G:N7 | 2.87 | 0.43 |
| 22:DA:200:U:C5 | 22:DA:201:C:C4 | 3.06 | 0.43 |
| 22:DA:216:A:OP2 | 22:DA:429:A:OP1 | 2.37 | 0.43 |
| 22:DA:480:A:O3' | 42:DU:44:LYS:HG3 | 2.19 | 0.43 |
| 22:DA:553:G:H2' | 22:DA:554:U:O4' | 2.19 | 0.43 |
| 22:DA:563:A:C2 | 22:DA:2018:G:H1' | 2.53 | 0.43 |
| 22:DA:614:A:H2' | 22:DA:614:A:OP2 | 2.19 | 0.43 |
| 22:DA:623:C:H2' | 22:DA:624:C:O4' | 2.19 | 0.43 |
| 22:DA:696:G:C6 | 22:DA:767:U:C2 | 3.07 | 0.43 |
| 22:DA:771:G:N3 | 22:DA:771:G:H2' | 2.33 | 0.43 |
| 22:DA:982:C:H5'' | 22:DA:983:A:OP1 | 2.18 | 0.43 |
| 22:DA:1178:C:C2 | 22:DA:1179:G:N7 | 2.87 | 0.43 |
| 22:DA:1219:U:H2' | 22:DA:1220:G:C8 | 2.54 | 0.43 |
| 22:DA:1267:U:N3 | 22:DA:2013:A:N7 | 2.65 | 0.43 |
| 22:DA:1324:G:C1' | 22:DA:1616:A:N6 | 2.81 | 0.43 |
| 22:DA:1403:A:H2' | 22:DA:1404:C:C6 | 2.54 | 0.43 |
| 22:DA:1422:G:N2 | 22:DA:1577:C:H1' | 2.33 | 0.43 |
| 22:DA:1445:G:C2 | 22:DA:1446:C:C2 | 3.07 | 0.43 |
| 22:DA:1677:A:N6 | 22:DA:1678:A:C2 | 2.87 | 0.43 |
| 22:DA:1749:A:C2 | 22:DA:1750:G:C4 | 3.07 | 0.43 |
| 22:DA:1789:A:H5'' | 24:DC:219:THR:O | 2.19 | 0.43 |
| 22:DA:2104:C:C2 | 22:DA:2186:G:N2 | 2.86 | 0.43 |
| 22:DA:2114:A:C2 | 22:DA:2115:G:H1' | 2.54 | 0.43 |
| 22:DA:2333:A:OP2 | 44:DW:77:ARG:NH2 | 2.42 | 0.43 |
| 22:DA:2415:G:C6 | 22:DA:2416:C:N4 | 2.87 | 0.43 |
| 22:DA:2643:G:C2' | 22:DA:2644:G:H5' | 2.49 | 0.43 |
| 22:DA:2756:U:N3 | 22:DA:2759:G:O6 | 2.52 | 0.43 |
| 23:DB:52:A:C4 | 36:DO:33:ARG:NH2 | 2.86 | 0.43 |
| 24:DC:124:ILE:CD1 | 24:DC:136:PRO:HD3 | 2.48 | 0.43 |
| 25:DD:33:ARG:HA | 25:DD:95:SER:HA | 2.01 | 0.43 |
| 27:DF:44:ILE:CG2 | 27:DF:79:ILE:HG22 | 2.49 | 0.43 |
| 32:DK:91:SER:O | 32:DK:92:GLU:C | 2.56 | 0.43 |
| 32:DK:92:GLU:O | 32:DK:93:GLN:HB2 | 2.18 | 0.43 |
| 38:DQ:90:ILE:CG2 | 38:DQ:94:ILE:CG2 | 2.97 | 0.43 |
| 1:AA:29:U:O2' | 1:AA:30:U:H5' | 2.18 | 0.43 |
| 1:AA:112:G:C2 | 1:AA:113:G:C8 | 3.07 | 0.43 |
| 1:AA:670:G:H2' | 1:AA:671:G:O5' | 2.18 | 0.43 |
| 1:AA:903:G:H2' | 1:AA:904:U:H6 | 1.83 | 0.43 |
| 1:AA:1130:A:C4 | 1:AA:1146:A:C2 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AA:1145:A:O2' | 1:AA:1146:A:P | 2.77 | 0.43 |
| 3:AC:72:ARG:N | 3:AC:73:PRO:HD3 | 2.32 | 0.43 |
| 6:AF:51:ILE:O | 6:AF:52:ASN:HB2 | 2.19 | 0.43 |
| 9:AI:49:ARG:C | 9:AI:51:PRO:HD2 | 2.39 | 0.43 |
| 9:AI:52:LEU:HB3 | 9:AI:57:MET:HG3 | 2.00 | 0.43 |
| 10:AJ:56:HIS:C | 10:AJ:57:VAL:CG1 | 2.87 | 0.43 |
| 11:AK:38:GLN:O | 11:AK:38:GLN:HG2 | 2.19 | 0.43 |
| 20:AT:4:ILE:HA | 20:AT:8:LYS:HD3 | 2.00 | 0.43 |
| 22:BA:404:A:H1' | 22:BA:405:U:OP2 | 2.18 | 0.43 |
| 22:BA:1082:U:H5' | 30:BI:119:GLY:N | 2.34 | 0.43 |
| 22:BA:1142:A:C2 | 22:BA:1144:A:O4' | 2.72 | 0.43 |
| 22:BA:1439:A:C2 | 22:BA:1553:A:C4 | 3.06 | 0.43 |
| 22:BA:1464:G:C6 | 22:BA:1465:G:C6 | 3.06 | 0.43 |
| 22:BA:1734:G:H2' | 22:BA:1735:A:O4' | 2.19 | 0.43 |
| 22:BA:1916:A:H2' | 22:BA:1917:U:C4' | 2.49 | 0.43 |
| 22:BA:2196:C:C2' | 22:BA:2197:U:H5' | 2.48 | 0.43 |
| 22:BA:2244:U:H2' | 22:BA:2245:U:O4' | 2.18 | 0.43 |
| 34:BM:78:LEU:O | 34:BM:80:VAL:HG23 | 2.19 | 0.43 |
| 37:BP:21:ARG:HB2 | 37:BP:22:PRO:HD2 | 2.01 | 0.43 |
| 37:BP:31:TRP:CD2 | 37:BP:40:LEU:HD12 | 2.53 | 0.43 |
| 53:B5:76:LEU:O | 53:B5:76:LEU:HD13 | 2.18 | 0.43 |
| 1:CA:60:A:H4' | 1:CA:61:G:O5' | 2.19 | 0.43 |
| 1:CA:923:A:H2' | 1:CA:924:C:O4' | 2.19 | 0.43 |
| 1:CA:957:U:H4' | 19:CS:79:THR:O | 2.18 | 0.43 |
| 1:CA:971:G:N2 | 1:CA:1363:A:C8 | 2.87 | 0.43 |
| 1:CA:1197:A:C2' | 1:CA:1198:G:H5' | 2.48 | 0.43 |
| 1:CA:1361:G:C3' | 1:CA:1362:A:H5'' | 2.48 | 0.43 |
| 2:CB:18:HIS:O | 2:CB:19:GLN:CB | 2.67 | 0.43 |
| 3:CC:36:ASP:OD2 | 3:CC:57:ILE:HG12 | 2.19 | 0.43 |
| 6:CF:70:VAL:HG23 | 6:CF:71:ILE:CD1 | 2.49 | 0.43 |
| 8:CH:88:ARG:O | 8:CH:92:LEU:HD12 | 2.18 | 0.43 |
| 14:CN:46:LEU:HG | 14:CN:46:LEU:O | 2.18 | 0.43 |
| 22:DA:116:C:C4 | 22:DA:117:G:N7 | 2.86 | 0.43 |
| 22:DA:153:U:H2' | 22:DA:154:U:C6 | 2.53 | 0.43 |
| 22:DA:377:G:O6 | 22:DA:378:C:N4 | 2.51 | 0.43 |
| 22:DA:828:U:H2' | 22:DA:829:A:C8 | 2.53 | 0.43 |
| 22:DA:1060:U:OP2 | 30:DI:75:PRO:HA | 2.18 | 0.43 |
| 22:DA:1063:G:C4' | 30:DI:77:ALA:HB1 | 2.49 | 0.43 |
| 22:DA:1241:A:N3 | 22:DA:1241:A:H2' | 2.32 | 0.43 |
| 22:DA:1272:A:C5 | 22:DA:1618:A:H1' | 2.53 | 0.43 |
| 22:DA:1272:A:N3 | 22:DA:1618:A:C4 | 2.87 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1544:A:N6 | 22:DA:1545:A:C6 | 2.86 | 0.43 |
| 22:DA:1616:A:H2 | 22:DA:1647:U:C5 | 2.37 | 0.43 |
| 22:DA:1874:C:C5' | 22:DA:1875:G:OP2 | 2.67 | 0.43 |
| 22:DA:2326:C:C1' | 22:DA:2327:A:OP1 | 2.67 | 0.43 |
| 22:DA:2598:A:OP1 | 24:DC:234:GLY:O | 2.36 | 0.43 |
| 23:DB:31:C:O2' | 23:DB:53:A:N1 | 2.48 | 0.43 |
| 25:DD:193:VAL:HB | 25:DD:194:PRO:CD | 2.49 | 0.43 |
| 26:DE:15:SER:OG | 26:DE:197:GLU:OE2 | 2.32 | 0.43 |
| 26:DE:48:THR:OG1 | 26:DE:49:ARG:N | 2.51 | 0.43 |
| 31:DJ:15:TRP:CD2 | 31:DJ:53:TYR:HB2 | 2.54 | 0.43 |
| 31:DJ:57:LEU:O | 31:DJ:58:ASN:HB2 | 2.18 | 0.43 |
| 1:AA:474:G:C6 | 1:AA:475:C:C5 | 3.06 | 0.43 |
| 1:AA:567:G:C2 | 1:AA:568:G:H1' | 2.54 | 0.43 |
| 1:AA:597:G:N7 | 1:AA:598:U:C5 | 2.86 | 0.43 |
| 1:AA:751:U:C4 | 1:AA:752:G:C6 | 3.06 | 0.43 |
| 1:AA:914:A:C4 | 1:AA:915:A:C8 | 3.07 | 0.43 |
| 1:AA:1313:U:OP2 | 19:AS:6:LYS:HB3 | 2.19 | 0.43 |
| 3:AC:22:TRP:CD1 | 3:AC:59:ARG:CD | 3.02 | 0.43 |
| 3:AC:167:TRP:C | 3:AC:167:TRP:CE3 | 2.92 | 0.43 |
| 4:AD:27:ALA:O | 4:AD:28:ILE:C | 2.57 | 0.43 |
| 4:AD:78:GLU:CG | 4:AD:93:LEU:HD21 | 2.48 | 0.43 |
| 4:AD:78:GLU:O | 4:AD:79:ALA:C | 2.57 | 0.43 |
| 5:AE:72:ILE:CD1 | 5:AE:145:GLU:OE2 | 2.67 | 0.43 |
| 6:AF:38:ARG:HB3 | 6:AF:63:ASN:HB2 | 2.01 | 0.43 |
| 8:AH:7:ILE:O | 8:AH:11:LEU:HG | 2.18 | 0.43 |
| 12:AL:63:VAL:HG21 | 12:AL:95:TYR:CE2 | 2.54 | 0.43 |
| 19:AS:65:GLU:OE2 | 19:AS:66:MET:N | 2.52 | 0.43 |
| 20:AT:51:PHE:HA | 20:AT:54:MET:HG2 | 2.00 | 0.43 |
| 22:BA:118:A:C8 | 22:BA:119:A:C8 | 3.06 | 0.43 |
| 22:BA:242:G:N7 | 51:B3:5:LYS:HG2 | 2.34 | 0.43 |
| 22:BA:282:A:H2' | 22:BA:283:G:C8 | 2.54 | 0.43 |
| 22:BA:483:A:H1' | 42:BU:58:ILE:CD1 | 2.49 | 0.43 |
| 22:BA:572:A:P | 58:BA:3569:HOH:O | 2.77 | 0.43 |
| 22:BA:580:U:O3' | 38:BQ:31:VAL:HG13 | 2.18 | 0.43 |
| 22:BA:735:A:H3' | 22:BA:736:C:C6 | 2.54 | 0.43 |
| 22:BA:753:A:H2' | 22:BA:754:U:C6 | 2.54 | 0.43 |
| 22:BA:971:G:OP2 | 22:BA:974:G:N2 | 2.52 | 0.43 |
| 22:BA:1097:U:H3' | 22:BA:1098:A:H4' | 2.01 | 0.43 |
| 22:BA:1607:C:N4 | 22:BA:1622:G:C5 | 2.86 | 0.43 |
| 22:BA:1916:A:O3' | 22:BA:1917:U:H4' | 2.18 | 0.43 |
| 22:BA:1937:A:C2 | 22:BA:1939:U:C4 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2116:G:C6 | 22:BA:2171:A:N6 | 2.87 | 0.43 |
| 22:BA:2190:G:C4 | 22:BA:2191:A:C8 | 3.07 | 0.43 |
| 22:BA:2356:U:O3' | 44:BW:20:ARG:HD3 | 2.18 | 0.43 |
| 22:BA:2435:A:C2' | 22:BA:2436:G:O5' | 2.67 | 0.43 |
| 22:BA:2636:C:H2' | 22:BA:2637:U:C6 | 2.53 | 0.43 |
| 22:BA:2820:A:N1 | 25:BD:197:THR:CG2 | 2.81 | 0.43 |
| 26:BE:1:MET:N | 26:BE:14:VAL:O | 2.50 | 0.43 |
| 41:BT:28:ASN:HD21 | 41:BT:91:GLN:HB2 | 1.84 | 0.43 |
| 42:BU:12:ILE:HG13 | 42:BU:22:ARG:HG3 | 2.00 | 0.43 |
| 53:B5:50:ILE:CB | 53:B5:52:PRO:HD3 | 2.48 | 0.43 |
| 1:CA:21:G:H2' | 1:CA:22:G:C8 | 2.54 | 0.43 |
| 1:CA:32:A:N1 | 1:CA:33:A:C6 | 2.87 | 0.43 |
| 1:CA:91:U:C4 | 1:CA:92:U:C4 | 3.07 | 0.43 |
| 1:CA:461:A:H2' | 1:CA:462:G:O4' | 2.19 | 0.43 |
| 1:CA:582:C:C4 | 1:CA:760:G:C6 | 3.07 | 0.43 |
| 1:CA:741:G:C6 | 1:CA:742:G:C5 | 3.07 | 0.43 |
| 1:CA:824:G:H1' | 8:CH:2:SER:CA | 2.49 | 0.43 |
| 1:CA:1137:C:H1' | 1:CA:1138:G:N2 | 2.33 | 0.43 |
| 1:CA:1203:C:H4' | 14:CN:67:THR:HG22 | 2.00 | 0.43 |
| 1:CA:1314:C:OP2 | 19:CS:6:LYS:HG2 | 2.19 | 0.43 |
| 3:CC:9:GLY:HA3 | 14:CN:89:MET:SD | 2.59 | 0.43 |
| 3:CC:156:ARG:NH1 | 3:CC:159:GLY:O | 2.52 | 0.43 |
| 5:CE:109:GLY:O | 5:CE:110:ALA:CB | 2.67 | 0.43 |
| 5:CE:156:LYS:HD3 | 8:CH:71:VAL:HG13 | 2.01 | 0.43 |
| 6:CF:92:THR:HG22 | 6:CF:93:LYS:N | 2.33 | 0.43 |
| 12:CL:16:VAL:HG23 | 12:CL:16:VAL:O | 2.19 | 0.43 |
| 12:CL:80:ILE:HD12 | 12:CL:97:THR:HG21 | 2.01 | 0.43 |
| 19:CS:53:ASN:OD1 | 19:CS:55:ARG:HG2 | 2.19 | 0.43 |
| 22:DA:245:G:O6 | 51:D3:8:ARG:HD2 | 2.19 | 0.43 |
| 22:DA:288:U:H2' | 22:DA:289:G:C8 | 2.54 | 0.43 |
| 22:DA:349:U:O2' | 22:DA:350:G:H5' | 2.18 | 0.43 |
| 22:DA:599:A:H1' | 22:DA:659:G:N2 | 2.34 | 0.43 |
| 22:DA:1109:C:C5 | 22:DA:1110:G:O6 | 2.72 | 0.43 |
| 22:DA:1179:G:H2' | 22:DA:1180:U:H4' | 2.00 | 0.43 |
| 22:DA:1249:U:H4' | 38:DQ:4:VAL:HB | 2.00 | 0.43 |
| 22:DA:1464:G:C4 | 22:DA:1465:G:C8 | 3.06 | 0.43 |
| 22:DA:1502:A:C2 | 22:DA:1503:A:C4 | 3.07 | 0.43 |
| 22:DA:1663:G:H3' | 58:DA:3423:HOH:O | 2.17 | 0.43 |
| 22:DA:1715:G:O2' | 22:DA:1716:U:OP2 | 2.36 | 0.43 |
| 22:DA:1794:A:H2' | 22:DA:1795:C:C6 | 2.54 | 0.43 |
| 22:DA:1874:C:N4 | 22:DA:1875:G:C6 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2156:G:C6 | 22:DA:2157:G:N2 | 2.87 | 0.43 |
| 22:DA:2819:G:N3 | 22:DA:2828:G:C2 | 2.86 | 0.43 |
| 22:DA:2849:U:C3' | 22:DA:2850:A:H5' | 2.49 | 0.43 |
| 24:DC:17:VAL:N | 24:DC:204:VAL:HG22 | 2.34 | 0.43 |
| 24:DC:75:PRO:HB2 | 24:DC:97:LYS:CG | 2.49 | 0.43 |
| 24:DC:251:GLN:CG | 24:DC:255:LYS:HB2 | 2.49 | 0.43 |
| 25:DD:106:LYS:HA | 25:DD:175:LEU:O | 2.19 | 0.43 |
| 27:DF:16:LEU:HD11 | 27:DF:169:LEU:HD13 | 2.01 | 0.43 |
| 27:DF:31:VAL:O | 27:DF:31:VAL:HG13 | 2.19 | 0.43 |
| 29:DH:62:LEU:HD13 | 29:DH:63:ALA:N | 2.34 | 0.43 |
| 29:DH:82:SER:O | 29:DH:83:LYS:C | 2.57 | 0.43 |
| 30:DI:80:LEU:HA | 30:DI:84:ALA:HB3 | 2.01 | 0.43 |
| 31:DJ:38:GLY:O | 31:DJ:44:TYR:HB2 | 2.18 | 0.43 |
| 31:DJ:114:LEU:O | 31:DJ:118:MET:HG2 | 2.18 | 0.43 |
| 33:DL:82:LEU:HA | 33:DL:85:VAL:HG13 | 1.99 | 0.43 |
| 38:DQ:76:TYR:CE1 | 38:DQ:80:ILE:HD11 | 2.54 | 0.43 |
| 39:DR:67:GLY:C | 39:DR:93:PHE:CE2 | 2.92 | 0.43 |
| 42:DU:46:GLN:HG2 | 42:DU:47:LYS:N | 2.34 | 0.43 |
| 45:DX:30:LEU:HB3 | 45:DX:31:PRO:CD | 2.49 | 0.43 |
| 1:AA:188:C:N3 | 1:AA:189:A:C2 | 2.86 | 0.43 |
| 1:AA:209:U:C4' | 1:AA:210:C:OP2 | 2.64 | 0.43 |
| 1:AA:258:G:C5 | 1:AA:259:G:C8 | 3.06 | 0.43 |
| 1:AA:1367:C:C4 | 1:AA:1368:A:N7 | 2.87 | 0.43 |
| 1:AA:1508:A:H2' | 1:AA:1509:C:O4' | 2.18 | 0.43 |
| 2:AB:47:VAL:C | 2:AB:49:MET:N | 2.71 | 0.43 |
| 4:AD:150:LYS:O | 4:AD:152:GLN:NE2 | 2.51 | 0.43 |
| 10:AJ:40:ILE:HB | 10:AJ:73:LEU:HB2 | 2.00 | 0.43 |
| 13:AM:66:GLU:O | 13:AM:69:LEU:N | 2.51 | 0.43 |
| 13:AM:83:LEU:HD21 | 19:AS:65:GLU:HG2 | 1.99 | 0.43 |
| 22:BA:460:A:H2' | 22:BA:461:C:O4' | 2.18 | 0.43 |
| 22:BA:818:G:H5' | 22:BA:839:U:OP1 | 2.19 | 0.43 |
| 22:BA:1243:C:H2' | 22:BA:1244:A:O4' | 2.19 | 0.43 |
| 22:BA:1442:U:H2' | 22:BA:1443:U:H6 | 1.84 | 0.43 |
| 22:BA:1535:A:H5' | 22:BA:1536:C:C5 | 2.54 | 0.43 |
| 22:BA:1637:A:H4' | 22:BA:2711:A:O2' | 2.19 | 0.43 |
| 22:BA:1675:C:N3 | 25:BD:133:THR:HG21 | 2.34 | 0.43 |
| 22:BA:2029:G:N1 | 22:BA:2033:A:OP2 | 2.36 | 0.43 |
| 29:BH:45:GLU:HA | 29:BH:48:GLU:HB2 | 2.01 | 0.43 |
| 35:BN:38:LEU:HB3 | 35:BN:39:PRO:HD3 | 2.01 | 0.43 |
| 37:BP:31:TRP:CE2 | 37:BP:40:LEU:HD12 | 2.54 | 0.43 |
| 41:BT:29:THR:OG1 | 41:BT:86:THR:CG2 | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:57:VAL:HG22 | 41:BT:58:VAL:N | 2.34 | 0.43 |
| 53:B5:218:THR:O | 53:B5:219:MET:CB | 2.65 | 0.43 |
| 1:CA:94:G:H4' | 1:CA:95:C:C5 | 2.54 | 0.43 |
| 1:CA:378:G:N2 | 1:CA:386:C:O2 | 2.51 | 0.43 |
| 1:CA:552:U:H4' | 12:CL:83:ARG:HG3 | 2.00 | 0.43 |
| 1:CA:786:G:N2 | 1:CA:787:A:H1' | 2.34 | 0.43 |
| 1:CA:959:A:O3' | 1:CA:960:U:H4' | 2.19 | 0.43 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:C5 | 3.07 | 0.43 |
| 1:CA:1160:G:O6 | 1:CA:1181:G:C5 | 2.72 | 0.43 |
| 1:CA:1386:G:H2' | 1:CA:1387:G:H8 | 1.84 | 0.43 |
| 5:CE:56:VAL:N | 5:CE:57:PRO:CD | 2.81 | 0.43 |
| 8:CH:59:LEU:HD12 | 8:CH:60:GLU:N | 2.34 | 0.43 |
| 10:CJ:80:THR:O | 10:CJ:84:VAL:HG12 | 2.19 | 0.43 |
| 12:CL:14:ARG:NH1 | 12:CL:15:LYS:HG3 | 2.34 | 0.43 |
| 14:CN:46:LEU:HD23 | 19:CS:10:PHE:HB2 | 2.01 | 0.43 |
| 16:CP:37:GLY:HA2 | 16:CP:51:ARG:NH1 | 2.34 | 0.43 |
| 22:DA:46:G:N1 | 22:DA:47:C:C4 | 2.87 | 0.43 |
| 22:DA:110:G:N2 | 22:DA:111:A:H1' | 2.34 | 0.43 |
| 22:DA:155:A:H2' | 22:DA:156:A:C8 | 2.53 | 0.43 |
| 22:DA:167:A:H2' | 22:DA:168:G:O4' | 2.19 | 0.43 |
| 22:DA:372:G:P | 45:DX:62:LYS:NZ | 2.92 | 0.43 |
| 22:DA:415:A:N1 | 22:DA:2409:G:C6 | 2.87 | 0.43 |
| 22:DA:571:U:H1' | 22:DA:573:U:C6 | 2.54 | 0.43 |
| 22:DA:668:A:C4 | 22:DA:670:A:N7 | 2.87 | 0.43 |
| 22:DA:668:A:H3' | 22:DA:669:G:H5'' | 2.00 | 0.43 |
| 22:DA:784:G:H5'' | 24:DC:226:ASN:OD1 | 2.18 | 0.43 |
| 22:DA:845:A:C6 | 22:DA:847:U:C6 | 3.07 | 0.43 |
| 22:DA:950:G:H2' | 22:DA:951:C:O4' | 2.19 | 0.43 |
| 22:DA:1056:G:N1 | 22:DA:1102:C:OP2 | 2.48 | 0.43 |
| 22:DA:1062:G:C2 | 22:DA:1063:G:N1 | 2.87 | 0.43 |
| 22:DA:1239:G:H2' | 22:DA:1240:U:O4' | 2.18 | 0.43 |
| 22:DA:1383:A:C2 | 22:DA:1384:A:C5 | 3.07 | 0.43 |
| 22:DA:1677:A:N6 | 22:DA:1678:A:N1 | 2.67 | 0.43 |
| 22:DA:1833:C:C4 | 22:DA:1834:U:C4 | 3.07 | 0.43 |
| 22:DA:2103:C:H2' | 22:DA:2104:C:C5 | 2.54 | 0.43 |
| 22:DA:2115:G:H2' | 22:DA:2117:A:N7 | 2.34 | 0.43 |
| 22:DA:2201:G:H2' | 22:DA:2202:U:C6 | 2.54 | 0.43 |
| 22:DA:2253:G:C5 | 22:DA:2254:C:C5 | 3.06 | 0.43 |
| 22:DA:2345:G:C4 | 22:DA:2381:A:C2 | 3.06 | 0.43 |
| 22:DA:2478:A:C8 | 22:DA:2529:G:C6 | 3.06 | 0.43 |
| 22:DA:2478:A:N7 | 22:DA:2529:G:C6 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2720:U:C5 | 22:DA:2872:A:N1 | 2.87 | 0.43 |
| 22:DA:2829:A:C2' | 22:DA:2830:C:H5' | 2.49 | 0.43 |
| 24:DC:187:ASP:O | 24:DC:188:CYS:C | 2.57 | 0.43 |
| 25:DD:167:ASN:O | 25:DD:168:GLU:HB3 | 2.18 | 0.43 |
| 31:DJ:94:ALA:O | 31:DJ:95:ARG:C | 2.57 | 0.43 |
| 32:DK:113:MET:HA | 32:DK:116:ILE:HG12 | 2.01 | 0.43 |
| 36:DO:11:ALA:O | 36:DO:13:ARG:N | 2.52 | 0.43 |
| 37:DP:79:PRO:O | 37:DP:80:VAL:C | 2.57 | 0.43 |
| 37:DP:100:LEU:HD22 | 37:DP:108:ALA:HB1 | 2.00 | 0.43 |
| 42:DU:71:ALA:HB3 | 42:DU:80:ALA:HB1 | 1.99 | 0.43 |
| 46:DY:20:ASN:HB3 | 46:DY:50:VAL:CG2 | 2.49 | 0.43 |
| 1:AA:65:A:C4 | 1:AA:381:C:C5 | 3.06 | 0.43 |
| 1:AA:104:G:N2 | 1:AA:105:G:C4 | 2.87 | 0.43 |
| 1:AA:259:G:C2 | 1:AA:268:U:O2 | 2.71 | 0.43 |
| 1:AA:625:U:H5'' | 16:AP:16:PHE:CD1 | 2.53 | 0.43 |
| 1:AA:1160:G:O6 | 1:AA:1181:G:C5 | 2.71 | 0.43 |
| 1:AA:1178:G:C8 | 9:AI:99:ARG:NH2 | 2.87 | 0.43 |
| 1:AA:1296:C:H4' | 1:AA:1302:C:N4 | 2.34 | 0.43 |
| 2:AB:23:TRP:CZ3 | 2:AB:25:PRO:HA | 2.54 | 0.43 |
| 4:AD:13:ARG:HD2 | 4:AD:34:ILE:HA | 2.01 | 0.43 |
| 12:AL:57:LEU:O | 12:AL:59:ASN:N | 2.52 | 0.43 |
| 15:AO:87:LEU:N | 15:AO:87:LEU:CD2 | 2.82 | 0.43 |
| 16:AP:67:ILE:HG23 | 16:AP:71:VAL:CG1 | 2.49 | 0.43 |
| 18:AR:67:LEU:O | 18:AR:68:LEU:HG | 2.19 | 0.43 |
| 20:AT:58:VAL:O | 20:AT:59:ASP:C | 2.58 | 0.43 |
| 22:BA:27:G:N2 | 22:BA:512:G:H1' | 2.34 | 0.43 |
| 22:BA:319:G:C4 | 22:BA:333:G:N2 | 2.86 | 0.43 |
| 22:BA:1062:G:OP1 | 22:BA:1070:A:H4' | 2.19 | 0.43 |
| 22:BA:1736:U:N3 | 22:BA:1737:G:C4 | 2.87 | 0.43 |
| 22:BA:1980:G:C4 | 22:BA:1982:U:C4 | 3.07 | 0.43 |
| 27:BF:146:VAL:HG23 | 27:BF:146:VAL:O | 2.19 | 0.43 |
| 30:BI:28:LEU:HG | 30:BI:35:ILE:HD12 | 2.00 | 0.43 |
| 32:BK:92:GLU:HG3 | 32:BK:111:LYS:NZ | 2.33 | 0.43 |
| 34:BM:42:THR:O | 34:BM:45:GLN:HB2 | 2.18 | 0.43 |
| 36:BO:28:VAL:HG11 | 36:BO:92:PHE:CZ | 2.54 | 0.43 |
| 38:BQ:86:ALA:O | 38:BQ:87:SER:CB | 2.66 | 0.43 |
| 39:BR:49:ILE:HB | 39:BR:52:PRO:O | 2.19 | 0.43 |
| 40:BS:28:LYS:O | 40:BS:30:SER:N | 2.51 | 0.43 |
| 41:BT:69:ARG:HB3 | 41:BT:74:ILE:HG22 | 2.01 | 0.43 |
| 49:B1:6:ARG:HD3 | 49:B1:24:THR:OG1 | 2.19 | 0.43 |
| 53:B5:59:VAL:HG23 | 53:B5:167:ASP:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:40:C:H2' | 1:CA:41:G:O4' | 2.18 | 0.43 |
| 1:CA:451:A:H4' | 1:CA:452:A:O4' | 2.19 | 0.43 |
| 1:CA:560:A:N7 | 1:CA:566:G:C4 | 2.87 | 0.43 |
| 1:CA:706:A:H4' | 11:CK:31:ILE:HD11 | 2.01 | 0.43 |
| 1:CA:755:G:C2 | 1:CA:756:C:C6 | 3.07 | 0.43 |
| 1:CA:783:C:C2 | 1:CA:784:A:C8 | 3.07 | 0.43 |
| 1:CA:847:G:C2 | 1:CA:848:C:C2 | 3.07 | 0.43 |
| 1:CA:1362:A:OP1 | 1:CA:1362:A:H4' | 2.17 | 0.43 |
| 2:CB:21:ARG:O | 2:CB:22:TYR:C | 2.57 | 0.43 |
| 2:CB:140:GLU:O | 2:CB:141:LEU:C | 2.57 | 0.43 |
| 7:CG:12:ILE:HD12 | 7:CG:24:ALA:C | 2.39 | 0.43 |
| 7:CG:40:GLU:O | 7:CG:44:TYR:CD2 | 2.72 | 0.43 |
| 8:CH:51:VAL:O | 8:CH:51:VAL:HG22 | 2.19 | 0.43 |
| 10:CJ:33:GLY:HA3 | 10:CJ:83:THR:HB | 2.00 | 0.43 |
| 12:CL:87:VAL:HG11 | 12:CL:90:LEU:HD23 | 2.00 | 0.43 |
| 12:CL:111:LYS:O | 12:CL:114:ARG:HG3 | 2.19 | 0.43 |
| 13:CM:40:ALA:O | 13:CM:41:GLU:C | 2.58 | 0.43 |
| 14:CN:31:ILE:HG22 | 14:CN:32:SER:N | 2.34 | 0.43 |
| 22:DA:447:A:H5' | 22:DA:449:A:C5 | 2.53 | 0.43 |
| 22:DA:483:A:H4' | 42:DU:47:LYS:HA | 2.00 | 0.43 |
| 22:DA:546:U:O2 | 22:DA:546:U:C2' | 2.67 | 0.43 |
| 22:DA:609:A:H2' | 22:DA:610:C:O4' | 2.19 | 0.43 |
| 22:DA:629:G:O4' | 22:DA:638:G:N2 | 2.52 | 0.43 |
| 22:DA:687:C:C2 | 22:DA:788:A:H5' | 2.54 | 0.43 |
| 22:DA:704:G:H1' | 22:DA:726:G:N2 | 2.34 | 0.43 |
| 22:DA:776:G:C8 | 22:DA:793:A:C2 | 3.07 | 0.43 |
| 22:DA:980:A:N6 | 22:DA:981:A:N1 | 2.67 | 0.43 |
| 22:DA:1431:A:C6 | 22:DA:1432:G:C5 | 3.07 | 0.43 |
| 22:DA:1537:G:H3' | 22:DA:1537:G:N3 | 2.34 | 0.43 |
| 22:DA:2067:G:C4 | 22:DA:2444:G:N2 | 2.87 | 0.43 |
| 22:DA:2199:A:C1' | 29:DH:28:ASN:ND2 | 2.81 | 0.43 |
| 22:DA:2291:U:H2' | 22:DA:2292:U:C6 | 2.53 | 0.43 |
| 22:DA:2756:U:H1' | 22:DA:2757:A:H5'' | 2.01 | 0.43 |
| 22:DA:2803:G:C2 | 22:DA:2804:U:C4 | 3.07 | 0.43 |
| 23:DB:40:U:C2 | 23:DB:44:G:OP2 | 2.70 | 0.43 |
| 24:DC:129:THR:CG2 | 24:DC:130:LEU:N | 2.82 | 0.43 |
| 27:DF:9:LYS:O | 27:DF:13:VAL:HG23 | 2.19 | 0.43 |
| 27:DF:110:ARG:CZ | 27:DF:110:ARG:HB3 | 2.49 | 0.43 |
| 27:DF:169:LEU:HG | 27:DF:169:LEU:O | 2.18 | 0.43 |
| 30:DI:59:ILE:CG2 | 30:DI:60:THR:N | 2.81 | 0.43 |
| 31:DJ:17:VAL:HG22 | 31:DJ:55:ILE:HB | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:DK:99:ILE:CG2 | 32:DK:119:ALA:HB2 | 2.49 | 0.43 |
| 33:DL:56:PRO:HD2 | 33:DL:59:ARG:HB2 | 2.01 | 0.43 |
| 34:DM:62:LYS:HD3 | 34:DM:64:TRP:CZ2 | 2.54 | 0.43 |
| 37:DP:60:THR:HA | 37:DP:73:VAL:HA | 2.01 | 0.43 |
| 40:DS:10:ALA:HB3 | 40:DS:101:SER:O | 2.19 | 0.43 |
| 41:DT:38:ALA:O | 41:DT:39:THR:HB | 2.18 | 0.43 |
| 1:AA:33:A:H2' | 1:AA:34:C:C6 | 2.54 | 0.42 |
| 1:AA:408:A:C2 | 1:AA:435:A:C2 | 3.07 | 0.42 |
| 1:AA:457:G:C6 | 1:AA:458:U:C2 | 3.07 | 0.42 |
| 1:AA:580:C:H2' | 1:AA:581:G:O4' | 2.19 | 0.42 |
| 1:AA:776:G:HO2' | 1:AA:777:A:H8 | 1.64 | 0.42 |
| 1:AA:827:U:H2' | 1:AA:870:U:O4 | 2.19 | 0.42 |
| 1:AA:832:G:C2 | 1:AA:833:G:C8 | 3.06 | 0.42 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.54 | 0.42 |
| 1:AA:1202:U:C4 | 1:AA:1203:C:C5 | 3.08 | 0.42 |
| 1:AA:1368:A:OP2 | 9:AI:114:LYS:HD2 | 2.19 | 0.42 |
| 1:AA:1370:G:C5' | 9:AI:111:VAL:HG21 | 2.49 | 0.42 |
| 1:AA:1392:G:C5 | 1:AA:1393:U:C5 | 3.07 | 0.42 |
| 1:AA:1419:G:C6 | 1:AA:1420:U:C4 | 3.07 | 0.42 |
| 2:AB:68:LEU:HD12 | 2:AB:154:MET:HE1 | 2.01 | 0.42 |
| 2:AB:131:LYS:HA | 2:AB:131:LYS:HE2 | 2.01 | 0.42 |
| 4:AD:190:ASP:O | 4:AD:191:LEU:O | 2.37 | 0.42 |
| 7:AG:46:ALA:CB | 7:AG:120:LEU:HD12 | 2.49 | 0.42 |
| 13:AM:15:ALA:O | 13:AM:16:VAL:C | 2.56 | 0.42 |
| 17:AQ:8:LEU:N | 17:AQ:8:LEU:CD1 | 2.82 | 0.42 |
| 19:AS:37:ARG:O | 19:AS:70:LYS:HD2 | 2.19 | 0.42 |
| 19:AS:40:ILE:CG1 | 19:AS:71:LEU:HD22 | 2.49 | 0.42 |
| 21:AU:12:PHE:CD1 | 21:AU:16:LEU:CD1 | 3.02 | 0.42 |
| 22:BA:123:G:H2' | 22:BA:124:G:O4' | 2.18 | 0.42 |
| 22:BA:973:A:H5' | 22:BA:1188:U:C1' | 2.48 | 0.42 |
| 22:BA:999:U:C5 | 22:BA:1154:G:C5 | 3.07 | 0.42 |
| 22:BA:1313:U:H2' | 22:BA:1610:A:C2 | 2.55 | 0.42 |
| 22:BA:1853:A:N1 | 22:BA:2087:G:H1' | 2.34 | 0.42 |
| 22:BA:1925:C:C4' | 22:BA:1926:U:OP1 | 2.66 | 0.42 |
| 22:BA:2166:U:O4 | 22:BA:2170:A:N7 | 2.52 | 0.42 |
| 22:BA:2275:C:O2 | 34:BM:84:LYS:CD | 2.67 | 0.42 |
| 22:BA:2452:C:C4 | 22:BA:2453:A:C6 | 3.07 | 0.42 |
| 22:BA:2576:G:O2' | 22:BA:2579:C:OP2 | 2.23 | 0.42 |
| 22:BA:2615:U:H2' | 22:BA:2616:C:H5' | 2.01 | 0.42 |
| 24:BC:257:THR:O | 24:BC:258:ARG:C | 2.56 | 0.42 |
| 27:BF:5:HIS:O | 27:BF:8:TYR:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BF:55:ALA:HA | 27:BF:58:ALA:HB3 | 2.00 | 0.42 |
| 28:BG:168:VAL:O | 28:BG:168:VAL:HG13 | 2.19 | 0.42 |
| 29:BH:79:THR:CG2 | 29:BH:147:VAL:CG2 | 2.97 | 0.42 |
| 29:BH:97:ARG:NH1 | 1:CA:370:C:O4' | 2.52 | 0.42 |
| 37:BP:93:ARG:O | 37:BP:94:LYS:HB2 | 2.18 | 0.42 |
| 42:BU:7:ARG:O | 42:BU:8:ASP:O | 2.37 | 0.42 |
| 45:BX:7:VAL:HG23 | 45:BX:51:VAL:HG12 | 2.00 | 0.42 |
| 1:CA:75:G:N2 | 1:CA:96:U:H1' | 2.34 | 0.42 |
| 2:CB:146:ASN:OD1 | 2:CB:147:SER:N | 2.51 | 0.42 |
| 4:CD:119:SER:O | 4:CD:131:ASN:OD1 | 2.36 | 0.42 |
| 6:CF:66:ALA:HB3 | 6:CF:71:ILE:HD11 | 2.00 | 0.42 |
| 11:CK:118:HIS:O | 11:CK:119:ASN:HB2 | 2.19 | 0.42 |
| 22:DA:14:A:H5'' | 22:DA:15:G:OP2 | 2.18 | 0.42 |
| 22:DA:389:G:C2 | 22:DA:2413:G:H1' | 2.54 | 0.42 |
| 22:DA:578:G:C5 | 22:DA:2018:G:H5' | 2.54 | 0.42 |
| 22:DA:579:G:C2 | 22:DA:1262:A:C5 | 3.06 | 0.42 |
| 22:DA:847:U:O4 | 22:DA:932:U:C4 | 2.72 | 0.42 |
| 22:DA:1109:C:H3' | 22:DA:1110:G:C8 | 2.54 | 0.42 |
| 22:DA:1384:A:O4' | 22:DA:1405:U:O4' | 2.35 | 0.42 |
| 22:DA:1415:U:O2' | 22:DA:1416:G:H4' | 2.18 | 0.42 |
| 22:DA:1434:A:H2' | 22:DA:1435:G:C8 | 2.54 | 0.42 |
| 22:DA:1453:A:C2 | 35:DN:77:ALA:HB2 | 2.54 | 0.42 |
| 22:DA:1975:G:N2 | 22:DA:1976:U:H1' | 2.34 | 0.42 |
| 22:DA:2235:G:C2 | 22:DA:2236:U:C2 | 3.07 | 0.42 |
| 22:DA:2297:A:C8 | 22:DA:2320:U:C4 | 3.06 | 0.42 |
| 22:DA:2840:C:H5'' | 35:DN:53:THR:OG1 | 2.19 | 0.42 |
| 24:DC:3:VAL:HG11 | 24:DC:202:LEU:HD23 | 2.00 | 0.42 |
| 28:DG:121:ILE:HD12 | 28:DG:141:ILE:HG22 | 2.00 | 0.42 |
| 30:DI:10:LYS:HB2 | 30:DI:56:PRO:HB2 | 2.01 | 0.42 |
| 32:DK:21:CYS:HA | 32:DK:41:ILE:HG22 | 2.01 | 0.42 |
| 33:DL:29:LYS:O | 33:DL:30:THR:HG23 | 2.19 | 0.42 |
| 47:DZ:3:LYS:O | 47:DZ:4:THR:HG22 | 2.19 | 0.42 |
| 1:AA:78:A:C5 | 1:AA:79:G:H1' | 2.55 | 0.42 |
| 1:AA:79:G:N2 | 1:AA:91:U:O4 | 2.52 | 0.42 |
| 1:AA:464:U:N3 | 1:AA:466:A:H5'' | 2.33 | 0.42 |
| 1:AA:549:C:C2 | 1:AA:550:G:C8 | 3.07 | 0.42 |
| 1:AA:1296:C:H4' | 1:AA:1302:C:C5 | 2.54 | 0.42 |
| 1:AA:1452:C:O4' | 1:AA:1453:G:N2 | 2.52 | 0.42 |
| 1:AA:1485:U:O2' | 1:AA:1486:G:H5' | 2.20 | 0.42 |
| 2:AB:50:PHE:CE2 | 2:AB:51:ASN:OD1 | 2.73 | 0.42 |
| 2:AB:83:ALA:O | 2:AB:87:CYS:SG | 2.77 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:AC:25:ASN:O | 3:AC:27:LYS:HG2 | 2.19 | 0.42 |
| 5:AE:56:VAL:O | 5:AE:60:ILE:HG23 | 2.19 | 0.42 |
| 5:AE:115:LEU:HG | 5:AE:120:VAL:HG21 | 2.01 | 0.42 |
| 9:AI:51:PRO:HG2 | 9:AI:83:ILE:HD13 | 2.02 | 0.42 |
| 10:AJ:52:LEU:CB | 14:AN:81:ARG:HE | 2.32 | 0.42 |
| 11:AK:35:THR:HA | 11:AK:42:LEU:HG | 2.01 | 0.42 |
| 13:AM:74:SER:O | 13:AM:78:LYS:HG3 | 2.19 | 0.42 |
| 20:AT:35:VAL:CG1 | 20:AT:79:LEU:HD22 | 2.49 | 0.42 |
| 22:BA:83:A:C6 | 22:BA:101:A:C4 | 3.06 | 0.42 |
| 22:BA:195:A:C4 | 22:BA:198:C:N4 | 2.86 | 0.42 |
| 22:BA:419:U:H2' | 22:BA:420:C:C6 | 2.54 | 0.42 |
| 22:BA:451:U:H4' | 26:BE:47:LYS:NZ | 2.34 | 0.42 |
| 22:BA:468:G:N7 | 50:B2:39:ARG:NH2 | 2.65 | 0.42 |
| 22:BA:915:C:C2' | 22:BA:916:G:H5' | 2.49 | 0.42 |
| 22:BA:996:A:N6 | 22:BA:1160:G:N1 | 2.67 | 0.42 |
| 22:BA:1194:A:H2' | 22:BA:1195:G:O5' | 2.19 | 0.42 |
| 22:BA:1510:G:H2' | 22:BA:1511:G:O4' | 2.19 | 0.42 |
| 22:BA:1635:A:C6 | 22:BA:1636:U:C2 | 3.08 | 0.42 |
| 22:BA:2060:A:O4' | 22:BA:2502:G:H1' | 2.18 | 0.42 |
| 22:BA:2271:G:H2' | 22:BA:2272:U:O4' | 2.20 | 0.42 |
| 22:BA:2552:U:C2 | 22:BA:2554:U:C5' | 3.03 | 0.42 |
| 24:BC:141:VAL:HG13 | 24:BC:191:THR:O | 2.19 | 0.42 |
| 25:BD:127:PHE:CZ | 25:BD:160:LYS:HB2 | 2.54 | 0.42 |
| 26:BE:152:GLU:OE1 | 26:BE:152:GLU:HA | 2.20 | 0.42 |
| 30:BI:101:ILE:HG22 | 30:BI:102:SER:N | 2.34 | 0.42 |
| 32:BK:66:LYS:HA | 32:BK:79:PHE:O | 2.19 | 0.42 |
| 33:BL:62:PRO:HG2 | 51:B3:25:LYS:CD | 2.48 | 0.42 |
| 34:BM:65:ILE:HG12 | 34:BM:103:TYR:CE2 | 2.54 | 0.42 |
| 36:BO:51:ALA:HB3 | 36:BO:78:VAL:HG13 | 2.02 | 0.42 |
| 1:CA:102:G:C2 | 1:CA:103:U:C5 | 3.07 | 0.42 |
| 1:CA:401:C:O2' | 1:CA:402:G:H5' | 2.18 | 0.42 |
| 1:CA:590:U:O2' | 1:CA:591:U:H5' | 2.18 | 0.42 |
| 1:CA:678:U:H2' | 1:CA:679:C:O4' | 2.20 | 0.42 |
| 1:CA:728:A:C6 | 1:CA:729:A:C6 | 3.08 | 0.42 |
| 1:CA:1175:G:O6 | 1:CA:1182:G:O6 | 2.37 | 0.42 |
| 1:CA:1424:U:H2' | 1:CA:1425:U:O4' | 2.17 | 0.42 |
| 1:CA:1426:G:C4 | 1:CA:1475:G:C2 | 3.07 | 0.42 |
| 2:CB:87:CYS:HB3 | 2:CB:222:ARG:HA | 2.02 | 0.42 |
| 4:CD:168:PRO:HB2 | 4:CD:171:LEU:CD1 | 2.49 | 0.42 |
| 6:CF:38:ARG:CG | 6:CF:63:ASN:CB | 2.97 | 0.42 |
| 6:CF:45:ARG:HD2 | 6:CF:59:TYR:CD2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:CG:42:ILE:HG21 | 7:CG:116:MET:CG | 2.49 | 0.42 |
| 7:CG:148:ASN:C | 7:CG:150:ALA:N | 2.72 | 0.42 |
| 8:CH:67:GLN:C | 8:CH:69:LYS:N | 2.72 | 0.42 |
| 10:CJ:17:LEU:HD21 | 10:CJ:96:VAL:HG22 | 2.01 | 0.42 |
| 13:CM:64:VAL:O | 13:CM:69:LEU:HB2 | 2.18 | 0.42 |
| 21:CU:9:ASN:C | 21:CU:10:GLU:HG3 | 2.39 | 0.42 |
| 21:CU:20:LYS:C | 21:CU:22:SER:H | 2.21 | 0.42 |
| 22:DA:268:C:O2' | 22:DA:269:C:H5' | 2.20 | 0.42 |
| 22:DA:280:U:O4 | 22:DA:361:G:N2 | 2.52 | 0.42 |
| 22:DA:905:A:H2' | 22:DA:906:U:H5' | 2.02 | 0.42 |
| 22:DA:1097:U:O2 | 30:DI:9:VAL:CG1 | 2.67 | 0.42 |
| 22:DA:1210:G:C8 | 22:DA:1212:G:C2 | 3.08 | 0.42 |
| 22:DA:1332:G:C6 | 22:DA:1609:A:C5 | 3.07 | 0.42 |
| 22:DA:1364:G:C4 | 22:DA:1368:G:N2 | 2.87 | 0.42 |
| 22:DA:1501:G:H2' | 22:DA:1502:A:O4' | 2.19 | 0.42 |
| 22:DA:1509:A:O2' | 22:DA:1510:G:OP2 | 2.36 | 0.42 |
| 22:DA:1512:C:N3 | 22:DA:1513:U:C4 | 2.87 | 0.42 |
| 22:DA:1595:C:H2' | 22:DA:1596:A:O4' | 2.20 | 0.42 |
| 22:DA:1956:U:O2 | 22:DA:1985:C:H4' | 2.19 | 0.42 |
| 22:DA:2059:A:H2' | 22:DA:2503:A:N1 | 2.34 | 0.42 |
| 22:DA:2201:G:C6 | 22:DA:2202:U:C4 | 3.07 | 0.42 |
| 22:DA:2331:G:N2 | 22:DA:2385:C:N1 | 2.68 | 0.42 |
| 22:DA:2425:A:H4' | 22:DA:2426:A:O5' | 2.20 | 0.42 |
| 22:DA:2699:C:O2 | 22:DA:2709:G:C2 | 2.72 | 0.42 |
| 22:DA:2740:A:N6 | 22:DA:2764:A:C8 | 2.87 | 0.42 |
| 22:DA:2886:A:N1 | 48:D0:29:SER:OG | 2.49 | 0.42 |
| 23:DB:11:C:C5 | 23:DB:12:C:C5 | 3.07 | 0.42 |
| 26:DE:130:LYS:CB | 26:DE:133:LEU:HB2 | 2.49 | 0.42 |
| 27:DF:69:LYS:HG3 | 27:DF:84:PRO:HA | 2.00 | 0.42 |
| 27:DF:136:ILE:HA | 27:DF:141:ILE:CG2 | 2.48 | 0.42 |
| 31:DJ:36:LEU:HD23 | 31:DJ:121:LYS:HB2 | 2.00 | 0.42 |
| 33:DL:41:ARG:O | 33:DL:44:GLY:N | 2.50 | 0.42 |
| 33:DL:111:ILE:HG22 | 33:DL:112:LEU:N | 2.34 | 0.42 |
| 33:DL:135:ILE:O | 33:DL:140:GLY:HA3 | 2.19 | 0.42 |
| 34:DM:49:ALA:CB | 34:DM:124:LEU:HD21 | 2.49 | 0.42 |
| 34:DM:78:LEU:O | 34:DM:79:ALA:HB3 | 2.19 | 0.42 |
| 40:DS:25:ARG:CZ | 40:DS:25:ARG:HB2 | 2.49 | 0.42 |
| 41:DT:2:ILE:HG12 | 41:DT:7:LEU:HD12 | 1.99 | 0.42 |
| 41:DT:37:ASP:CG | 41:DT:38:ALA:N | 2.72 | 0.42 |
| 47:DZ:3:LYS:N | 47:DZ:3:LYS:HD3 | 2.34 | 0.42 |
| 1:AA:38:G:C2 | 1:AA:397:A:C2 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:AA:55:A:C6 | 1:AA:56:U:C2 | 3.08 | 0.42 |
| 1:AA:96:U:O2' | 1:AA:97:G:P | 2.77 | 0.42 |
| 1:AA:457:G:C5 | 1:AA:458:U:C5 | 3.07 | 0.42 |
| 1:AA:692:U:O2 | 1:AA:694:A:C8 | 2.72 | 0.42 |
| 1:AA:722:G:H2' | 1:AA:723:U:OP2 | 2.20 | 0.42 |
| 1:AA:1134:G:H2' | 1:AA:1135:U:O4' | 2.19 | 0.42 |
| 1:AA:1181:G:H4' | 1:AA:1182:G:OP1 | 2.19 | 0.42 |
| 1:AA:1210:C:N4 | 1:AA:1211:U:O4 | 2.52 | 0.42 |
| 1:AA:1461:G:H2' | 1:AA:1462:C:H6 | 1.84 | 0.42 |
| 3:AC:132:ARG:O | 3:AC:136:ARG:HG2 | 2.20 | 0.42 |
| 5:AE:84:PRO:HA | 5:AE:98:PRO:HD3 | 2.01 | 0.42 |
| 9:AI:36:GLU:OE2 | 9:AI:36:GLU:CA | 2.68 | 0.42 |
| 15:AO:81:LEU:CD1 | 15:AO:85:LEU:CD2 | 2.98 | 0.42 |
| 17:AQ:48:ASP:CG | 17:AQ:52:GLU:OE1 | 2.58 | 0.42 |
| 22:BA:360:U:H3' | 22:BA:361:G:C8 | 2.54 | 0.42 |
| 22:BA:391:A:C5 | 22:BA:392:U:C5 | 3.07 | 0.42 |
| 22:BA:1047:G:C2 | 22:BA:1110:G:C4 | 3.07 | 0.42 |
| 22:BA:1232:G:C4 | 22:BA:1233:C:C6 | 3.07 | 0.42 |
| 22:BA:1474:U:O4 | 22:BA:1475:G:N2 | 2.52 | 0.42 |
| 22:BA:1507:C:H2' | 22:BA:1508:A:C4' | 2.50 | 0.42 |
| 22:BA:1912:A:C2 | 22:BA:1919:A:C6 | 3.08 | 0.42 |
| 22:BA:1916:A:H2' | 22:BA:1917:U:C2' | 2.49 | 0.42 |
| 22:BA:1924:C:N3 | 22:BA:1926:U:O4 | 2.52 | 0.42 |
| 22:BA:2191:A:C2 | 22:BA:2192:U:N3 | 2.88 | 0.42 |
| 22:BA:2191:A:C2 | 22:BA:2192:U:O4 | 2.72 | 0.42 |
| 22:BA:2637:U:H2' | 22:BA:2638:G:H5' | 2.01 | 0.42 |
| 22:BA:2776:A:H4' | 22:BA:2777:G:O5' | 2.19 | 0.42 |
| 25:BD:30:GLU:O | 25:BD:31:ALA:C | 2.57 | 0.42 |
| 26:BE:134:LEU:HD23 | 26:BE:160:ALA:O | 2.19 | 0.42 |
| 27:BF:69:LYS:N | 27:BF:69:LYS:CD | 2.83 | 0.42 |
| 32:BK:91:SER:O | 32:BK:92:GLU:C | 2.58 | 0.42 |
| 35:BN:49:GLU:N | 35:BN:50:PRO:CD | 2.82 | 0.42 |
| 38:BQ:94:ILE:HG21 | 39:BR:4:VAL:HG11 | 2.01 | 0.42 |
| 39:BR:21:ARG:CZ | 39:BR:93:PHE:CE1 | 3.02 | 0.42 |
| 39:BR:76:LYS:O | 39:BR:84:ARG:HA | 2.19 | 0.42 |
| 1:CA:130:A:C2 | 1:CA:264:C:N1 | 2.88 | 0.42 |
| 1:CA:156:C:C4 | 1:CA:157:U:C4 | 3.08 | 0.42 |
| 1:CA:302:G:O2' | 1:CA:556:C:H5'' | 2.19 | 0.42 |
| 1:CA:455:G:C2 | 1:CA:478:A:N1 | 2.88 | 0.42 |
| 1:CA:938:A:C2 | 1:CA:1345:U:O4 | 2.73 | 0.42 |
| 1:CA:1068:G:C6 | 1:CA:1069:C:C4 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CA:1149:C:N4 | 1:CA:1150:A:N6 | 2.67 | 0.42 |
| 1:CA:1213:A:C8 | 1:CA:1215:G:C6 | 3.07 | 0.42 |
| 1:CA:1385:G:N7 | 58:CA:1873:HOH:O | 2.37 | 0.42 |
| 2:CB:62:SER:C | 2:CB:64:LYS:H | 2.22 | 0.42 |
| 4:CD:48:LEU:HD23 | 4:CD:53:VAL:N | 2.34 | 0.42 |
| 6:CF:86:ARG:CG | 6:CF:86:ARG:NH1 | 2.78 | 0.42 |
| 15:CO:73:LYS:HA | 15:CO:73:LYS:CE | 2.49 | 0.42 |
| 16:CP:4:ILE:N | 16:CP:4:ILE:HD12 | 2.34 | 0.42 |
| 18:CR:23:TYR:CB | 18:CR:58:ALA:HB1 | 2.50 | 0.42 |
| 20:CT:67:ILE:O | 20:CT:68:HIS:O | 2.37 | 0.42 |
| 22:DA:35:G:H1' | 22:DA:454:A:C4 | 2.55 | 0.42 |
| 22:DA:86:G:O2' | 22:DA:104:A:H4' | 2.19 | 0.42 |
| 22:DA:482:A:H1' | 22:DA:498:G:N2 | 2.34 | 0.42 |
| 22:DA:607:U:O4 | 22:DA:619:G:H2' | 2.18 | 0.42 |
| 22:DA:1049:C:C2' | 22:DA:1050:A:H5' | 2.49 | 0.42 |
| 22:DA:1084:A:C8 | 22:DA:1085:A:C8 | 3.07 | 0.42 |
| 22:DA:1120:G:C5 | 22:DA:1121:C:C5 | 3.07 | 0.42 |
| 22:DA:1355:G:C6 | 22:DA:1356:G:C8 | 3.08 | 0.42 |
| 22:DA:1500:G:N1 | 22:DA:1501:G:C5 | 2.87 | 0.42 |
| 22:DA:1606:C:O2' | 22:DA:1607:C:P | 2.77 | 0.42 |
| 22:DA:1652:A:H3' | 22:DA:1653:G:C8 | 2.54 | 0.42 |
| 22:DA:2010:G:C6 | 22:DA:2011:U:N3 | 2.87 | 0.42 |
| 22:DA:2024:G:C2 | 22:DA:2040:G:N3 | 2.87 | 0.42 |
| 22:DA:2044:C:N3 | 22:DA:2045:C:C5 | 2.88 | 0.42 |
| 22:DA:2234:G:C5 | 22:DA:2235:G:N7 | 2.87 | 0.42 |
| 22:DA:2323:G:C6 | 22:DA:2324:U:C4 | 3.07 | 0.42 |
| 22:DA:2341:G:C6 | 22:DA:2342:C:N3 | 2.87 | 0.42 |
| 22:DA:2370:G:C6 | 22:DA:2371:G:C6 | 3.08 | 0.42 |
| 22:DA:2793:C:H2' | 22:DA:2794:C:C1' | 2.50 | 0.42 |
| 26:DE:25:GLU:HA | 26:DE:28:VAL:HB | 1.99 | 0.42 |
| 26:DE:170:ARG:N | 26:DE:170:ARG:HD3 | 2.34 | 0.42 |
| 28:DG:2:SER:OG | 28:DG:3:ARG:N | 2.50 | 0.42 |
| 42:DU:3:ALA:O | 42:DU:6:ARG:NH1 | 2.53 | 0.42 |
| 42:DU:60:GLU:O | 42:DU:60:GLU:CG | 2.67 | 0.42 |
| 1:AA:174:A:C2' | 1:AA:175:C:H5' | 2.50 | 0.42 |
| 1:AA:322:C:O2' | 20:AT:18:ARG:HG3 | 2.20 | 0.42 |
| 1:AA:451:A:H61 | 1:AA:481:G:H5' | 1.84 | 0.42 |
| 1:AA:457:G:H2' | 1:AA:457:G:N3 | 2.34 | 0.42 |
| 1:AA:616:G:O2' | 1:AA:617:G:H5' | 2.19 | 0.42 |
| 1:AA:842:U:H3' | 1:AA:843:U:C5' | 2.49 | 0.42 |
| 1:AA:891:U:H2' | 1:AA:892:A:H5' | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1072:G:C5 | 1:AA:1073:U:C4 | 3.07 | 0.42 |
| 1:AA:1253:G:N3 | 1:AA:1254:A:C8 | 2.88 | 0.42 |
| 1:AA:1410:A:C4 | 1:AA:1491:G:N2 | 2.87 | 0.42 |
| 2:AB:132:LYS:HA | 2:AB:132:LYS:HE3 | 2.00 | 0.42 |
| 5:AE:151:GLU:HG2 | 5:AE:152:MET:H | 1.84 | 0.42 |
| 6:AF:12:PRO:O | 6:AF:15:SER:N | 2.50 | 0.42 |
| 6:AF:85:ILE:O | 6:AF:86:ARG:HG2 | 2.19 | 0.42 |
| 8:AH:89:LYS:HG3 | 8:AH:90:ASP:H | 1.84 | 0.42 |
| 10:AJ:57:VAL:CG2 | 10:AJ:58:ASN:H | 2.32 | 0.42 |
| 16:AP:36:VAL:CG2 | 16:AP:57:ILE:HG13 | 2.49 | 0.42 |
| 19:AS:42:PRO:C | 19:AS:44:MET:H | 2.21 | 0.42 |
| 22:BA:517:C:P | 48:B0:10:ARG:NH2 | 2.91 | 0.42 |
| 22:BA:863:A:O2' | 22:BA:864:G:H5' | 2.19 | 0.42 |
| 22:BA:969:G:C6 | 22:BA:970:U:C4 | 3.07 | 0.42 |
| 22:BA:1060:U:C1' | 22:BA:1062:G:OP2 | 2.67 | 0.42 |
| 22:BA:1438:U:C5 | 22:BA:1552:A:C2 | 3.07 | 0.42 |
| 22:BA:1813:G:H1' | 24:BC:50:THR:OG1 | 2.18 | 0.42 |
| 22:BA:1845:G:P | 24:BC:256:LYS:HZ3 | 2.43 | 0.42 |
| 22:BA:2190:G:N2 | 22:BA:2191:A:H1' | 2.34 | 0.42 |
| 22:BA:2672:U:C2' | 22:BA:2673:G:O5' | 2.68 | 0.42 |
| 22:BA:2683:C:H5'' | 37:BP:56:HIS:HB3 | 2.00 | 0.42 |
| 22:BA:2820:A:N1 | 25:BD:197:THR:HG22 | 2.34 | 0.42 |
| 22:BA:2838:G:C6 | 22:BA:2839:G:C5 | 3.08 | 0.42 |
| 22:BA:2885:G:H2' | 22:BA:2886:A:H5' | 2.02 | 0.42 |
| 30:BI:125:MET:HA | 30:BI:128:SER:HB3 | 2.02 | 0.42 |
| 32:BK:64:ARG:HB2 | 32:BK:83:ALA:HB3 | 2.01 | 0.42 |
| 34:BM:132:THR:HG22 | 34:BM:133:LYS:N | 2.34 | 0.42 |
| 40:BS:59:GLU:HA | 40:BS:64:ALA:CB | 2.50 | 0.42 |
| 45:BX:41:GLU:OE2 | 45:BX:44:LYS:NZ | 2.47 | 0.42 |
| 47:BZ:24:LEU:HD11 | 47:BZ:54:MET:CE | 2.49 | 0.42 |
| 49:B1:17:THR:CG2 | 49:B1:43:VAL:HG13 | 2.49 | 0.42 |
| 1:CA:207:C:O2 | 1:CA:207:C:H2' | 2.20 | 0.42 |
| 1:CA:375:U:O3' | 16:CP:6:LEU:HB2 | 2.20 | 0.42 |
| 1:CA:780:A:H1' | 1:CA:803:G:N2 | 2.34 | 0.42 |
| 1:CA:1049:U:H4' | 1:CA:1050:G:O5' | 2.19 | 0.42 |
| 2:CB:118:GLU:HA | 2:CB:121:SER:OG | 2.20 | 0.42 |
| 4:CD:130:VAL:HG11 | 4:CD:135:TYR:CG | 2.55 | 0.42 |
| 11:CK:127:ARG:HB2 | 21:CU:34:ARG:NH1 | 2.34 | 0.42 |
| 15:CO:37:ASN:O | 15:CO:40:GLN:CB | 2.68 | 0.42 |
| 17:CQ:49:GLU:C | 17:CQ:50:ASN:CG | 2.77 | 0.42 |
| 19:CS:44:MET:O | 19:CS:45:ILE:C | 2.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:77:G:H2' | 22:DA:78:U:O4' | 2.19 | 0.42 |
| 22:DA:485:C:H2' | 22:DA:486:C:O4' | 2.18 | 0.42 |
| 22:DA:751:A:C6 | 22:DA:789:A:C5 | 3.08 | 0.42 |
| 22:DA:841:G:H2' | 22:DA:842:U:O4' | 2.20 | 0.42 |
| 22:DA:1003:G:O2' | 22:DA:1010:A:N1 | 2.40 | 0.42 |
| 22:DA:1026:G:H1' | 22:DA:1134:A:C2 | 2.53 | 0.42 |
| 22:DA:1085:A:H2' | 22:DA:1086:A:C4 | 2.54 | 0.42 |
| 22:DA:1255:U:H2' | 22:DA:1256:G:OP1 | 2.20 | 0.42 |
| 22:DA:1265:A:N1 | 22:DA:2013:A:H5'' | 2.34 | 0.42 |
| 22:DA:1386:C:H2' | 22:DA:1387:A:C8 | 2.55 | 0.42 |
| 22:DA:1519:G:N3 | 22:DA:1519:G:H2' | 2.33 | 0.42 |
| 22:DA:1525:A:C6 | 22:DA:1526:C:C4 | 3.07 | 0.42 |
| 22:DA:1668:A:H4' | 22:DA:1669:A:O5' | 2.19 | 0.42 |
| 22:DA:1829:A:HO2' | 24:DC:15:HIS:CD2 | 2.37 | 0.42 |
| 22:DA:2116:G:C6 | 22:DA:2171:A:N6 | 2.87 | 0.42 |
| 22:DA:2291:U:O2' | 22:DA:2292:U:H5' | 2.19 | 0.42 |
| 22:DA:2397:G:N3 | 22:DA:2397:G:H2' | 2.35 | 0.42 |
| 22:DA:2480:C:N4 | 22:DA:2481:G:C6 | 2.87 | 0.42 |
| 23:DB:26:C:C5 | 23:DB:27:C:C4 | 3.08 | 0.42 |
| 24:DC:62:TYR:CD1 | 24:DC:63:ARG:N | 2.86 | 0.42 |
| 26:DE:152:GLU:O | 26:DE:154:ASP:N | 2.52 | 0.42 |
| 27:DF:117:LEU:HG | 27:DF:130:MET:SD | 2.58 | 0.42 |
| 27:DF:131:GLY:HA2 | 27:DF:153:ASP:HA | 2.00 | 0.42 |
| 30:DI:56:PRO:HD2 | 30:DI:75:PRO:HD3 | 2.01 | 0.42 |
| 32:DK:31:ARG:CB | 32:DK:32:TYR:CE2 | 3.02 | 0.42 |
| 33:DL:77:ILE:HG23 | 33:DL:81:ASP:OD2 | 2.20 | 0.42 |
| 34:DM:17:ASN:O | 34:DM:38:ARG:HD3 | 2.19 | 0.42 |
| 42:DU:33:LYS:HB3 | 42:DU:64:ALA:HB1 | 2.01 | 0.42 |
| 46:DY:27:ASN:O | 46:DY:31:GLN:HB2 | 2.19 | 0.42 |
| 1:AA:200:G:N2 | 1:AA:218:U:C2 | 2.87 | 0.42 |
| 1:AA:666:G:C6 | 1:AA:741:G:C6 | 3.07 | 0.42 |
| 1:AA:925:G:C2 | 1:AA:927:G:C8 | 3.07 | 0.42 |
| 1:AA:1031:C:O2' | 1:AA:1032:G:P | 2.77 | 0.42 |
| 1:AA:1074:G:O2' | 1:AA:1101:A:N1 | 2.46 | 0.42 |
| 5:AE:115:LEU:CD2 | 5:AE:123:VAL:HG21 | 2.49 | 0.42 |
| 9:AI:30:ILE:HG22 | 9:AI:65:ILE:CD1 | 2.49 | 0.42 |
| 10:AJ:11:LYS:HA | 10:AJ:70:HIS:O | 2.20 | 0.42 |
| 10:AJ:17:LEU:HD21 | 10:AJ:96:VAL:HG22 | 2.01 | 0.42 |
| 12:AL:106:GLY:HA3 | 12:AL:118:GLY:O | 2.19 | 0.42 |
| 22:BA:37:C:H4' | 22:BA:451:U:OP1 | 2.19 | 0.42 |
| 22:BA:144:A:C6 | 22:BA:145:C:C4 | 3.06 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:555:G:HO2' | 22:BA:556:A:P | 2.38 | 0.42 |
| 22:BA:1059:G:C5 | 22:BA:1080:A:C2 | 3.07 | 0.42 |
| 22:BA:1075:C:H2' | 22:BA:1076:C:N1 | 2.35 | 0.42 |
| 22:BA:1848:A:C2' | 22:BA:1849:G:O5' | 2.67 | 0.42 |
| 22:BA:2275:C:O2 | 34:BM:84:LYS:HD3 | 2.20 | 0.42 |
| 22:BA:2804:U:H2' | 22:BA:2805:C:H6 | 1.84 | 0.42 |
| 22:BA:2805:C:C4 | 22:BA:2806:C:C4 | 3.08 | 0.42 |
| 23:BB:17:C:H2' | 23:BB:18:G:O4' | 2.19 | 0.42 |
| 23:BB:78:A:H2' | 23:BB:79:G:O4' | 2.19 | 0.42 |
| 24:BC:21:ASN:C | 24:BC:21:ASN:OD1 | 2.56 | 0.42 |
| 24:BC:174:LEU:N | 24:BC:174:LEU:CD1 | 2.83 | 0.42 |
| 27:BF:28:VAL:O | 27:BF:28:VAL:CG1 | 2.68 | 0.42 |
| 28:BG:11:VAL:O | 28:BG:11:VAL:HG22 | 2.19 | 0.42 |
| 28:BG:40:ALA:CB | 28:BG:58:TYR:HB3 | 2.49 | 0.42 |
| 28:BG:174:ALA:O | 28:BG:175:LYS:HB2 | 2.20 | 0.42 |
| 29:BH:45:GLU:C | 29:BH:47:PHE:N | 2.72 | 0.42 |
| 30:BI:22:PRO:HB2 | 30:BI:23:PRO:HD3 | 2.01 | 0.42 |
| 42:BU:48:PRO:CB | 42:BU:54:GLN:O | 2.67 | 0.42 |
| 44:BW:40:GLN:OE1 | 44:BW:44:LYS:N | 2.52 | 0.42 |
| 44:BW:41:ARG:HH11 | 44:BW:41:ARG:HG3 | 1.84 | 0.42 |
| 44:BW:75:LYS:O | 44:BW:76:ASN:HB2 | 2.18 | 0.42 |
| 48:B0:10:ARG:HB2 | 48:B0:13:ARG:NH2 | 2.34 | 0.42 |
| 1:CA:64:G:H4' | 1:CA:65:A:O5' | 2.18 | 0.42 |
| 1:CA:428:G:OP2 | 4:CD:10:LYS:HE3 | 2.20 | 0.42 |
| 1:CA:1149:C:N4 | 1:CA:1150:A:C6 | 2.87 | 0.42 |
| 1:CA:1489:G:C5 | 1:CA:1490:U:C5 | 3.08 | 0.42 |
| 2:CB:25:PRO:O | 2:CB:28:LYS:HB2 | 2.19 | 0.42 |
| 2:CB:55:ALA:O | 2:CB:59:LYS:HB2 | 2.20 | 0.42 |
| 2:CB:71:GLY:O | 2:CB:93:ASN:HA | 2.19 | 0.42 |
| 4:CD:198:HIS:CE1 | 4:CD:199:LEU:HD21 | 2.54 | 0.42 |
| 6:CF:80:PHE:O | 6:CF:80:PHE:CD2 | 2.72 | 0.42 |
| 7:CG:51:ALA:HB2 | 7:CG:58:GLU:HA | 2.01 | 0.42 |
| 9:CI:49:ARG:NH2 | 9:CI:52:LEU:O | 2.53 | 0.42 |
| 11:CK:25:ALA:O | 11:CK:89:PRO:O | 2.37 | 0.42 |
| 11:CK:60:PRO:HD3 | 11:CK:91:PRO:HB3 | 2.00 | 0.42 |
| 14:CN:93:ILE:HG21 | 14:CN:96:LEU:HD22 | 2.02 | 0.42 |
| 16:CP:21:VAL:HG23 | 16:CP:36:VAL:HG21 | 2.02 | 0.42 |
| 17:CQ:19:LYS:HD3 | 17:CQ:49:GLU:HA | 2.01 | 0.42 |
| 19:CS:40:ILE:HG21 | 19:CS:66:MET:HB3 | 2.01 | 0.42 |
| 22:DA:7:G:H4' | 31:DJ:15:TRP:HH2 | 1.85 | 0.42 |
| 22:DA:219:A:C6 | 22:DA:220:G:C6 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:232:G:N2 | 22:DA:420:C:OP1 | 2.52 | 0.42 |
| 22:DA:322:A:O4' | 22:DA:340:A:H1' | 2.20 | 0.42 |
| 22:DA:675:A:N3 | 22:DA:2443:C:O2' | 2.43 | 0.42 |
| 22:DA:695:G:C6 | 22:DA:768:G:C5 | 3.08 | 0.42 |
| 22:DA:705:A:C2 | 22:DA:727:A:O4' | 2.72 | 0.42 |
| 22:DA:848:C:O2 | 22:DA:933:A:C2 | 2.72 | 0.42 |
| 22:DA:1036:G:C6 | 22:DA:1120:G:C5 | 3.08 | 0.42 |
| 22:DA:1154:G:OP1 | 38:DQ:58:ARG:HD3 | 2.20 | 0.42 |
| 22:DA:1248:G:C5 | 38:DQ:3:ARG:HB2 | 2.55 | 0.42 |
| 22:DA:1277:G:H2' | 22:DA:1278:C:O4' | 2.19 | 0.42 |
| 22:DA:1310:G:H1' | 22:DA:1611:C:C5' | 2.49 | 0.42 |
| 22:DA:1350:C:O2 | 22:DA:1382:G:N3 | 2.53 | 0.42 |
| 22:DA:1400:U:H2' | 22:DA:1401:G:O4' | 2.20 | 0.42 |
| 22:DA:2059:A:C2 | 54:D6:5:MHU:HD1 | 2.53 | 0.42 |
| 22:DA:2108:A:H2' | 22:DA:2109:U:H5' | 2.01 | 0.42 |
| 22:DA:2114:A:C4 | 22:DA:2167:U:H4' | 2.54 | 0.42 |
| 22:DA:2410:G:C2 | 22:DA:2411:A:H1' | 2.54 | 0.42 |
| 22:DA:2428:G:H5'' | 22:DA:2429:G:P | 2.59 | 0.42 |
| 22:DA:2825:G:H2' | 22:DA:2826:A:H5' | 2.02 | 0.42 |
| 24:DC:130:LEU:HD11 | 24:DC:135:ILE:HG12 | 2.01 | 0.42 |
| 25:DD:60:VAL:HG13 | 25:DD:60:VAL:O | 2.19 | 0.42 |
| 25:DD:107:VAL:HB | 25:DD:204:LYS:O | 2.18 | 0.42 |
| 26:DE:40:ARG:NH2 | 26:DE:92:HIS:CE1 | 2.87 | 0.42 |
| 31:DJ:25:LEU:HA | 31:DJ:62:VAL:HG21 | 2.02 | 0.42 |
| 32:DK:56:ASP:OD2 | 32:DK:56:ASP:N | 2.53 | 0.42 |
| 35:DN:95:THR:HG23 | 35:DN:96:ARG:N | 2.34 | 0.42 |
| 42:DU:59:VAL:HG12 | 42:DU:61:LYS:HB2 | 2.00 | 0.42 |
| 1:AA:73:C:O2' | 1:AA:74:A:P | 2.77 | 0.42 |
| 1:AA:444:G:N1 | 1:AA:445:G:C5 | 2.87 | 0.42 |
| 1:AA:499:A:H4' | 1:AA:500:G:OP1 | 2.20 | 0.42 |
| 1:AA:695:A:N1 | 1:AA:696:A:C2 | 2.87 | 0.42 |
| 1:AA:945:G:H2' | 1:AA:945:G:N3 | 2.34 | 0.42 |
| 1:AA:986:U:C2 | 1:AA:987:G:C8 | 3.07 | 0.42 |
| 1:AA:1109:C:P | 3:AC:176:HIS:CE1 | 3.13 | 0.42 |
| 1:AA:1141:C:C2 | 1:AA:1142:G:C8 | 3.07 | 0.42 |
| 1:AA:1157:A:C4 | 1:AA:1181:G:C6 | 3.08 | 0.42 |
| 1:AA:1160:G:O2' | 1:AA:1161:C:O5' | 2.35 | 0.42 |
| 1:AA:1375:A:C6 | 1:AA:1376:U:C4 | 3.08 | 0.42 |
| 2:AB:112:LYS:O | 2:AB:116:ASP:HB2 | 2.20 | 0.42 |
| 2:AB:184:PHE:CE1 | 2:AB:198:PHE:CD2 | 3.07 | 0.42 |
| 4:AD:53:VAL:CG2 | 4:AD:54:GLN:N | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AD:58:LYS:HG2 | 4:AD:203:LEU:HD22 | 2.01 | 0.42 |
| 4:AD:147:GLU:O | 4:AD:150:LYS:N | 2.53 | 0.42 |
| 12:AL:46:ASN:ND2 | 12:AL:89:ASP:OD1 | 2.51 | 0.42 |
| 17:AQ:17:MET:HG2 | 17:AQ:20:SER:HB3 | 2.02 | 0.42 |
| 17:AQ:50:ASN:O | 17:AQ:51:ASN:O | 2.36 | 0.42 |
| 17:AQ:59:VAL:HG23 | 17:AQ:77:ARG:O | 2.20 | 0.42 |
| 19:AS:64:ASP:HB3 | 27:BF:115:ARG:NH2 | 2.34 | 0.42 |
| 20:AT:8:LYS:O | 20:AT:11:ALA:HB3 | 2.19 | 0.42 |
| 21:AU:53:VAL:O | 21:AU:54:LYS:HB2 | 2.18 | 0.42 |
| 22:BA:872:U:H2' | 22:BA:873:C:C6 | 2.54 | 0.42 |
| 22:BA:934:U:H2' | 22:BA:935:C:H6 | 1.85 | 0.42 |
| 22:BA:1380:G:N2 | 22:BA:1570:A:N1 | 2.65 | 0.42 |
| 22:BA:1923:U:H2' | 22:BA:1923:U:O2 | 2.19 | 0.42 |
| 22:BA:2602:A:H4' | 22:BA:2603:G:OP2 | 2.18 | 0.42 |
| 22:BA:2727:A:C2' | 22:BA:2728:U:H5' | 2.50 | 0.42 |
| 23:BB:2:G:C6 | 23:BB:119:A:C2 | 3.08 | 0.42 |
| 23:BB:101:A:H2' | 23:BB:102:G:O4' | 2.20 | 0.42 |
| 24:BC:142:HIS:CD2 | 24:BC:142:HIS:C | 2.93 | 0.42 |
| 27:BF:134:GLU:HG2 | 27:BF:136:ILE:HD12 | 2.00 | 0.42 |
| 29:BH:114:GLU:CB | 29:BH:133:GLN:O | 2.66 | 0.42 |
| 31:BJ:77:HIS:CD2 | 31:BJ:79:GLY:H | 2.38 | 0.42 |
| 38:BQ:62:ILE:HG23 | 38:BQ:76:TYR:CE1 | 2.54 | 0.42 |
| 45:BX:71:LEU:HB3 | 45:BX:76:GLU:O | 2.19 | 0.42 |
| 48:B0:25:VAL:HG13 | 48:B0:26:THR:N | 2.34 | 0.42 |
| 53:B5:67:HIS:CD2 | 53:B5:69:LEU:HD23 | 2.54 | 0.42 |
| 1:CA:209:U:O2 | 1:CA:209:U:H2' | 2.18 | 0.42 |
| 1:CA:784:A:C2 | 1:CA:785:G:C4 | 3.07 | 0.42 |
| 1:CA:853:C:H2' | 1:CA:854:U:O4' | 2.20 | 0.42 |
| 1:CA:1321:U:C4 | 1:CA:1322:C:H5 | 2.37 | 0.42 |
| 1:CA:1459:G:H2' | 1:CA:1460:C:O4' | 2.20 | 0.42 |
| 2:CB:32:PHE:N | 2:CB:40:ILE:O | 2.45 | 0.42 |
| 4:CD:5:LEU:CD1 | 4:CD:5:LEU:N | 2.82 | 0.42 |
| 4:CD:30:THR:O | 4:CD:31:LYS:HD3 | 2.19 | 0.42 |
| 4:CD:42:GLY:C | 4:CD:44:ARG:H | 2.23 | 0.42 |
| 7:CG:43:VAL:HG12 | 7:CG:44:TYR:CD1 | 2.54 | 0.42 |
| 7:CG:51:ALA:HB1 | 7:CG:57:SER:O | 2.20 | 0.42 |
| 8:CH:83:LEU:HD22 | 8:CH:83:LEU:C | 2.40 | 0.42 |
| 8:CH:105:SER:O | 8:CH:123:GLY:HA3 | 2.20 | 0.42 |
| 9:CI:114:LYS:HG3 | 9:CI:120:LYS:HA | 2.01 | 0.42 |
| 9:CI:116:VAL:CG2 | 10:CJ:60:ASP:O | 2.68 | 0.42 |
| 10:CJ:83:THR:O | 10:CJ:83:THR:HG23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CK:107:ILE:HG23 | 11:CK:107:ILE:O | 2.18 | 0.42 |
| 13:CM:37:ALA:CB | 13:CM:56:LEU:HG | 2.48 | 0.42 |
| 21:CU:36:GLU:O | 21:CU:37:PHE:HB2 | 2.19 | 0.42 |
| 22:DA:24:G:C6 | 22:DA:25:U:C4 | 3.07 | 0.42 |
| 22:DA:237:C:N4 | 22:DA:238:C:C5 | 2.88 | 0.42 |
| 22:DA:298:G:N2 | 22:DA:341:C:C4 | 2.87 | 0.42 |
| 22:DA:450:G:H2' | 22:DA:451:U:H5'' | 2.02 | 0.42 |
| 22:DA:1043:C:C5 | 22:DA:1044:C:C5 | 3.07 | 0.42 |
| 22:DA:1163:G:C2 | 22:DA:1164:C:C5 | 3.08 | 0.42 |
| 22:DA:1262:A:C6 | 22:DA:1263:U:C2 | 3.07 | 0.42 |
| 22:DA:1358:G:O6 | 22:DA:1371:G:C8 | 2.72 | 0.42 |
| 22:DA:2079:U:C2' | 22:DA:2080:A:O4' | 2.66 | 0.42 |
| 22:DA:2191:A:C6 | 22:DA:2192:U:C4 | 3.07 | 0.42 |
| 22:DA:2511:U:C5 | 22:DA:2512:C:C5 | 3.08 | 0.42 |
| 22:DA:2722:G:H4' | 35:DN:4:ARG:HB2 | 2.00 | 0.42 |
| 22:DA:2834:G:O6 | 22:DA:2879:A:C2' | 2.66 | 0.42 |
| 25:DD:15:PHE:CE2 | 37:DP:78:SER:HA | 2.55 | 0.42 |
| 25:DD:122:VAL:HG21 | 25:DD:141:ARG:HB3 | 2.01 | 0.42 |
| 25:DD:177:VAL:CG2 | 25:DD:187:LEU:HD11 | 2.49 | 0.42 |
| 26:DE:8:ALA:HB2 | 26:DE:122:GLU:CG | 2.49 | 0.42 |
| 26:DE:112:LEU:HD11 | 26:DE:180:LEU:O | 2.20 | 0.42 |
| 26:DE:170:ARG:NH2 | 26:DE:176:ASP:OD1 | 2.52 | 0.42 |
| 27:DF:17:MET:SD | 27:DF:22:TYR:HB2 | 2.60 | 0.42 |
| 29:DH:31:VAL:HG12 | 29:DH:32:PRO:HD3 | 2.02 | 0.42 |
| 29:DH:69:ALA:HB2 | 29:DH:138:VAL:HG12 | 2.02 | 0.42 |
| 29:DH:72:ILE:O | 29:DH:72:ILE:CG2 | 2.67 | 0.42 |
| 30:DI:8:TYR:HB2 | 30:DI:59:ILE:H | 1.85 | 0.42 |
| 39:DR:39:LEU:O | 39:DR:49:ILE:HG23 | 2.19 | 0.42 |
| 40:DS:29:VAL:CG1 | 40:DS:55:ILE:HD11 | 2.49 | 0.42 |
| 42:DU:96:PHE:CE1 | 42:DU:103:ILE:HG13 | 2.54 | 0.42 |
| 44:DW:67:VAL:HG12 | 44:DW:68:LYS:N | 2.35 | 0.42 |
| 1:AA:639:G:N3 | 1:AA:639:G:H2' | 2.34 | 0.42 |
| 1:AA:955:U:O4' | 1:AA:1227:A:N6 | 2.51 | 0.42 |
| 1:AA:1072:G:H2' | 1:AA:1073:U:C6 | 2.55 | 0.42 |
| 1:AA:1216:A:H2' | 1:AA:1217:C:C6 | 2.54 | 0.42 |
| 1:AA:1269:A:N1 | 1:AA:1313:U:O4' | 2.53 | 0.42 |
| 2:AB:222:ARG:HB3 | 2:AB:222:ARG:NH1 | 2.35 | 0.42 |
| 4:AD:121:LYS:HB3 | 4:AD:129:VAL:HG21 | 2.02 | 0.42 |
| 4:AD:190:ASP:O | 4:AD:191:LEU:HD12 | 2.18 | 0.42 |
| 17:AQ:26:GLU:OE2 | 17:AQ:39:LYS:HD3 | 2.20 | 0.42 |
| 22:BA:477:A:H2' | 22:BA:478:A:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:532:A:N3 | 22:BA:532:A:H2' | 2.35 | 0.42 |
| 22:BA:536:G:C2 | 22:BA:537:G:H1' | 2.55 | 0.42 |
| 22:BA:598:U:O2' | 22:BA:599:A:H5' | 2.20 | 0.42 |
| 22:BA:670:A:H4' | 22:BA:671:C:O5' | 2.20 | 0.42 |
| 22:BA:874:G:OP1 | 34:BM:62:LYS:NZ | 2.53 | 0.42 |
| 22:BA:1071:G:O4' | 22:BA:1089:A:N7 | 2.52 | 0.42 |
| 22:BA:1458:U:H5' | 22:BA:1459:G:N3 | 2.35 | 0.42 |
| 22:BA:2187:U:H2' | 22:BA:2188:U:H1' | 2.00 | 0.42 |
| 22:BA:2371:G:C2 | 22:BA:2372:U:C6 | 3.07 | 0.42 |
| 22:BA:2543:G:H2' | 22:BA:2544:G:O4' | 2.20 | 0.42 |
| 56:BA:3001:DOL:C37 | 56:BA:3001:DOL:C29 | 2.98 | 0.42 |
| 25:BD:177:VAL:O | 25:BD:177:VAL:CG2 | 2.67 | 0.42 |
| 26:BE:79:ARG:CG | 26:BE:79:ARG:NH1 | 2.83 | 0.42 |
| 32:BK:107:LEU:C | 32:BK:109:SER:N | 2.72 | 0.42 |
| 34:BM:132:THR:HG22 | 34:BM:133:LYS:O | 2.20 | 0.42 |
| 35:BN:24:MET:HG2 | 35:BN:44:LEU:HD13 | 2.01 | 0.42 |
| 39:BR:79:ARG:O | 39:BR:80:ARG:HB3 | 2.20 | 0.42 |
| 41:BT:47:VAL:CG1 | 41:BT:55:VAL:CG2 | 2.98 | 0.42 |
| 41:BT:88:LYS:O | 41:BT:89:GLU:CG | 2.68 | 0.42 |
| 41:BT:91:GLN:HG3 | 41:BT:91:GLN:O | 2.19 | 0.42 |
| 1:CA:68:G:C5 | 1:CA:69:G:H1' | 2.55 | 0.42 |
| 1:CA:754:C:OP1 | 15:CO:72:ARG:NH2 | 2.53 | 0.42 |
| 1:CA:756:C:C2 | 1:CA:757:U:C6 | 3.07 | 0.42 |
| 1:CA:1107:C:C4 | 1:CA:1108:G:N7 | 2.87 | 0.42 |
| 1:CA:1124:G:C2' | 1:CA:1145:A:H62 | 2.32 | 0.42 |
| 4:CD:192:SER:HB2 | 4:CD:195:ILE:HG12 | 2.00 | 0.42 |
| 6:CF:64:VAL:HG12 | 6:CF:65:GLU:H | 1.84 | 0.42 |
| 6:CF:97:THR:O | 6:CF:98:GLU:CG | 2.68 | 0.42 |
| 8:CH:95:VAL:O | 8:CH:99:LEU:O | 2.38 | 0.42 |
| 9:CI:49:ARG:C | 9:CI:51:PRO:HD2 | 2.39 | 0.42 |
| 9:CI:88:MET:HA | 9:CI:92:GLU:OE2 | 2.19 | 0.42 |
| 10:CJ:5:ARG:O | 10:CJ:102:LEU:CD1 | 2.68 | 0.42 |
| 11:CK:124:PRO:O | 21:CU:35:ARG:N | 2.48 | 0.42 |
| 13:CM:3:ARG:HA | 13:CM:8:ASN:O | 2.19 | 0.42 |
| 13:CM:20:THR:HG23 | 13:CM:26:GLY:O | 2.19 | 0.42 |
| 14:CN:67:THR:HG23 | 14:CN:83:LYS:CE | 2.50 | 0.42 |
| 22:DA:42:A:C2 | 22:DA:438:G:C2 | 3.07 | 0.42 |
| 22:DA:80:G:O2' | 22:DA:346:A:C8 | 2.67 | 0.42 |
| 22:DA:192:C:P | 58:DA:3739:HOH:O | 2.75 | 0.42 |
| 22:DA:479:A:N3 | 22:DA:481:G:H5'' | 2.35 | 0.42 |
| 22:DA:481:G:C2 | 22:DA:507:A:C4 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:669:G:C2 | 22:DA:801:G:C6 | 3.08 | 0.42 |
| 22:DA:669:G:N3 | 22:DA:801:G:C2 | 2.88 | 0.42 |
| 22:DA:826:U:H2' | 22:DA:828:U:O4' | 2.18 | 0.42 |
| 22:DA:1428:C:C5 | 22:DA:1569:A:C5' | 3.03 | 0.42 |
| 22:DA:1439:A:C8 | 22:DA:1440:U:C5 | 3.08 | 0.42 |
| 22:DA:1601:G:C5 | 22:DA:1602:U:C4 | 3.08 | 0.42 |
| 22:DA:1668:A:N3 | 22:DA:1670:C:C4 | 2.88 | 0.42 |
| 22:DA:1833:C:N3 | 22:DA:1834:U:C4 | 2.87 | 0.42 |
| 22:DA:1867:G:O6 | 22:DA:1875:G:N2 | 2.52 | 0.42 |
| 22:DA:2093:G:N7 | 22:DA:2225:A:H2' | 2.35 | 0.42 |
| 22:DA:2217:G:C6 | 22:DA:2218:G:C5 | 3.08 | 0.42 |
| 22:DA:2583:G:H2' | 22:DA:2584:U:O4' | 2.19 | 0.42 |
| 22:DA:2599:G:C8 | 24:DC:236:GLU:HB2 | 2.55 | 0.42 |
| 22:DA:2807:U:H1' | 22:DA:2892:G:N2 | 2.34 | 0.42 |
| 22:DA:2837:A:H2' | 22:DA:2838:G:O4' | 2.20 | 0.42 |
| 22:DA:2883:A:P | 48:D0:49:TYR:HH | 2.41 | 0.42 |
| 23:DB:92:C:H2' | 23:DB:93:C:C6 | 2.54 | 0.42 |
| 25:DD:62:LYS:N | 25:DD:63:PRO:CD | 2.82 | 0.42 |
| 25:DD:186:LEU:HD11 | 37:DP:8:LEU:HD12 | 2.02 | 0.42 |
| 28:DG:52:PHE:CE2 | 28:DG:69:ARG:HA | 2.54 | 0.42 |
| 29:DH:41:LYS:HE2 | 29:DH:44:ILE:CD1 | 2.50 | 0.42 |
| 31:DJ:41:LYS:HD2 | 31:DJ:50:THR:O | 2.19 | 0.42 |
| 33:DL:29:LYS:O | 33:DL:30:THR:CB | 2.67 | 0.42 |
| 33:DL:77:ILE:HG22 | 33:DL:78:ARG:N | 2.34 | 0.42 |
| 33:DL:90:VAL:O | 33:DL:123:ARG:N | 2.50 | 0.42 |
| 35:DN:51:LEU:N | 35:DN:51:LEU:HD23 | 2.34 | 0.42 |
| 42:DU:49:VAL:HG13 | 42:DU:53:ASN:O | 2.20 | 0.42 |
| 44:DW:37:ILE:HG22 | 44:DW:38:VAL:CG2 | 2.49 | 0.42 |
| 45:DX:54:LYS:CA | 45:DX:57:ARG:HB2 | 2.50 | 0.42 |
| 50:D2:10:LEU:HD11 | 50:D2:14:ARG:NH1 | 2.35 | 0.42 |
| 1:AA:79:G:N2 | 1:AA:91:U:C4 | 2.88 | 0.42 |
| 1:AA:695:A:H2' | 1:AA:696:A:O4' | 2.20 | 0.42 |
| 1:AA:1081:A:OP1 | 5:AE:21:VAL:HG23 | 2.19 | 0.42 |
| 1:AA:1173:U:H2' | 1:AA:1174:G:C8 | 2.55 | 0.42 |
| 1:AA:1307:U:H2' | 1:AA:1308:U:H6 | 1.85 | 0.42 |
| 1:AA:1370:G:C2 | 1:AA:1371:G:C8 | 3.08 | 0.42 |
| 2:AB:41:ILE:N | 2:AB:41:ILE:CD1 | 2.83 | 0.42 |
| 3:AC:112:ASP:O | 3:AC:116:VAL:HG23 | 2.20 | 0.42 |
| 4:AD:17:THR:HG22 | 4:AD:18:ASP:N | 2.32 | 0.42 |
| 4:AD:171:LEU:C | 4:AD:171:LEU:HD12 | 2.40 | 0.42 |
| 8:AH:78:VAL:HG11 | 8:AH:125:ILE:HD11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:AK:128:ARG:HG2 | 11:AK:128:ARG:NH1 | 2.32 | 0.42 |
| 12:AL:50:ARG:HG3 | 12:AL:90:LEU:HD11 | 2.02 | 0.42 |
| 14:AN:46:LEU:HG | 14:AN:47:LYS:N | 2.34 | 0.42 |
| 14:AN:50:THR:O | 14:AN:50:THR:OG1 | 2.34 | 0.42 |
| 17:AQ:81:LYS:N | 17:AQ:81:LYS:CD | 2.82 | 0.42 |
| 20:AT:54:MET:CE | 20:AT:58:VAL:CG2 | 2.98 | 0.42 |
| 22:BA:226:A:N6 | 22:BA:227:A:C6 | 2.88 | 0.42 |
| 22:BA:475:C:C5 | 22:BA:481:G:O6 | 2.73 | 0.42 |
| 22:BA:784:G:H5' | 24:BC:226:ASN:OD1 | 2.19 | 0.42 |
| 22:BA:859:G:O2' | 22:BA:860:U:P | 2.78 | 0.42 |
| 22:BA:1071:G:C4 | 22:BA:1089:A:C5 | 3.08 | 0.42 |
| 22:BA:1754:A:N6 | 22:BA:1755:A:N6 | 2.67 | 0.42 |
| 22:BA:1998:A:O3' | 22:BA:2724:U:H4' | 2.19 | 0.42 |
| 22:BA:2459:A:C5 | 22:BA:2460:U:C5 | 3.07 | 0.42 |
| 22:BA:2725:A:C4 | 22:BA:2727:A:C8 | 3.08 | 0.42 |
| 26:BE:149:ILE:HD12 | 26:BE:150:THR:O | 2.20 | 0.42 |
| 29:BH:89:LYS:O | 29:BH:90:LEU:C | 2.58 | 0.42 |
| 29:BH:116:ARG:HB3 | 29:BH:131:SER:O | 2.20 | 0.42 |
| 29:BH:118:PRO:O | 29:BH:119:ASN:CB | 2.68 | 0.42 |
| 31:BJ:62:VAL:HG22 | 31:BJ:63:ALA:N | 2.35 | 0.42 |
| 32:BK:21:CYS:HA | 32:BK:41:ILE:HG22 | 2.02 | 0.42 |
| 32:BK:108:ARG:O | 32:BK:109:SER:C | 2.57 | 0.42 |
| 33:BL:101:ILE:HG13 | 33:BL:102:GLY:N | 2.35 | 0.42 |
| 34:BM:11:LYS:HE2 | 34:BM:87:GLY:O | 2.19 | 0.42 |
| 38:BQ:83:LEU:HD22 | 38:BQ:88:VAL:HG11 | 2.02 | 0.42 |
| 1:CA:32:A:C2 | 1:CA:33:A:C6 | 3.07 | 0.42 |
| 1:CA:104:G:H4' | 1:CA:174:A:O4' | 2.19 | 0.42 |
| 1:CA:260:G:C6 | 1:CA:261:U:C4 | 3.08 | 0.42 |
| 1:CA:406:G:C2 | 1:CA:407:U:C5 | 3.08 | 0.42 |
| 1:CA:431:A:H2' | 1:CA:432:A:O4' | 2.20 | 0.42 |
| 1:CA:463:U:H5' | 1:CA:464:U:OP2 | 2.20 | 0.42 |
| 1:CA:632:U:H2' | 1:CA:633:G:OP1 | 2.20 | 0.42 |
| 1:CA:723:U:C5 | 21:CU:49:LYS:HB3 | 2.55 | 0.42 |
| 1:CA:857:C:H2' | 1:CA:858:G:O4' | 2.19 | 0.42 |
| 1:CA:993:G:H2' | 1:CA:995:C:N4 | 2.35 | 0.42 |
| 1:CA:1060:U:H5'' | 10:CJ:53:ILE:CG2 | 2.50 | 0.42 |
| 1:CA:1225:A:OP1 | 13:CM:101:ARG:HA | 2.19 | 0.42 |
| 1:CA:1493:A:H4' | 22:DA:1913:A:N1 | 2.35 | 0.42 |
| 3:CC:71:ALA:O | 3:CC:73:PRO:HD3 | 2.19 | 0.42 |
| 7:CG:37:SER:OG | 9:CI:43:THR:HG23 | 2.20 | 0.42 |
| 7:CG:57:SER:O | 7:CG:61:ALA:HB2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:CK:126:LYS:C | 21:CU:34:ARG:NH2 | 2.73 | 0.42 |
| 15:CO:89:ARG:NH1 | 22:DA:716:A:OP1 | 2.53 | 0.42 |
| 22:DA:110:G:H2' | 22:DA:110:G:N3 | 2.34 | 0.42 |
| 22:DA:135:U:H2' | 22:DA:136:G:C8 | 2.55 | 0.42 |
| 22:DA:447:A:C2 | 22:DA:454:A:H2' | 2.55 | 0.42 |
| 22:DA:972:A:N1 | 22:DA:973:A:C6 | 2.87 | 0.42 |
| 22:DA:1339:G:O4' | 22:DA:1393:A:C2 | 2.73 | 0.42 |
| 22:DA:1855:U:C6 | 22:DA:1856:U:C5 | 3.08 | 0.42 |
| 22:DA:1869:G:C2 | 22:DA:1873:G:C6 | 3.07 | 0.42 |
| 22:DA:2012:G:P | 40:DS:98:LYS:HZ2 | 2.42 | 0.42 |
| 22:DA:2204:G:C4 | 22:DA:2205:A:C8 | 3.08 | 0.42 |
| 22:DA:2345:G:C8 | 22:DA:2381:A:C2 | 3.08 | 0.42 |
| 22:DA:2347:C:C2 | 22:DA:2371:G:N2 | 2.87 | 0.42 |
| 22:DA:2357:G:H5' | 22:DA:2358:A:OP2 | 2.20 | 0.42 |
| 22:DA:2603:G:C5 | 22:DA:2604:U:C5 | 3.08 | 0.42 |
| 22:DA:2722:G:H2' | 22:DA:2723:C:O4' | 2.20 | 0.42 |
| 22:DA:2810:A:H2' | 22:DA:2811:G:O4' | 2.19 | 0.42 |
| 24:DC:18:LYS:O | 24:DC:19:VAL:HB | 2.19 | 0.42 |
| 24:DC:25:HIS:HB2 | 24:DC:80:ARG:HG3 | 2.00 | 0.42 |
| 25:DD:114:LYS:HE2 | 25:DD:196:ALA:CB | 2.50 | 0.42 |
| 28:DG:9:VAL:O | 28:DG:49:THR:HA | 2.20 | 0.42 |
| 30:DI:21:SER:HB3 | 30:DI:22:PRO:HD3 | 2.00 | 0.42 |
| 32:DK:113:MET:O | 32:DK:116:ILE:CG1 | 2.68 | 0.42 |
| 36:DO:111:ARG:NH2 | 36:DO:117:PHE:OXT | 2.52 | 0.42 |
| 38:DQ:11:ARG:O | 38:DQ:11:ARG:HG3 | 2.20 | 0.42 |
| 41:DT:65:GLY:O | 41:DT:66:LYS:C | 2.58 | 0.42 |
| 46:DY:16:THR:O | 46:DY:19:LEU:HB2 | 2.20 | 0.42 |
| 51:D3:31:HIS:CE1 | 51:D3:32:ILE:HD12 | 2.54 | 0.42 |
| 1:AA:22:G:C5 | 1:AA:23:C:C5 | 3.07 | 0.42 |
| 1:AA:137:U:H1' | 1:AA:227:G:N2 | 2.35 | 0.42 |
| 1:AA:760:G:C8 | 1:AA:761:G:C8 | 3.07 | 0.42 |
| 1:AA:1053:G:N7 | 1:AA:1200:C:H5'' | 2.35 | 0.42 |
| 1:AA:1119:C:OP1 | 9:AI:85:ARG:NH2 | 2.53 | 0.42 |
| 6:AF:55:HIS:O | 6:AF:56:LYS:HB2 | 2.19 | 0.42 |
| 6:AF:99:ALA:O | 6:AF:100:SER:HB2 | 2.20 | 0.42 |
| 9:AI:50:GLN:OE1 | 9:AI:80:ARG:NH1 | 2.53 | 0.42 |
| 11:AK:112:ASP:CB | 21:AU:20:LYS:HD2 | 2.49 | 0.42 |
| 15:AO:17:ARG:HB3 | 15:AO:18:ASP:H | 1.71 | 0.42 |
| 18:AR:71:THR:OG1 | 18:AR:73:ARG:HB2 | 2.19 | 0.42 |
| 22:BA:150:U:H2' | 22:BA:151:C:C6 | 2.55 | 0.42 |
| 22:BA:195:A:C5 | 22:BA:198:C:C5 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:340:A:H2' | 22:BA:341:C:O4' | 2.20 | 0.42 |
| 22:BA:983:A:C6 | 22:BA:984:A:N1 | 2.87 | 0.42 |
| 22:BA:1027:A:C5 | 22:BA:1126:A:C2 | 3.07 | 0.42 |
| 22:BA:1176:U:H3' | 22:BA:1177:G:C8 | 2.55 | 0.42 |
| 22:BA:1179:G:O6 | 22:BA:1180:U:C2 | 2.73 | 0.42 |
| 22:BA:1380:G:N3 | 22:BA:1380:G:H2' | 2.35 | 0.42 |
| 22:BA:1839:G:C4 | 22:BA:1840:G:C8 | 3.08 | 0.42 |
| 22:BA:1922:G:C6 | 22:BA:1923:U:C5 | 3.08 | 0.42 |
| 22:BA:2352:A:H2' | 22:BA:2353:G:H5' | 2.02 | 0.42 |
| 22:BA:2722:G:H2' | 22:BA:2723:C:C6 | 2.54 | 0.42 |
| 24:BC:14:ARG:HG2 | 24:BC:15:HIS:ND1 | 2.34 | 0.42 |
| 30:BI:99:GLY:C | 30:BI:100:LYS:HG2 | 2.40 | 0.42 |
| 31:BJ:98:GLU:CD | 31:BJ:126:ALA:HB2 | 2.39 | 0.42 |
| 32:BK:86:LEU:N | 32:BK:86:LEU:HD23 | 2.34 | 0.42 |
| 33:BL:82:LEU:HD21 | 33:BL:120:VAL:HG11 | 2.02 | 0.42 |
| 43:BV:92:VAL:O | 43:BV:92:VAL:HG12 | 2.20 | 0.42 |
| 45:BX:45:ARG:HG2 | 45:BX:46:PHE:N | 2.34 | 0.42 |
| 53:B5:64:SER:O | 53:B5:65:LEU:CB | 2.68 | 0.42 |
| 1:CA:6:G:O6 | 5:CE:100:SER:N | 2.52 | 0.42 |
| 1:CA:47:C:H4' | 1:CA:48:C:OP1 | 2.18 | 0.42 |
| 1:CA:49:U:O4 | 1:CA:362:G:N2 | 2.52 | 0.42 |
| 1:CA:112:G:H5' | 1:CA:389:A:O2' | 2.19 | 0.42 |
| 1:CA:182:A:C4 | 1:CA:184:G:C8 | 3.08 | 0.42 |
| 1:CA:213:G:C5 | 1:CA:214:C:C2 | 3.08 | 0.42 |
| 1:CA:268:U:H2' | 1:CA:269:C:H6 | 1.83 | 0.42 |
| 1:CA:411:A:C5 | 1:CA:429:U:C5 | 3.08 | 0.42 |
| 1:CA:518:C:H4' | 1:CA:519:C:O5' | 2.20 | 0.42 |
| 1:CA:716:A:N3 | 11:CK:120:GLY:HA2 | 2.35 | 0.42 |
| 1:CA:1012:A:C2 | 1:CA:1018:G:N2 | 2.88 | 0.42 |
| 1:CA:1055:A:C5 | 1:CA:1206:G:C6 | 3.08 | 0.42 |
| 1:CA:1158:C:O2 | 1:CA:1158:C:C2' | 2.67 | 0.42 |
| 1:CA:1259:C:C5 | 1:CA:1260:G:C8 | 3.08 | 0.42 |
| 3:CC:167:TRP:C | 3:CC:167:TRP:HE3 | 2.23 | 0.42 |
| 4:CD:188:ARG:HD2 | 4:CD:191:LEU:HD11 | 2.01 | 0.42 |
| 7:CG:14:PRO:O | 7:CG:15:ASP:C | 2.58 | 0.42 |
| 7:CG:136:LYS:O | 7:CG:136:LYS:CG | 2.68 | 0.42 |
| 7:CG:145:ALA:O | 7:CG:146:GLU:HB2 | 2.18 | 0.42 |
| 8:CH:11:LEU:HD22 | 8:CH:75:ILE:HD11 | 2.02 | 0.42 |
| 11:CK:97:ILE:HG13 | 11:CK:98:ARG:N | 2.33 | 0.42 |
| 12:CL:64:THR:HG23 | 12:CL:93:VAL:HA | 2.02 | 0.42 |
| 21:CU:15:ALA:O | 21:CU:17:ARG:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:9:G:C6 | 22:DA:2629:U:C6 | 3.07 | 0.42 |
| 22:DA:483:A:C1' | 42:DU:45:HIS:HB2 | 2.50 | 0.42 |
| 22:DA:538:A:O2' | 31:DJ:8:PRO:HG3 | 2.19 | 0.42 |
| 22:DA:600:G:H2' | 22:DA:601:C:C6 | 2.55 | 0.42 |
| 22:DA:892:A:N3 | 22:DA:892:A:C2' | 2.82 | 0.42 |
| 22:DA:1511:G:O2' | 22:DA:1512:C:H5' | 2.19 | 0.42 |
| 22:DA:1525:A:H2' | 22:DA:1526:C:O4' | 2.20 | 0.42 |
| 22:DA:1607:C:O2 | 22:DA:1621:U:C5 | 2.72 | 0.42 |
| 22:DA:1989:G:H2' | 22:DA:1990:C:H5' | 2.02 | 0.42 |
| 22:DA:2127:G:O2' | 22:DA:2173:A:C4 | 2.72 | 0.42 |
| 22:DA:2230:G:C5 | 22:DA:2231:U:C4 | 3.08 | 0.42 |
| 22:DA:2333:A:C8 | 22:DA:2335:A:C4 | 3.07 | 0.42 |
| 22:DA:2691:C:N3 | 22:DA:2718:G:O6 | 2.53 | 0.42 |
| 23:DB:109:A:C6 | 23:DB:110:C:N3 | 2.88 | 0.42 |
| 25:DD:146:ILE:O | 25:DD:146:ILE:HG13 | 2.20 | 0.42 |
| 28:DG:174:ALA:O | 28:DG:175:LYS:O | 2.37 | 0.42 |
| 29:DH:121:VAL:O | 29:DH:122:LEU:CB | 2.67 | 0.42 |
| 29:DH:127:GLU:HA | 29:DH:144:VAL:O | 2.19 | 0.42 |
| 33:DL:135:ILE:HG22 | 33:DL:140:GLY:CA | 2.49 | 0.42 |
| 35:DN:71:ARG:HH21 | 35:DN:71:ARG:HG2 | 1.82 | 0.42 |
| 39:DR:11:GLN:NE2 | 39:DR:39:LEU:CD2 | 2.82 | 0.42 |
| 40:DS:66:ILE:O | 40:DS:69:LEU:HB2 | 2.20 | 0.42 |
| 41:DT:93:LEU:N | 41:DT:93:LEU:HD22 | 2.34 | 0.42 |
| 43:DV:51:GLN:HB3 | 43:DV:56:PHE:CD2 | 2.55 | 0.42 |
| 45:DX:40:VAL:CG1 | 45:DX:68:LEU:CD1 | 2.97 | 0.42 |
| 45:DX:71:LEU:HA | 45:DX:74:ARG:CG | 2.50 | 0.42 |
| 47:DZ:52:SER:O | 47:DZ:55:VAL:N | 2.52 | 0.42 |
| 49:D1:11:LEU:HB2 | 49:D1:21:TYR:HB2 | 2.02 | 0.42 |
| 1:AA:223:A:C6 | 1:AA:224:U:O4 | 2.72 | 0.42 |
| 1:AA:230:G:C5 | 1:AA:231:U:C5 | 3.08 | 0.42 |
| 1:AA:614:C:C2' | 1:AA:615:G:O5' | 2.67 | 0.42 |
| 1:AA:657:U:O2 | 15:AO:22:THR:HG22 | 2.19 | 0.42 |
| 1:AA:1067:A:N3 | 1:AA:1068:G:H1' | 2.35 | 0.42 |
| 1:AA:1139:G:N2 | 1:AA:1141:C:C5 | 2.88 | 0.42 |
| 1:AA:1141:C:HO2' | 1:AA:1142:G:P | 2.43 | 0.42 |
| 1:AA:1263:C:H2' | 1:AA:1264:U:C6 | 2.55 | 0.42 |
| 2:AB:118:GLU:O | 2:AB:121:SER:CB | 2.67 | 0.42 |
| 3:AC:155:GLY:N | 3:AC:164:ARG:O | 2.51 | 0.42 |
| 4:AD:34:ILE:O | 4:AD:34:ILE:HD13 | 2.20 | 0.42 |
| 4:AD:98:LEU:O | 4:AD:101:VAL:N | 2.53 | 0.42 |
| 10:AJ:33:GLY:HA3 | 10:AJ:83:THR:OG1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:AK:65:VAL:O | 11:AK:65:VAL:HG23 | 2.20 | 0.42 |
| 11:AK:112:ASP:OD1 | 11:AK:114:THR:HG23 | 2.19 | 0.42 |
| 12:AL:3:THR:HG22 | 12:AL:4:VAL:N | 2.35 | 0.42 |
| 14:AN:25:ALA:C | 14:AN:27:LEU:N | 2.73 | 0.42 |
| 14:AN:84:VAL:HG12 | 14:AN:85:ARG:N | 2.34 | 0.42 |
| 17:AQ:16:LYS:C | 17:AQ:17:MET:CE | 2.88 | 0.42 |
| 17:AQ:82:ALA:O | 17:AQ:83:VAL:C | 2.58 | 0.42 |
| 19:AS:15:LEU:HD12 | 19:AS:33:THR:HG21 | 2.02 | 0.42 |
| 20:AT:24:ARG:O | 20:AT:25:ARG:C | 2.58 | 0.42 |
| 21:AU:10:GLU:OE2 | 3:CC:72:ARG:NH2 | 2.53 | 0.42 |
| 22:BA:189:G:H2' | 22:BA:205:G:N2 | 2.35 | 0.42 |
| 22:BA:451:U:C2 | 22:BA:453:A:N7 | 2.87 | 0.42 |
| 22:BA:481:G:N3 | 22:BA:507:A:C2 | 2.88 | 0.42 |
| 22:BA:735:A:H3' | 22:BA:736:C:H6 | 1.85 | 0.42 |
| 22:BA:826:U:O2' | 33:BL:53:GLY:CA | 2.68 | 0.42 |
| 22:BA:1737:G:C6 | 22:BA:1738:G:C2 | 3.08 | 0.42 |
| 22:BA:1829:A:O2' | 24:BC:15:HIS:CD2 | 2.73 | 0.42 |
| 22:BA:1922:G:N1 | 22:BA:1923:U:C6 | 2.88 | 0.42 |
| 22:BA:2021:C:P | 48:B0:9:THR:HG21 | 2.60 | 0.42 |
| 22:BA:2233:U:H2' | 22:BA:2234:G:C8 | 2.54 | 0.42 |
| 22:BA:2680:U:C2 | 22:BA:2681:C:C5 | 3.08 | 0.42 |
| 22:BA:2861:U:O2 | 22:BA:2862:G:C8 | 2.72 | 0.42 |
| 22:BA:2896:C:H2' | 22:BA:2897:U:H6 | 1.85 | 0.42 |
| 24:BC:72:ASP:HA | 24:BC:118:SER:O | 2.20 | 0.42 |
| 25:BD:106:LYS:HA | 25:BD:175:LEU:O | 2.20 | 0.42 |
| 31:BJ:124:VAL:O | 31:BJ:124:VAL:HG22 | 2.20 | 0.42 |
| 37:BP:73:VAL:O | 37:BP:73:VAL:CG2 | 2.67 | 0.42 |
| 39:BR:39:LEU:O | 39:BR:49:ILE:HG23 | 2.20 | 0.42 |
| 39:BR:51:VAL:CB | 39:BR:52:PRO:CD | 2.98 | 0.42 |
| 41:BT:2:ILE:HG12 | 41:BT:7:LEU:HD11 | 2.02 | 0.42 |
| 45:BX:11:ARG:HB2 | 45:BX:12:PRO:CD | 2.50 | 0.42 |
| 46:BY:22:LEU:O | 46:BY:23:ARG:C | 2.59 | 0.42 |
| 1:CA:33:A:H2' | 1:CA:34:C:C6 | 2.55 | 0.42 |
| 1:CA:73:C:C2 | 1:CA:74:A:H8 | 2.37 | 0.42 |
| 1:CA:147:G:C2 | 1:CA:148:G:C6 | 3.08 | 0.42 |
| 1:CA:291:U:O2 | 1:CA:291:U:H2' | 2.19 | 0.42 |
| 1:CA:407:U:H2' | 1:CA:408:A:H8 | 1.84 | 0.42 |
| 1:CA:445:G:N1 | 1:CA:446:G:C5 | 2.88 | 0.42 |
| 1:CA:604:G:C2 | 1:CA:635:A:C2 | 3.08 | 0.42 |
| 1:CA:701:U:H4' | 1:CA:703:G:C8 | 2.55 | 0.42 |
| 1:CA:707:U:H4' | 11:CK:22:HIS:ND1 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:CA:938:A:N6 | 1:CA:939:G:C5 | 2.88 | 0.42 |
| 1:CA:1004:A:H2' | 1:CA:1005:A:C8 | 2.54 | 0.42 |
| 1:CA:1126:U:O4 | 10:CJ:73:LEU:CD1 | 2.68 | 0.42 |
| 1:CA:1280:A:OP1 | 1:CA:1281:C:C5 | 2.73 | 0.42 |
| 1:CA:1314:C:N3 | 1:CA:1315:U:C4 | 2.88 | 0.42 |
| 2:CB:15:HIS:CD2 | 2:CB:209:ALA:HB2 | 2.55 | 0.42 |
| 2:CB:16:PHE:CZ | 2:CB:18:HIS:NE2 | 2.88 | 0.42 |
| 2:CB:222:ARG:HE | 2:CB:223:GLU:N | 2.17 | 0.42 |
| 3:CC:169:ARG:HD2 | 3:CC:169:ARG:C | 2.40 | 0.42 |
| 5:CE:90:THR:HG22 | 5:CE:91:GLY:N | 2.35 | 0.42 |
| 5:CE:104:GLY:O | 5:CE:105:ILE:HG23 | 2.19 | 0.42 |
| 5:CE:104:GLY:HA3 | 5:CE:122:ASN:HA | 2.01 | 0.42 |
| 15:CO:73:LYS:HA | 15:CO:73:LYS:HE2 | 2.02 | 0.42 |
| 22:DA:162:U:H4' | 22:DA:163:C:OP1 | 2.20 | 0.42 |
| 22:DA:294:A:N6 | 22:DA:345:A:N9 | 2.68 | 0.42 |
| 22:DA:389:G:N9 | 22:DA:2413:G:H4' | 2.34 | 0.42 |
| 22:DA:602:A:H2' | 22:DA:602:A:N3 | 2.34 | 0.42 |
| 22:DA:611:C:N3 | 22:DA:618:G:C2 | 2.87 | 0.42 |
| 22:DA:752:A:N3 | 22:DA:752:A:H2' | 2.35 | 0.42 |
| 22:DA:845:A:H5' | 22:DA:846:U:OP2 | 2.19 | 0.42 |
| 22:DA:957:C:C4 | 22:DA:2459:A:C1' | 3.02 | 0.42 |
| 22:DA:965:C:C4' | 22:DA:2273:A:H1' | 2.49 | 0.42 |
| 22:DA:1073:A:H2' | 22:DA:1074:G:H5' | 2.02 | 0.42 |
| 22:DA:1257:C:N4 | 22:DA:1258:U:O4 | 2.52 | 0.42 |
| 22:DA:1282:U:C4 | 22:DA:1283:G:C6 | 3.07 | 0.42 |
| 22:DA:1310:G:N2 | 22:DA:1605:C:C2 | 2.87 | 0.42 |
| 22:DA:1359:A:N1 | 22:DA:1360:G:H1' | 2.35 | 0.42 |
| 22:DA:1394:U:H4' | 22:DA:1603:A:H4' | 2.02 | 0.42 |
| 22:DA:1480:C:C4 | 22:DA:1481:U:C4 | 3.08 | 0.42 |
| 22:DA:1754:A:N6 | 22:DA:1755:A:N6 | 2.68 | 0.42 |
| 22:DA:1863:G:H2' | 22:DA:1864:U:O4' | 2.19 | 0.42 |
| 22:DA:2013:A:N1 | 22:DA:2014:A:C2 | 2.87 | 0.42 |
| 22:DA:2016:U:O2 | 48:D0:4:GLN:NE2 | 2.52 | 0.42 |
| 22:DA:2186:G:C5 | 22:DA:2187:U:C5 | 3.08 | 0.42 |
| 22:DA:2262:U:N3 | 22:DA:2279:G:C2 | 2.88 | 0.42 |
| 22:DA:2305:U:C5 | 22:DA:2306:C:C5 | 3.07 | 0.42 |
| 22:DA:2351:G:H1' | 22:DA:2367:G:N2 | 2.35 | 0.42 |
| 22:DA:2440:C:N3 | 22:DA:2441:U:H1' | 2.35 | 0.42 |
| 22:DA:2683:C:C5 | 22:DA:2684:U:C5 | 3.08 | 0.42 |
| 23:DB:90:C:H5' | 34:DM:18:ARG:HG2 | 2.02 | 0.42 |
| 27:DF:117:LEU:O | 27:DF:118:SER:C | 2.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DH:31:VAL:HB | 29:DH:32:PRO:HD2 | 2.00 | 0.42 |
| 32:DK:121:GLU:HG2 | 32:DK:122:VAL:HG23 | 2.01 | 0.42 |
| 33:DL:78:ARG:CZ | 33:DL:113:ALA:HB1 | 2.50 | 0.42 |
| 33:DL:78:ARG:CB | 33:DL:113:ALA:CB | 2.98 | 0.42 |
| 41:DT:65:GLY:O | 41:DT:66:LYS:O | 2.38 | 0.42 |
| 42:DU:40:ASN:O | 42:DU:41:LEU:C | 2.58 | 0.42 |
| 43:DV:30:ILE:O | 43:DV:37:PRO:HA | 2.20 | 0.42 |
| 45:DX:40:VAL:CG2 | 45:DX:45:ARG:O | 2.68 | 0.42 |
| 1:AA:22:G:H2' | 1:AA:23:C:H6 | 1.85 | 0.41 |
| 1:AA:243:A:C2 | 1:AA:246:A:C8 | 3.08 | 0.41 |
| 1:AA:325:A:H2' | 1:AA:326:G:O4' | 2.20 | 0.41 |
| 1:AA:375:U:C2 | 1:AA:376:G:C8 | 3.08 | 0.41 |
| 1:AA:402:G:C5 | 1:AA:403:C:C5 | 3.08 | 0.41 |
| 1:AA:466:A:H5' | 1:AA:467:U:OP2 | 2.20 | 0.41 |
| 1:AA:468:A:N1 | 1:AA:469:C:C4 | 2.88 | 0.41 |
| 1:AA:748:G:N1 | 1:AA:749:A:C5 | 2.88 | 0.41 |
| 1:AA:757:U:O2' | 1:AA:879:C:O2 | 2.33 | 0.41 |
| 1:AA:781:A:C4 | 1:AA:802:A:C2 | 3.08 | 0.41 |
| 1:AA:1264:U:O2 | 1:AA:1272:G:N2 | 2.53 | 0.41 |
| 1:AA:1346:A:C8 | 7:AG:10:ARG:NH2 | 2.88 | 0.41 |
| 1:AA:1347:G:N2 | 1:AA:1373:G:H2' | 2.34 | 0.41 |
| 1:AA:1513:A:H2' | 1:AA:1514:G:C8 | 2.55 | 0.41 |
| 2:AB:24:ASN:HA | 2:AB:25:PRO:HD2 | 1.79 | 0.41 |
| 2:AB:186:ILE:HG22 | 2:AB:200:ILE:HB | 2.02 | 0.41 |
| 4:AD:19:LEU:HD22 | 4:AD:64:ILE:CG1 | 2.49 | 0.41 |
| 11:AK:53:ARG:O | 11:AK:56:ARG:HG3 | 2.20 | 0.41 |
| 14:AN:73:PHE:CZ | 14:AN:78:GLY:HA2 | 2.55 | 0.41 |
| 19:AS:29:LYS:HG2 | 19:AS:30:PRO:HD2 | 2.02 | 0.41 |
| 20:AT:34:LYS:HD3 | 20:AT:34:LYS:HA | 1.84 | 0.41 |
| 22:BA:468:G:O6 | 22:BA:469:G:C2 | 2.73 | 0.41 |
| 22:BA:483:A:H1' | 42:BU:58:ILE:HD12 | 2.02 | 0.41 |
| 22:BA:574:A:C6 | 22:BA:2033:A:H5' | 2.55 | 0.41 |
| 22:BA:586:A:C2 | 22:BA:1254:A:C2 | 3.08 | 0.41 |
| 22:BA:1513:U:H2' | 22:BA:1514:G:O4' | 2.20 | 0.41 |
| 22:BA:1563:U:H2' | 22:BA:1564:C:H6 | 1.82 | 0.41 |
| 22:BA:1992:G:N2 | 22:BA:1996:C:O2' | 2.53 | 0.41 |
| 22:BA:2190:G:C5 | 22:BA:2191:A:C5 | 3.08 | 0.41 |
| 22:BA:2341:G:H2' | 22:BA:2342:C:C6 | 2.55 | 0.41 |
| 22:BA:2418:A:C6 | 22:BA:2419:U:C4 | 3.08 | 0.41 |
| 22:BA:2469:A:H4' | 34:BM:55:ARG:HH12 | 1.86 | 0.41 |
| 22:BA:2517:C:O2' | 22:BA:2542:A:N7 | 2.43 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2540:C:H2' | 22:BA:2541:A:O4' | 2.20 | 0.41 |
| 22:BA:2592:G:C5 | 22:BA:2593:U:C4 | 3.08 | 0.41 |
| 22:BA:2673:G:C2 | 22:BA:2674:G:C8 | 3.08 | 0.41 |
| 22:BA:2845:U:H5'' | 37:BP:52:ASN:O | 2.18 | 0.41 |
| 24:BC:141:VAL:CG1 | 24:BC:142:HIS:N | 2.83 | 0.41 |
| 25:BD:1:MET:HG3 | 25:BD:205:PRO:HG2 | 2.01 | 0.41 |
| 25:BD:125:TRP:CE3 | 25:BD:160:LYS:HD2 | 2.55 | 0.41 |
| 28:BG:125:CYS:HB3 | 28:BG:127:THR:O | 2.20 | 0.41 |
| 29:BH:82:SER:HG | 29:BH:90:LEU:HG | 1.85 | 0.41 |
| 29:BH:104:THR:CG2 | 29:BH:110:VAL:O | 2.68 | 0.41 |
| 29:BH:139:PHE:O | 29:BH:140:ALA:HB3 | 2.20 | 0.41 |
| 30:BI:116:ASP:O | 30:BI:117:MET:CG | 2.68 | 0.41 |
| 31:BJ:76:HIS:CE1 | 31:BJ:85:LYS:HB2 | 2.55 | 0.41 |
| 32:BK:63:VAL:HG12 | 32:BK:107:LEU:HD11 | 2.02 | 0.41 |
| 34:BM:62:LYS:HG2 | 34:BM:63:ILE:N | 2.35 | 0.41 |
| 36:BO:83:LEU:HD22 | 36:BO:88:LYS:HB2 | 2.02 | 0.41 |
| 43:BV:89:ILE:HG21 | 43:BV:91:PHE:CZ | 2.55 | 0.41 |
| 53:B5:36:ALA:O | 53:B5:37:LYS:HB2 | 2.19 | 0.41 |
| 1:CA:208:U:H2' | 1:CA:210:C:O4' | 2.21 | 0.41 |
| 1:CA:504:C:H1' | 1:CA:510:A:C4 | 2.54 | 0.41 |
| 1:CA:583:A:C6 | 1:CA:759:A:N7 | 2.88 | 0.41 |
| 1:CA:793:U:HO2' | 1:CA:1516:G:C1' | 2.33 | 0.41 |
| 1:CA:999:C:H2' | 1:CA:1000:A:C8 | 2.55 | 0.41 |
| 1:CA:1240:U:OP2 | 7:CG:116:MET:HB3 | 2.19 | 0.41 |
| 1:CA:1379:G:C6 | 1:CA:1380:U:O4 | 2.73 | 0.41 |
| 1:CA:1380:U:C4 | 7:CG:3:ARG:HA | 2.54 | 0.41 |
| 4:CD:9:LEU:HD22 | 4:CD:22:LYS:HD2 | 2.01 | 0.41 |
| 4:CD:116:GLN:CG | 4:CD:120:HIS:CE1 | 3.02 | 0.41 |
| 6:CF:9:MET:HE2 | 6:CF:59:TYR:CD1 | 2.55 | 0.41 |
| 7:CG:133:THR:HA | 7:CG:136:LYS:HB3 | 2.02 | 0.41 |
| 10:CJ:15:HIS:HB3 | 10:CJ:70:HIS:NE2 | 2.35 | 0.41 |
| 10:CJ:37:ARG:O | 10:CJ:38:GLY:O | 2.38 | 0.41 |
| 10:CJ:47:GLU:O | 10:CJ:66:GLU:HA | 2.19 | 0.41 |
| 13:CM:18:ALA:HB2 | 13:CM:45:ILE:HD11 | 2.01 | 0.41 |
| 14:CN:34:VAL:HG12 | 14:CN:34:VAL:O | 2.20 | 0.41 |
| 15:CO:41:GLY:O | 15:CO:42:HIS:C | 2.57 | 0.41 |
| 22:DA:46:G:C2 | 22:DA:47:C:C4 | 3.08 | 0.41 |
| 22:DA:253:C:C2' | 22:DA:254:G:H5' | 2.50 | 0.41 |
| 22:DA:554:U:O4 | 22:DA:555:G:C6 | 2.73 | 0.41 |
| 22:DA:620:G:H2' | 22:DA:620:G:N3 | 2.34 | 0.41 |
| 22:DA:629:G:H4' | 22:DA:650:C:O2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:1051:G:H4' | 22:DA:2752:C:O2' | 2.20 | 0.41 |
| 22:DA:1140:C:C2' | 22:DA:1141:U:H5' | 2.50 | 0.41 |
| 22:DA:1190:G:OP1 | 33:DL:32:GLY:HA2 | 2.19 | 0.41 |
| 22:DA:1337:G:C2 | 22:DA:1338:G:H1' | 2.55 | 0.41 |
| 22:DA:1379:U:OP1 | 22:DA:1379:U:C6 | 2.73 | 0.41 |
| 22:DA:1453:A:N3 | 35:DN:77:ALA:HB2 | 2.35 | 0.41 |
| 22:DA:1737:G:C6 | 22:DA:1738:G:C6 | 3.08 | 0.41 |
| 22:DA:1810:A:H5'' | 22:DA:1811:G:OP2 | 2.19 | 0.41 |
| 22:DA:1851:U:H2' | 22:DA:1852:U:O4' | 2.20 | 0.41 |
| 22:DA:2127:G:H4' | 22:DA:2128:G:OP1 | 2.20 | 0.41 |
| 22:DA:2305:U:O4' | 27:DF:131:GLY:HA3 | 2.19 | 0.41 |
| 22:DA:2451:A:N3 | 56:DA:3001:DOL:HC12 | 2.34 | 0.41 |
| 22:DA:2454:G:N2 | 22:DA:2499:C:C2 | 2.88 | 0.41 |
| 22:DA:2560:A:H2' | 22:DA:2561:U:O4' | 2.20 | 0.41 |
| 22:DA:2884:U:O2 | 22:DA:2884:U:O4' | 2.38 | 0.41 |
| 22:DA:2887:A:C2 | 22:DA:2888:C:H1' | 2.55 | 0.41 |
| 23:DB:39:A:H2' | 23:DB:40:U:H6 | 1.85 | 0.41 |
| 25:DD:2:ILE:HG23 | 25:DD:88:GLU:OE2 | 2.19 | 0.41 |
| 25:DD:48:ILE:HG23 | 25:DD:84:LEU:HD11 | 2.02 | 0.41 |
| 27:DF:9:LYS:O | 27:DF:13:VAL:CG2 | 2.67 | 0.41 |
| 27:DF:77:PHE:C | 27:DF:78:LYS:HG3 | 2.41 | 0.41 |
| 30:DI:29:GLY:HA2 | 30:DI:33:VAL:HB | 2.02 | 0.41 |
| 33:DL:100:ILE:O | 33:DL:100:ILE:HG13 | 2.14 | 0.41 |
| 35:DN:72:ASP:O | 35:DN:75:ILE:N | 2.52 | 0.41 |
| 39:DR:49:ILE:HD12 | 39:DR:52:PRO:HA | 2.02 | 0.41 |
| 41:DT:2:ILE:HG12 | 41:DT:7:LEU:CD1 | 2.50 | 0.41 |
| 41:DT:7:LEU:HD21 | 41:DT:45:ALA:CB | 2.50 | 0.41 |
| 41:DT:21:SER:O | 41:DT:24:MET:N | 2.53 | 0.41 |
| 41:DT:24:MET:CG | 41:DT:29:THR:O | 2.68 | 0.41 |
| 42:DU:45:HIS:HB3 | 42:DU:58:ILE:HG12 | 2.02 | 0.41 |
| 42:DU:74:ASN:O | 42:DU:75:ALA:HB3 | 2.20 | 0.41 |
| 42:DU:83:VAL:HG11 | 42:DU:94:ARG:HD2 | 2.01 | 0.41 |
| 50:D2:26:ASN:O | 50:D2:30:VAL:HG23 | 2.20 | 0.41 |
| 1:AA:78:A:H2' | 1:AA:79:G:O4' | 2.18 | 0.41 |
| 1:AA:340:U:C2 | 1:AA:341:C:C5 | 3.08 | 0.41 |
| 1:AA:390:U:H2' | 1:AA:391:G:H8 | 1.82 | 0.41 |
| 1:AA:787:A:C5 | 1:AA:788:U:C5 | 3.08 | 0.41 |
| 1:AA:1118:U:O4' | 1:AA:1179:A:H1' | 2.20 | 0.41 |
| 1:AA:1368:A:OP2 | 9:AI:114:LYS:CD | 2.69 | 0.41 |
| 1:AA:1377:A:C5 | 7:AG:7:ILE:CD1 | 3.03 | 0.41 |
| 2:AB:164:ILE:HG12 | 2:AB:165:ASP:N | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 5:AE:136:VAL:O | 5:AE:140:THR:HG23 | 2.20 | 0.41 |
| 7:AG:69:VAL:HG21 | 7:AG:104:ILE:HD11 | 2.01 | 0.41 |
| 9:AI:26:GLY:CA | 9:AI:59:GLU:HA | 2.50 | 0.41 |
| 12:AL:108:LYS:O | 12:AL:109:ASP:HB2 | 2.19 | 0.41 |
| 17:AQ:45:HIS:CG | 17:AQ:70:THR:HG22 | 2.55 | 0.41 |
| 17:AQ:46:VAL:HG21 | 17:AQ:61:ILE:HG12 | 2.02 | 0.41 |
| 19:AS:58:VAL:HG11 | 19:AS:75:ALA:HA | 2.03 | 0.41 |
| 21:AU:12:PHE:N | 21:AU:12:PHE:HD2 | 2.16 | 0.41 |
| 22:BA:71:A:OP2 | 22:BA:71:A:H3' | 2.20 | 0.41 |
| 22:BA:785:G:C6 | 22:BA:786:C:C4 | 3.08 | 0.41 |
| 22:BA:1006:C:C2 | 22:BA:1138:G:N2 | 2.87 | 0.41 |
| 22:BA:1820:U:O2 | 24:BC:200:HIS:HB3 | 2.20 | 0.41 |
| 22:BA:1921:G:N2 | 22:BA:1922:G:C8 | 2.88 | 0.41 |
| 22:BA:1999:C:H2' | 22:BA:2000:C:O4' | 2.20 | 0.41 |
| 22:BA:2190:G:C2' | 22:BA:2191:A:H5' | 2.50 | 0.41 |
| 22:BA:2504:U:C5 | 56:BA:3001:DOL:H161 | 2.54 | 0.41 |
| 22:BA:2888:C:O2 | 22:BA:2888:C:H2' | 2.20 | 0.41 |
| 23:BB:37:C:C6 | 23:BB:38:C:C5 | 3.08 | 0.41 |
| 28:BG:94:TYR:C | 28:BG:95:ARG:HG2 | 2.40 | 0.41 |
| 30:BI:18:ALA:O | 30:BI:19:ASN:CB | 2.66 | 0.41 |
| 35:BN:55:ALA:HA | 35:BN:80:PHE:CE1 | 2.55 | 0.41 |
| 36:BO:2:ASP:OD1 | 36:BO:3:LYS:N | 2.53 | 0.41 |
| 39:BR:64:VAL:CG2 | 39:BR:65:ALA:N | 2.83 | 0.41 |
| 41:BT:51:PHE:O | 41:BT:52:GLU:C | 2.57 | 0.41 |
| 46:BY:13:GLU:HG3 | 46:BY:53:VAL:HG13 | 2.01 | 0.41 |
| 1:CA:376:G:H5' | 16:CP:5:ARG:CB | 2.46 | 0.41 |
| 1:CA:399:G:C6 | 1:CA:400:C:C4 | 3.08 | 0.41 |
| 1:CA:456:A:C6 | 1:CA:457:G:C5 | 3.07 | 0.41 |
| 1:CA:734:G:C4 | 1:CA:735:C:C6 | 3.08 | 0.41 |
| 1:CA:862:C:N3 | 1:CA:863:U:C5 | 2.88 | 0.41 |
| 1:CA:1239:A:N7 | 1:CA:1298:U:H5 | 2.17 | 0.41 |
| 1:CA:1251:A:H2' | 1:CA:1252:A:O4' | 2.20 | 0.41 |
| 2:CB:41:ILE:C | 2:CB:41:ILE:HD12 | 2.41 | 0.41 |
| 3:CC:42:TYR:CZ | 3:CC:90:VAL:HG21 | 2.54 | 0.41 |
| 7:CG:69:VAL:HG21 | 7:CG:104:ILE:HD11 | 2.01 | 0.41 |
| 7:CG:92:ARG:CZ | 7:CG:93:PRO:HD3 | 2.51 | 0.41 |
| 12:CL:90:LEU:HB2 | 12:CL:93:VAL:CG2 | 2.49 | 0.41 |
| 16:CP:23:ASP:O | 16:CP:25:ARG:N | 2.52 | 0.41 |
| 18:CR:58:ALA:O | 18:CR:59:ILE:C | 2.58 | 0.41 |
| 21:CU:36:GLU:O | 21:CU:37:PHE:CB | 2.67 | 0.41 |
| 22:DA:141:G:H3' | 22:DA:142:A:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:379:G:C4 | 22:DA:396:G:C2 | 3.08 | 0.41 |
| 22:DA:627:A:C6 | 22:DA:637:A:C8 | 3.08 | 0.41 |
| 22:DA:770:G:C4 | 22:DA:771:G:C8 | 3.09 | 0.41 |
| 22:DA:871:U:H5'' | 34:DM:68:PHE:CZ | 2.56 | 0.41 |
| 22:DA:1218:G:H2' | 22:DA:1219:U:O4' | 2.20 | 0.41 |
| 22:DA:1413:A:C2 | 22:DA:1590:A:C2 | 3.08 | 0.41 |
| 22:DA:1613:G:O2' | 50:D2:3:ARG:HD2 | 2.20 | 0.41 |
| 22:DA:2115:G:N3 | 22:DA:2117:A:N7 | 2.68 | 0.41 |
| 22:DA:2146:C:OP2 | 22:DA:2146:C:O4' | 2.39 | 0.41 |
| 22:DA:2185:U:H2' | 22:DA:2186:G:C8 | 2.55 | 0.41 |
| 22:DA:2345:G:H4' | 22:DA:2346:A:H5'' | 2.02 | 0.41 |
| 23:DB:20:G:N2 | 23:DB:64:G:C4 | 2.88 | 0.41 |
| 24:DC:131:PRO:HB2 | 24:DC:133:ARG:HG2 | 2.02 | 0.41 |
| 25:DD:115:GLY:O | 35:DN:3:HIS:CE1 | 2.74 | 0.41 |
| 29:DH:40:THR:OG1 | 29:DH:43:ASN:ND2 | 2.53 | 0.41 |
| 31:DJ:35:ARG:HB3 | 31:DJ:54:ILE:HD11 | 2.02 | 0.41 |
| 34:DM:63:ILE:HG22 | 34:DM:64:TRP:N | 2.34 | 0.41 |
| 34:DM:110:GLU:O | 34:DM:114:ARG:HG3 | 2.19 | 0.41 |
| 36:DO:27:VAL:HG21 | 36:DO:40:ILE:HD12 | 2.02 | 0.41 |
| 36:DO:28:VAL:CG1 | 36:DO:94:ARG:HA | 2.50 | 0.41 |
| 37:DP:110:ILE:HD13 | 37:DP:110:ILE:N | 2.35 | 0.41 |
| 37:DP:113:ARG:C | 37:DP:114:LEU:HD23 | 2.40 | 0.41 |
| 39:DR:21:ARG:NE | 39:DR:93:PHE:CE1 | 2.87 | 0.41 |
| 41:DT:15:HIS:CD2 | 41:DT:17:SER:OG | 2.74 | 0.41 |
| 41:DT:49:LYS:HD3 | 41:DT:49:LYS:N | 2.35 | 0.41 |
| 45:DX:39:TRP:CE3 | 45:DX:45:ARG:O | 2.73 | 0.41 |
| 45:DX:40:VAL:HG11 | 45:DX:68:LEU:CD1 | 2.50 | 0.41 |
| 48:D0:31:ASP:OD1 | 48:D0:48:TYR:HB3 | 2.20 | 0.41 |
| 1:AA:104:G:C2 | 1:AA:105:G:N7 | 2.88 | 0.41 |
| 1:AA:113:G:C6 | 1:AA:315:A:N6 | 2.88 | 0.41 |
| 1:AA:393:A:C2 | 1:AA:394:G:C8 | 3.09 | 0.41 |
| 1:AA:455:G:C2 | 1:AA:478:A:N1 | 2.88 | 0.41 |
| 1:AA:459:A:H2' | 1:AA:460:A:C8 | 2.55 | 0.41 |
| 1:AA:478:A:H2' | 1:AA:479:U:C5' | 2.50 | 0.41 |
| 1:AA:570:G:H1' | 1:AA:820:U:C4 | 2.55 | 0.41 |
| 1:AA:1154:G:C2 | 1:AA:1155:A:C5 | 3.08 | 0.41 |
| 2:AB:65:GLY:C | 2:AB:66:LYS:HD3 | 2.40 | 0.41 |
| 3:AC:23:PHE:CD2 | 3:AC:24:ALA:N | 2.88 | 0.41 |
| 3:AC:53:SER:HB2 | 3:AC:112:ASP:OD2 | 2.20 | 0.41 |
| 3:AC:120:ILE:O | 3:AC:124:LEU:HG | 2.20 | 0.41 |
| 4:AD:58:LYS:CE | 4:AD:69:GLU:OE2 | 2.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:AE:41:ASP:OD1 | 5:AE:42:GLY:N | 2.53 | 0.41 |
| 6:AF:63:ASN:OD1 | 6:AF:96:VAL:CG2 | 2.69 | 0.41 |
| 7:AG:74:GLU:HG2 | 7:AG:91:VAL:HB | 2.01 | 0.41 |
| 8:AH:25:VAL:O | 8:AH:25:VAL:CG1 | 2.67 | 0.41 |
| 10:AJ:56:HIS:O | 10:AJ:57:VAL:HG13 | 2.19 | 0.41 |
| 10:AJ:66:GLU:HG3 | 10:AJ:67:ILE:N | 2.34 | 0.41 |
| 12:AL:107:VAL:CG2 | 12:AL:117:TYR:HB3 | 2.50 | 0.41 |
| 15:AO:55:GLY:O | 15:AO:58:ARG:HB3 | 2.20 | 0.41 |
| 22:BA:616:A:H2' | 22:BA:617:G:O4' | 2.20 | 0.41 |
| 22:BA:668:A:C2' | 22:BA:669:G:OP1 | 2.67 | 0.41 |
| 22:BA:684:G:C6 | 22:BA:774:G:C4 | 3.09 | 0.41 |
| 22:BA:1414:C:C5 | 22:BA:1415:U:C5 | 3.08 | 0.41 |
| 22:BA:1496:A:C2 | 22:BA:1498:C:O2 | 2.73 | 0.41 |
| 22:BA:2262:U:H4' | 22:BA:2328:A:C2 | 2.55 | 0.41 |
| 23:BB:42:C:C6 | 27:BF:66:LEU:HD13 | 2.55 | 0.41 |
| 25:BD:172:VAL:HG21 | 25:BD:194:PRO:HD3 | 2.01 | 0.41 |
| 27:BF:44:ILE:HG21 | 27:BF:79:ILE:HG22 | 2.02 | 0.41 |
| 27:BF:53:ALA:O | 27:BF:56:ASP:HB2 | 2.21 | 0.41 |
| 27:BF:122:PHE:HB3 | 27:BF:163:ASP:OD2 | 2.19 | 0.41 |
| 28:BG:55:ARG:HG2 | 28:BG:58:TYR:CD1 | 2.54 | 0.41 |
| 32:BK:53:LYS:NZ | 32:BK:56:ASP:OD2 | 2.46 | 0.41 |
| 37:BP:43:PHE:CE2 | 37:BP:63:LYS:HD3 | 2.56 | 0.41 |
| 37:BP:53:ARG:HG3 | 37:BP:53:ARG:NH1 | 2.36 | 0.41 |
| 38:BQ:41:LYS:O | 38:BQ:41:LYS:HG3 | 2.19 | 0.41 |
| 44:BW:64:ASP:OD2 | 44:BW:64:ASP:N | 2.52 | 0.41 |
| 46:BY:7:ARG:O | 46:BY:7:ARG:HG3 | 2.19 | 0.41 |
| 46:BY:9:LYS:HB3 | 46:BY:12:GLU:HG2 | 2.02 | 0.41 |
| 51:B3:15:LYS:HD3 | 51:B3:23:LYS:CE | 2.51 | 0.41 |
| 53:B5:207:GLY:O | 53:B5:208:THR:C | 2.59 | 0.41 |
| 1:CA:112:G:C2' | 1:CA:113:G:H5' | 2.50 | 0.41 |
| 1:CA:135:C:O2 | 16:CP:1:MET:CB | 2.69 | 0.41 |
| 1:CA:198:G:H2' | 1:CA:199:A:C5' | 2.49 | 0.41 |
| 1:CA:302:G:C6 | 1:CA:303:A:C6 | 3.08 | 0.41 |
| 1:CA:445:G:N3 | 1:CA:445:G:H2' | 2.34 | 0.41 |
| 1:CA:821:G:C4 | 1:CA:822:U:C5 | 3.08 | 0.41 |
| 2:CB:161:LEU:CD2 | 2:CB:176:ALA:HB2 | 2.50 | 0.41 |
| 2:CB:207:ILE:HG12 | 2:CB:208:ARG:N | 2.35 | 0.41 |
| 4:CD:73:ARG:O | 4:CD:76:TYR:N | 2.53 | 0.41 |
| 4:CD:203:LEU:HD12 | 4:CD:203:LEU:O | 2.19 | 0.41 |
| 11:CK:25:ALA:N | 11:CK:87:LYS:O | 2.49 | 0.41 |
| 13:CM:22:ILE:HG22 | 13:CM:23:TYR:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:CM:106:ALA:O | 13:CM:110:LYS:HB3 | 2.20 | 0.41 |
| 17:CQ:29:VAL:O | 17:CQ:29:VAL:CG2 | 2.68 | 0.41 |
| 20:CT:33:LYS:HA | 20:CT:36:TYR:HD2 | 1.85 | 0.41 |
| 21:CU:26:ALA:O | 21:CU:27:GLY:C | 2.57 | 0.41 |
| 22:DA:117:G:N1 | 22:DA:119:A:N6 | 2.68 | 0.41 |
| 22:DA:226:A:H4' | 22:DA:258:G:OP1 | 2.20 | 0.41 |
| 22:DA:487:C:N4 | 22:DA:488:G:N1 | 2.68 | 0.41 |
| 22:DA:594:U:H2' | 22:DA:595:C:C6 | 2.55 | 0.41 |
| 22:DA:609:A:C6 | 22:DA:610:C:O2 | 2.72 | 0.41 |
| 22:DA:715:A:N1 | 22:DA:716:A:C2 | 2.89 | 0.41 |
| 22:DA:756:A:H2' | 22:DA:757:G:O4' | 2.19 | 0.41 |
| 22:DA:870:U:OP1 | 34:DM:6:ARG:CD | 2.68 | 0.41 |
| 22:DA:1063:G:O4' | 30:DI:77:ALA:HB1 | 2.19 | 0.41 |
| 22:DA:1274:A:N3 | 22:DA:1297:C:H1' | 2.35 | 0.41 |
| 22:DA:1298:C:N4 | 22:DA:1299:G:C6 | 2.88 | 0.41 |
| 22:DA:1302:A:H5' | 22:DA:1608:A:OP1 | 2.21 | 0.41 |
| 22:DA:1317:G:C6 | 22:DA:1318:U:N3 | 2.89 | 0.41 |
| 22:DA:1469:A:C2' | 22:DA:1470:A:C8 | 2.98 | 0.41 |
| 22:DA:1483:G:C6 | 22:DA:1484:U:C4 | 3.08 | 0.41 |
| 22:DA:1553:A:N7 | 22:DA:1555:G:C5 | 2.88 | 0.41 |
| 22:DA:1809:A:C5 | 22:DA:1810:A:C5 | 3.09 | 0.41 |
| 22:DA:2372:U:H2' | 22:DA:2373:G:H8 | 1.86 | 0.41 |
| 22:DA:2412:A:H3' | 22:DA:2413:G:H8 | 1.82 | 0.41 |
| 22:DA:2457:U:C4 | 22:DA:2458:G:C6 | 3.08 | 0.41 |
| 22:DA:2610:C:C6 | 54:D6:7:004:HD2 | 2.55 | 0.41 |
| 22:DA:2799:A:C2 | 22:DA:2801:G:H1' | 2.55 | 0.41 |
| 22:DA:2870:C:H5'' | 35:DN:65:LEU:CD2 | 2.49 | 0.41 |
| 40:DS:28:LYS:O | 40:DS:31:GLN:N | 2.50 | 0.41 |
| 45:DX:54:LYS:HA | 45:DX:57:ARG:CG | 2.50 | 0.41 |
| 1:AA:262:A:H2' | 1:AA:263:A:C8 | 2.54 | 0.41 |
| 1:AA:269:C:N4 | 1:AA:270:A:N6 | 2.67 | 0.41 |
| 1:AA:460:A:H2' | 1:AA:461:A:O4' | 2.20 | 0.41 |
| 1:AA:704:A:N6 | 1:AA:705:G:C6 | 2.89 | 0.41 |
| 1:AA:834:U:C4 | 1:AA:835:U:C4 | 3.09 | 0.41 |
| 1:AA:909:A:H2' | 1:AA:910:C:O5' | 2.19 | 0.41 |
| 1:AA:1225:A:N3 | 1:AA:1225:A:C2' | 2.83 | 0.41 |
| 1:AA:1277:C:O2' | 1:AA:1279:G:H8 | 2.01 | 0.41 |
| 1:AA:1327:C:O2' | 1:AA:1328:C:H5' | 2.20 | 0.41 |
| 1:AA:1381:U:C5 | 1:AA:1382:C:C5 | 3.09 | 0.41 |
| 1:AA:1401:G:N2 | 1:AA:1402:C:H1' | 2.34 | 0.41 |
| 5:AE:126:LYS:CD | 5:AE:128:TYR:HE2 | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:AI:44:ALA:O | 9:AI:47:VAL:HG22 | 2.20 | 0.41 |
| 9:AI:58:VAL:O | 9:AI:59:GLU:HB2 | 2.18 | 0.41 |
| 9:AI:61:LEU:HD23 | 9:AI:61:LEU:H | 1.85 | 0.41 |
| 10:AJ:34:ALA:O | 10:AJ:35:GLN:HB2 | 2.20 | 0.41 |
| 10:AJ:35:GLN:HG3 | 10:AJ:77:VAL:HB | 2.01 | 0.41 |
| 10:AJ:91:ASP:O | 10:AJ:92:LEU:HD12 | 2.20 | 0.41 |
| 12:AL:57:LEU:C | 12:AL:59:ASN:N | 2.74 | 0.41 |
| 12:AL:59:ASN:OD1 | 12:AL:59:ASN:C | 2.56 | 0.41 |
| 15:AO:24:SER:O | 15:AO:25:THR:C | 2.58 | 0.41 |
| 18:AR:63:ARG:HB3 | 18:AR:70:TYR:CZ | 2.56 | 0.41 |
| 22:BA:818:G:H2' | 22:BA:819:A:OP2 | 2.20 | 0.41 |
| 22:BA:1856:U:O4 | 22:BA:1857:G:C6 | 2.73 | 0.41 |
| 22:BA:1899:A:O2' | 22:BA:1900:A:H5'' | 2.21 | 0.41 |
| 22:BA:1915:U:H2' | 22:BA:1916:A:H8 | 1.85 | 0.41 |
| 22:BA:1932:A:H2 | 22:BA:1969:A:C2 | 2.38 | 0.41 |
| 22:BA:2075:U:C4 | 22:BA:2238:G:C6 | 3.09 | 0.41 |
| 22:BA:2190:G:C6 | 22:BA:2191:A:C4 | 3.08 | 0.41 |
| 22:BA:2192:U:H2' | 22:BA:2193:G:C5' | 2.46 | 0.41 |
| 22:BA:2280:G:O6 | 44:BW:14:ARG:HD2 | 2.20 | 0.41 |
| 22:BA:2311:A:H1' | 27:BF:85:ILE:HD11 | 2.01 | 0.41 |
| 22:BA:2331:G:C6 | 22:BA:2332:C:N3 | 2.88 | 0.41 |
| 22:BA:2380:C:P | 36:BO:17:LYS:NZ | 2.93 | 0.41 |
| 22:BA:2402:U:C2' | 22:BA:2403:C:OP2 | 2.68 | 0.41 |
| 22:BA:2564:A:C6 | 22:BA:2565:A:N1 | 2.89 | 0.41 |
| 22:BA:2650:U:C2' | 22:BA:2651:C:H5' | 2.50 | 0.41 |
| 22:BA:2885:G:H2' | 22:BA:2886:A:C5' | 2.49 | 0.41 |
| 25:BD:13:ARG:O | 25:BD:14:ILE:HD12 | 2.20 | 0.41 |
| 29:BH:33:GLN:O | 29:BH:35:LYS:N | 2.53 | 0.41 |
| 31:BJ:5:THR:HG22 | 31:BJ:6:ALA:O | 2.20 | 0.41 |
| 32:BK:64:ARG:O | 32:BK:82:ASN:HA | 2.20 | 0.41 |
| 32:BK:66:LYS:HE3 | 32:BK:66:LYS:O | 2.21 | 0.41 |
| 32:BK:107:LEU:O | 32:BK:108:ARG:C | 2.59 | 0.41 |
| 34:BM:20:LEU:HD12 | 43:BV:81:PRO:CG | 2.51 | 0.41 |
| 37:BP:53:ARG:CG | 37:BP:53:ARG:NH1 | 2.72 | 0.41 |
| 53:B5:43:GLU:HA | 53:B5:178:LYS:HA | 2.02 | 0.41 |
| 1:CA:182:A:C4 | 1:CA:184:G:N7 | 2.89 | 0.41 |
| 1:CA:568:G:O2' | 1:CA:574:A:N1 | 2.46 | 0.41 |
| 1:CA:784:A:H2' | 1:CA:785:G:C8 | 2.55 | 0.41 |
| 1:CA:932:C:H2' | 1:CA:933:G:C8 | 2.55 | 0.41 |
| 1:CA:968:A:C8 | 1:CA:1062:U:H4' | 2.55 | 0.41 |
| 1:CA:1015:G:O2' | 1:CA:1016:A:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1216:A:OP1 | 14:CN:5:SER:CB | 2.69 | 0.41 |
| 1:CA:1286:U:O2 | 1:CA:1286:U:H2' | 2.19 | 0.41 |
| 1:CA:1310:G:N2 | 1:CA:1328:C:O2 | 2.53 | 0.41 |
| 2:CB:68:LEU:HD12 | 2:CB:158:PRO:CG | 2.51 | 0.41 |
| 2:CB:141:LEU:O | 2:CB:143:LYS:N | 2.53 | 0.41 |
| 2:CB:187:VAL:O | 2:CB:187:VAL:HG22 | 2.21 | 0.41 |
| 10:CJ:31:ARG:HG2 | 10:CJ:31:ARG:O | 2.20 | 0.41 |
| 11:CK:82:LEU:HD23 | 11:CK:82:LEU:O | 2.21 | 0.41 |
| 13:CM:85:CYS:HB3 | 19:CS:74:PHE:CZ | 2.56 | 0.41 |
| 18:CR:62:ALA:HB1 | 18:CR:67:LEU:HB2 | 2.02 | 0.41 |
| 22:DA:543:G:N2 | 22:DA:551:G:C4 | 2.87 | 0.41 |
| 22:DA:590:A:H2' | 22:DA:591:U:O4' | 2.21 | 0.41 |
| 22:DA:681:G:N3 | 22:DA:682:G:C8 | 2.88 | 0.41 |
| 22:DA:830:G:C6 | 22:DA:2448:A:C8 | 3.09 | 0.41 |
| 22:DA:972:A:C2 | 22:DA:973:A:N6 | 2.88 | 0.41 |
| 22:DA:1436:G:C2 | 22:DA:1437:C:H1' | 2.55 | 0.41 |
| 22:DA:1662:U:O2 | 22:DA:2687:U:C5' | 2.69 | 0.41 |
| 22:DA:2094:A:C2 | 22:DA:2196:C:O2 | 2.73 | 0.41 |
| 22:DA:2361:G:H2' | 22:DA:2362:C:O4' | 2.20 | 0.41 |
| 22:DA:2379:G:H2' | 22:DA:2380:C:C6 | 2.55 | 0.41 |
| 22:DA:2665:A:N3 | 22:DA:2665:A:H2' | 2.35 | 0.41 |
| 22:DA:2815:C:H2' | 22:DA:2816:G:C8 | 2.56 | 0.41 |
| 23:DB:64:G:H2' | 23:DB:65:U:O4' | 2.20 | 0.41 |
| 24:DC:64:ILE:O | 24:DC:103:TYR:HB2 | 2.20 | 0.41 |
| 25:DD:47:ALA:HB2 | 25:DD:83:ARG:HA | 2.02 | 0.41 |
| 26:DE:170:ARG:CZ | 26:DE:176:ASP:OD1 | 2.68 | 0.41 |
| 27:DF:122:PHE:CE1 | 27:DF:166:GLY:C | 2.94 | 0.41 |
| 29:DH:135:HIS:CG | 29:DH:136:SER:N | 2.89 | 0.41 |
| 30:DI:19:ASN:OD1 | 30:DI:35:ILE:HG22 | 2.20 | 0.41 |
| 30:DI:54:PRO:HB2 | 30:DI:78:VAL:HG21 | 2.03 | 0.41 |
| 35:DN:2:ARG:O | 35:DN:3:HIS:C | 2.59 | 0.41 |
| 35:DN:38:LEU:HD11 | 35:DN:42:LYS:HE3 | 2.02 | 0.41 |
| 38:DQ:10:ALA:C | 38:DQ:12:ALA:N | 2.71 | 0.41 |
| 40:DS:19:LEU:HD13 | 40:DS:19:LEU:N | 2.35 | 0.41 |
| 40:DS:41:LYS:O | 40:DS:42:LYS:C | 2.59 | 0.41 |
| 49:D1:26:ASN:O | 49:D1:28:ARG:N | 2.53 | 0.41 |
| 1:AA:212:G:N1 | 1:AA:213:G:C5 | 2.89 | 0.41 |
| 1:AA:411:A:C6 | 1:AA:429:U:C4 | 3.07 | 0.41 |
| 1:AA:422:C:H1' | 1:AA:423:G:N2 | 2.35 | 0.41 |
| 1:AA:495:A:N3 | 1:AA:496:A:C6 | 2.88 | 0.41 |
| 1:AA:678:U:H2' | 1:AA:679:C:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:791:G:C5 | 1:AA:792:A:N7 | 2.88 | 0.41 |
| 1:AA:927:G:C2 | 1:AA:1391:U:O2 | 2.73 | 0.41 |
| 1:AA:974:A:H4' | 1:AA:975:A:O5' | 2.20 | 0.41 |
| 1:AA:1005:A:H3' | 1:AA:1006:G:C8 | 2.55 | 0.41 |
| 1:AA:1130:A:N3 | 1:AA:1146:A:C4 | 2.89 | 0.41 |
| 2:AB:81:LYS:HG2 | 2:AB:85:LEU:HD22 | 2.03 | 0.41 |
| 2:AB:91:PHE:CE2 | 2:AB:150:GLY:HA2 | 2.55 | 0.41 |
| 4:AD:62:ARG:NH1 | 4:AD:69:GLU:HG2 | 2.36 | 0.41 |
| 9:AI:50:GLN:N | 9:AI:51:PRO:HD2 | 2.35 | 0.41 |
| 9:AI:86:ALA:C | 9:AI:88:MET:N | 2.73 | 0.41 |
| 9:AI:115:LYS:O | 9:AI:116:VAL:C | 2.59 | 0.41 |
| 13:AM:114:LYS:HB3 | 13:AM:115:PRO:HD3 | 2.02 | 0.41 |
| 16:AP:30:GLY:O | 16:AP:31:ARG:C | 2.59 | 0.41 |
| 22:BA:185:G:H4' | 22:BA:218:A:H4' | 2.02 | 0.41 |
| 22:BA:257:C:H3' | 22:BA:258:G:H8 | 1.86 | 0.41 |
| 22:BA:345:A:N3 | 22:BA:346:A:N6 | 2.67 | 0.41 |
| 22:BA:769:U:N3 | 22:BA:770:G:N7 | 2.69 | 0.41 |
| 22:BA:1169:A:N1 | 22:BA:1180:U:O4 | 2.53 | 0.41 |
| 22:BA:1333:G:C2 | 22:BA:1334:G:C8 | 3.09 | 0.41 |
| 22:BA:1366:A:C6 | 22:BA:1367:A:C4 | 3.09 | 0.41 |
| 22:BA:1540:G:H2' | 22:BA:1541:C:O4' | 2.21 | 0.41 |
| 22:BA:1613:G:O2' | 50:B2:3:ARG:HD3 | 2.21 | 0.41 |
| 22:BA:1857:G:N2 | 22:BA:1884:G:H1' | 2.35 | 0.41 |
| 22:BA:1900:A:C2 | 22:BA:1970:A:C4 | 3.08 | 0.41 |
| 22:BA:1917:U:C5 | 22:BA:1918:A:C6 | 3.08 | 0.41 |
| 22:BA:2085:U:O2 | 22:BA:2235:G:C2 | 2.74 | 0.41 |
| 22:BA:2302:U:O2' | 22:BA:2303:G:H5' | 2.20 | 0.41 |
| 22:BA:2379:G:O3' | 36:BO:17:LYS:NZ | 2.53 | 0.41 |
| 23:BB:97:C:H2' | 23:BB:98:G:H5' | 2.03 | 0.41 |
| 25:BD:25:THR:HG22 | 25:BD:27:ILE:HG13 | 2.01 | 0.41 |
| 29:BH:90:LEU:HD13 | 29:BH:125:THR:HA | 2.03 | 0.41 |
| 32:BK:47:ILE:HB | 32:BK:48:PRO:CD | 2.50 | 0.41 |
| 34:BM:135:VAL:CG2 | 43:BV:57:TYR:CD1 | 3.04 | 0.41 |
| 35:BN:70:THR:OG1 | 35:BN:71:ARG:N | 2.53 | 0.41 |
| 40:BS:69:LEU:HG | 40:BS:107:VAL:HG22 | 2.02 | 0.41 |
| 51:B3:15:LYS:O | 51:B3:22:PHE:HA | 2.20 | 0.41 |
| 53:B5:28:ARG:O | 53:B5:28:ARG:CG | 2.69 | 0.41 |
| 53:B5:28:ARG:O | 53:B5:28:ARG:HG3 | 2.20 | 0.41 |
| 53:B5:212:SER:CB | 53:B5:221:PRO:CB | 2.98 | 0.41 |
| 1:CA:18:C:C4 | 1:CA:19:A:N7 | 2.88 | 0.41 |
| 1:CA:29:U:H4' | 1:CA:295:C:O3' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:312:C:H2' | 1:CA:313:A:O4' | 2.21 | 0.41 |
| 1:CA:552:U:N3 | 1:CA:553:A:C8 | 2.88 | 0.41 |
| 1:CA:686:U:C2 | 1:CA:687:A:N7 | 2.89 | 0.41 |
| 1:CA:803:G:N7 | 1:CA:804:U:C4 | 2.89 | 0.41 |
| 1:CA:1014:A:C8 | 1:CA:1015:G:C5 | 3.09 | 0.41 |
| 1:CA:1061:G:C2 | 1:CA:1197:A:C2 | 3.09 | 0.41 |
| 1:CA:1351:U:H2' | 1:CA:1352:C:C6 | 2.54 | 0.41 |
| 2:CB:80:VAL:O | 2:CB:84:ALA:HB3 | 2.20 | 0.41 |
| 3:CC:111:LEU:N | 3:CC:111:LEU:CD2 | 2.84 | 0.41 |
| 3:CC:173:VAL:O | 3:CC:173:VAL:HG12 | 2.20 | 0.41 |
| 5:CE:121:HIS:O | 5:CE:122:ASN:HB3 | 2.21 | 0.41 |
| 17:CQ:48:ASP:O | 17:CQ:49:GLU:C | 2.57 | 0.41 |
| 22:DA:84:A:C2 | 22:DA:103:A:C6 | 3.07 | 0.41 |
| 22:DA:426:C:H2' | 22:DA:427:U:O4' | 2.20 | 0.41 |
| 22:DA:489:G:C2 | 22:DA:491:G:H1' | 2.55 | 0.41 |
| 22:DA:870:U:OP1 | 34:DM:6:ARG:HD2 | 2.21 | 0.41 |
| 22:DA:892:A:N3 | 22:DA:892:A:H2' | 2.35 | 0.41 |
| 22:DA:1215:G:H2' | 22:DA:1216:G:O4' | 2.21 | 0.41 |
| 22:DA:1257:C:C4 | 22:DA:1258:U:O4 | 2.74 | 0.41 |
| 22:DA:1567:G:N7 | 24:DC:83:TYR:CE1 | 2.88 | 0.41 |
| 22:DA:1605:C:H4' | 22:DA:1610:A:C6 | 2.55 | 0.41 |
| 22:DA:1830:C:H5' | 24:DC:15:HIS:NE2 | 2.36 | 0.41 |
| 22:DA:1835:G:N3 | 22:DA:1836:C:C6 | 2.88 | 0.41 |
| 22:DA:1847:A:O2' | 22:DA:1848:A:P | 2.78 | 0.41 |
| 22:DA:2261:C:C2 | 22:DA:2280:G:C2 | 3.08 | 0.41 |
| 22:DA:2540:C:H2' | 22:DA:2541:A:H8 | 1.86 | 0.41 |
| 22:DA:2553:G:H2' | 22:DA:2554:U:H4' | 2.02 | 0.41 |
| 22:DA:2619:C:OP1 | 25:DD:157:LYS:HE2 | 2.21 | 0.41 |
| 22:DA:2864:G:C2' | 22:DA:2865:U:H5' | 2.51 | 0.41 |
| 23:DB:44:G:N2 | 23:DB:48:U:O2 | 2.53 | 0.41 |
| 23:DB:71:C:O2 | 23:DB:106:G:C2 | 2.74 | 0.41 |
| 25:DD:25:THR:HG22 | 25:DD:27:ILE:HG13 | 2.01 | 0.41 |
| 26:DE:94:GLN:O | 26:DE:95:LYS:C | 2.59 | 0.41 |
| 26:DE:108:ILE:HD11 | 26:DE:180:LEU:HB3 | 2.01 | 0.41 |
| 26:DE:131:THR:HG22 | 26:DE:160:ALA:HA | 2.02 | 0.41 |
| 27:DF:13:VAL:O | 27:DF:17:MET:HG2 | 2.21 | 0.41 |
| 30:DI:54:PRO:O | 30:DI:75:PRO:HD2 | 2.21 | 0.41 |
| 32:DK:36:GLY:HA2 | 32:DK:62:VAL:O | 2.20 | 0.41 |
| 33:DL:29:LYS:C | 33:DL:30:THR:HG23 | 2.41 | 0.41 |
| 38:DQ:47:TYR:C | 38:DQ:47:TYR:CD2 | 2.93 | 0.41 |
| 41:DT:11:LEU:HG | 41:DT:46:ALA:HB1 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DV:44:HIS:O | 43:DV:45:ASP:C | 2.58 | 0.41 |
| 45:DX:13:VAL:HG23 | 45:DX:29:PHE:HB2 | 2.03 | 0.41 |
| 49:D1:21:TYR:CE1 | 49:D1:38:LYS:HD2 | 2.56 | 0.41 |
| 49:D1:38:LYS:HB2 | 49:D1:49:TYR:CD2 | 2.56 | 0.41 |
| 52:D4:30:GLU:HG3 | 52:D4:32:LYS:HB2 | 2.01 | 0.41 |
| 1:AA:142:G:H5' | 1:AA:143:A:OP2 | 2.20 | 0.41 |
| 1:AA:719:C:O2' | 18:AR:39:ILE:O | 2.27 | 0.41 |
| 1:AA:864:A:H3' | 1:AA:865:A:C8 | 2.56 | 0.41 |
| 1:AA:923:A:H2' | 1:AA:924:C:C6 | 2.55 | 0.41 |
| 1:AA:956:U:C5 | 1:AA:957:U:C5 | 3.09 | 0.41 |
| 1:AA:1008:U:H5'' | 1:AA:1009:U:OP1 | 2.21 | 0.41 |
| 1:AA:1157:A:C6 | 1:AA:1180:A:C5 | 3.09 | 0.41 |
| 1:AA:1213:A:C5 | 1:AA:1215:G:C4 | 3.08 | 0.41 |
| 1:AA:1234:C:O2' | 1:AA:1235:U:H5' | 2.21 | 0.41 |
| 1:AA:1369:C:H2' | 1:AA:1370:G:C8 | 2.55 | 0.41 |
| 2:AB:50:PHE:CA | 2:AB:213:TYR:OH | 2.65 | 0.41 |
| 2:AB:182:PRO:O | 2:AB:183:VAL:HB | 2.20 | 0.41 |
| 4:AD:112:ALA:O | 4:AD:115:ARG:N | 2.53 | 0.41 |
| 6:AF:42:TRP:CZ2 | 6:AF:61:LEU:HB2 | 2.56 | 0.41 |
| 7:AG:9:GLN:HG3 | 7:AG:9:GLN:O | 2.21 | 0.41 |
| 7:AG:69:VAL:HG21 | 7:AG:104:ILE:CD1 | 2.49 | 0.41 |
| 10:AJ:10:LEU:O | 10:AJ:71:LEU:HA | 2.20 | 0.41 |
| 11:AK:111:THR:HA | 21:AU:4:ILE:O | 2.21 | 0.41 |
| 15:AO:32:LEU:O | 15:AO:33:THR:C | 2.59 | 0.41 |
| 22:BA:242:G:N7 | 51:B3:5:LYS:HD3 | 2.35 | 0.41 |
| 22:BA:807:U:OP2 | 33:BL:41:ARG:NH1 | 2.54 | 0.41 |
| 22:BA:1428:C:C5 | 22:BA:1569:A:H5'' | 2.56 | 0.41 |
| 22:BA:2201:G:C4 | 22:BA:2223:G:N2 | 2.89 | 0.41 |
| 22:BA:2311:A:C5 | 27:BF:77:PHE:HB3 | 2.56 | 0.41 |
| 22:BA:2592:G:C5 | 22:BA:2593:U:C5 | 3.09 | 0.41 |
| 22:BA:2831:G:P | 25:BD:56:LYS:NZ | 2.93 | 0.41 |
| 26:BE:79:ARG:O | 26:BE:80:SER:CB | 2.68 | 0.41 |
| 26:BE:108:ILE:CD1 | 26:BE:180:LEU:HB3 | 2.49 | 0.41 |
| 27:BF:8:TYR:CD2 | 27:BF:12:VAL:HB | 2.56 | 0.41 |
| 30:BI:57:VAL:HG23 | 30:BI:71:THR:HA | 2.02 | 0.41 |
| 31:BJ:17:VAL:HG23 | 31:BJ:137:PRO:CB | 2.51 | 0.41 |
| 34:BM:65:ILE:HG12 | 34:BM:103:TYR:CD2 | 2.56 | 0.41 |
| 35:BN:101:GLY:C | 35:BN:102:PHE:CD2 | 2.94 | 0.41 |
| 41:BT:29:THR:HG23 | 41:BT:86:THR:CA | 2.50 | 0.41 |
| 41:BT:71:GLY:O | 41:BT:73:ARG:N | 2.47 | 0.41 |
| 46:BY:35:GLY:O | 46:BY:36:GLN:O | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 46:BY:42:LEU:O | 46:BY:45:GLN:O | 2.38 | 0.41 |
| 53:B5:45:HIS:CD2 | 53:B5:176:VAL:HA | 2.56 | 0.41 |
| 1:CA:34:C:H2' | 1:CA:35:G:C8 | 2.56 | 0.41 |
| 1:CA:53:A:H2' | 1:CA:54:C:O4' | 2.21 | 0.41 |
| 1:CA:116:A:C8 | 1:CA:116:A:OP2 | 2.73 | 0.41 |
| 1:CA:282:A:C8 | 1:CA:283:U:C5 | 3.09 | 0.41 |
| 1:CA:296:U:C2 | 1:CA:297:G:C8 | 3.09 | 0.41 |
| 1:CA:413:G:O6 | 4:CD:32:CYS:N | 2.53 | 0.41 |
| 1:CA:445:G:C2 | 1:CA:446:G:C4 | 3.08 | 0.41 |
| 1:CA:554:A:H2' | 1:CA:555:U:H6 | 1.86 | 0.41 |
| 1:CA:630:A:H2' | 1:CA:631:C:C6 | 2.56 | 0.41 |
| 1:CA:977:A:O2' | 1:CA:1223:C:N4 | 2.53 | 0.41 |
| 1:CA:1144:G:N2 | 1:CA:1145:A:C2 | 2.88 | 0.41 |
| 1:CA:1291:U:OP1 | 7:CG:37:SER:HB3 | 2.20 | 0.41 |
| 1:CA:1315:U:C5 | 1:CA:1316:G:C5 | 3.09 | 0.41 |
| 8:CH:21:ASN:O | 8:CH:22:LYS:C | 2.59 | 0.41 |
| 11:CK:51:GLY:O | 11:CK:52:PHE:CD2 | 2.74 | 0.41 |
| 13:CM:18:ALA:CB | 13:CM:45:ILE:HD11 | 2.50 | 0.41 |
| 18:CR:20:GLU:O | 18:CR:21:ILE:C | 2.58 | 0.41 |
| 21:CU:29:LEU:O | 21:CU:30:ALA:C | 2.59 | 0.41 |
| 22:DA:149:A:C2' | 22:DA:150:U:H5' | 2.51 | 0.41 |
| 22:DA:311:A:OP1 | 22:DA:332:A:C2 | 2.73 | 0.41 |
| 22:DA:321:U:H4' | 26:DE:159:LEU:O | 2.20 | 0.41 |
| 22:DA:677:A:C2 | 22:DA:802:A:C2 | 3.09 | 0.41 |
| 22:DA:1178:C:H2' | 22:DA:1179:G:C8 | 2.55 | 0.41 |
| 22:DA:1265:A:C8 | 22:DA:1267:U:N3 | 2.89 | 0.41 |
| 22:DA:1276:A:N1 | 22:DA:1295:C:C2 | 2.88 | 0.41 |
| 22:DA:1358:G:N1 | 22:DA:1372:U:OP2 | 2.50 | 0.41 |
| 22:DA:1555:G:C2 | 22:DA:1556:C:C2 | 3.09 | 0.41 |
| 22:DA:1717:A:H2' | 22:DA:1718:G:O4' | 2.21 | 0.41 |
| 22:DA:1722:A:C2 | 22:DA:1739:A:H1' | 2.55 | 0.41 |
| 22:DA:1854:A:H2' | 22:DA:1855:U:H5' | 2.03 | 0.41 |
| 22:DA:2025:C:H2' | 22:DA:2026:U:C6 | 2.55 | 0.41 |
| 22:DA:2061:G:C6 | 56:DA:3001:DOL:H162 | 2.55 | 0.41 |
| 22:DA:2133:G:C6 | 22:DA:2157:G:C6 | 3.08 | 0.41 |
| 22:DA:2262:U:O2' | 22:DA:2263:C:H5' | 2.21 | 0.41 |
| 22:DA:2308:G:H5' | 22:DA:2309:A:OP2 | 2.21 | 0.41 |
| 22:DA:2447:G:C2 | 22:DA:2501:C:N4 | 2.89 | 0.41 |
| 22:DA:2725:A:C4 | 22:DA:2727:A:N7 | 2.87 | 0.41 |
| 22:DA:2751:G:N3 | 22:DA:2751:G:H2' | 2.36 | 0.41 |
| 22:DA:2820:A:C6 | 25:DD:197:THR:HB | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2836:U:H2' | 22:DA:2837:A:C8 | 2.54 | 0.41 |
| 22:DA:2889:C:C4 | 22:DA:2890:G:C6 | 3.08 | 0.41 |
| 25:DD:30:GLU:HG2 | 25:DD:185:ASN:ND2 | 2.35 | 0.41 |
| 25:DD:37:VAL:CG1 | 25:DD:38:LYS:N | 2.83 | 0.41 |
| 25:DD:179:ARG:HD2 | 25:DD:188:LEU:CD1 | 2.51 | 0.41 |
| 27:DF:174:ASP:O | 27:DF:175:PHE:O | 2.39 | 0.41 |
| 28:DG:80:THR:HG22 | 28:DG:81:GLU:N | 2.35 | 0.41 |
| 29:DH:130:VAL:CG1 | 29:DH:131:SER:N | 2.82 | 0.41 |
| 30:DI:84:ALA:HA | 30:DI:101:ILE:HD12 | 2.01 | 0.41 |
| 31:DJ:4:PHE:CD2 | 38:DQ:100:VAL:HG11 | 2.56 | 0.41 |
| 31:DJ:135:GLN:O | 31:DJ:136:GLN:C | 2.58 | 0.41 |
| 32:DK:7:MET:C | 32:DK:8:LEU:HD12 | 2.41 | 0.41 |
| 35:DN:63:ARG:HG3 | 35:DN:80:PHE:CE2 | 2.56 | 0.41 |
| 41:DT:20:ALA:HA | 41:DT:31:VAL:HG21 | 2.02 | 0.41 |
| 42:DU:13:VAL:CG2 | 42:DU:39:ILE:HG21 | 2.51 | 0.41 |
| 51:D3:32:ILE:HG22 | 51:D3:35:LYS:HD2 | 2.02 | 0.41 |
| 52:D4:3:VAL:HG23 | 52:D4:37:GLN:CD | 2.41 | 0.41 |
| 1:AA:102:G:C2 | 1:AA:103:U:C6 | 3.09 | 0.41 |
| 1:AA:397:A:C5 | 1:AA:548:G:N7 | 2.89 | 0.41 |
| 1:AA:504:C:H1' | 1:AA:510:A:C4 | 2.56 | 0.41 |
| 1:AA:604:G:C2 | 1:AA:635:A:N3 | 2.89 | 0.41 |
| 1:AA:604:G:C6 | 1:AA:635:A:N1 | 2.89 | 0.41 |
| 1:AA:707:U:H4' | 11:AK:22:HIS:CD2 | 2.56 | 0.41 |
| 1:AA:885:G:C2 | 1:AA:913:A:N1 | 2.89 | 0.41 |
| 1:AA:890:G:O2' | 1:AA:906:A:N6 | 2.54 | 0.41 |
| 1:AA:1068:G:N7 | 1:AA:1094:G:H2' | 2.35 | 0.41 |
| 1:AA:1151:A:O2' | 1:AA:1152:A:P | 2.78 | 0.41 |
| 1:AA:1438:G:OP1 | 20:AT:29:ARG:HD3 | 2.20 | 0.41 |
| 2:AB:24:ASN:O | 2:AB:25:PRO:C | 2.58 | 0.41 |
| 2:AB:210:VAL:O | 2:AB:211:THR:C | 2.59 | 0.41 |
| 3:AC:23:PHE:CD2 | 3:AC:23:PHE:C | 2.93 | 0.41 |
| 3:AC:77:ILE:HA | 3:AC:84:VAL:CG2 | 2.51 | 0.41 |
| 4:AD:173:VAL:HG22 | 4:AD:174:ASP:H | 1.85 | 0.41 |
| 8:AH:64:LYS:HB3 | 8:AH:64:LYS:HE2 | 1.93 | 0.41 |
| 10:AJ:5:ARG:HG2 | 10:AJ:79:PRO:HG3 | 2.01 | 0.41 |
| 10:AJ:8:ILE:O | 10:AJ:73:LEU:O | 2.38 | 0.41 |
| 10:AJ:53:ILE:HG22 | 10:AJ:61:ALA:HB3 | 2.01 | 0.41 |
| 11:AK:56:ARG:HA | 11:AK:56:ARG:HE | 1.85 | 0.41 |
| 17:AQ:7:THR:HG22 | 17:AQ:61:ILE:O | 2.20 | 0.41 |
| 17:AQ:14:SER:HB3 | 17:AQ:22:VAL:HG11 | 2.03 | 0.41 |
| 20:AT:74:ARG:O | 20:AT:78:ASN:OD1 | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:54:G:C5 | 22:BA:55:G:C8 | 3.09 | 0.41 |
| 22:BA:108:G:C2' | 22:BA:109:C:H5' | 2.50 | 0.41 |
| 22:BA:493:G:H2' | 22:BA:494:G:O4' | 2.21 | 0.41 |
| 22:BA:528:A:C2 | 22:BA:2042:A:H2' | 2.56 | 0.41 |
| 22:BA:934:U:H2' | 22:BA:935:C:C6 | 2.56 | 0.41 |
| 22:BA:948:C:O2 | 22:BA:984:A:O2' | 2.34 | 0.41 |
| 22:BA:1045:C:H3' | 22:BA:1046:A:C5' | 2.50 | 0.41 |
| 22:BA:1496:A:N3 | 22:BA:1577:C:O2' | 2.46 | 0.41 |
| 22:BA:1808:A:N1 | 45:BX:28:ARG:HD2 | 2.35 | 0.41 |
| 22:BA:1850:G:C6 | 22:BA:1851:U:C4 | 3.08 | 0.41 |
| 22:BA:1924:C:O2 | 22:BA:1926:U:C5 | 2.73 | 0.41 |
| 22:BA:1941:C:C4 | 22:BA:1942:C:C4 | 3.07 | 0.41 |
| 22:BA:2564:A:C6 | 22:BA:2565:A:C6 | 3.09 | 0.41 |
| 22:BA:2819:G:H2' | 22:BA:2821:A:N7 | 2.36 | 0.41 |
| 22:BA:2838:G:O3' | 35:BN:46:ARG:HD3 | 2.21 | 0.41 |
| 24:BC:7:LYS:HB3 | 24:BC:8:PRO:HD2 | 2.02 | 0.41 |
| 24:BC:30:PHE:CZ | 24:BC:32:PRO:HG2 | 2.55 | 0.41 |
| 24:BC:31:ALA:N | 24:BC:32:PRO:CD | 2.83 | 0.41 |
| 25:BD:61:THR:CB | 25:BD:63:PRO:HD2 | 2.50 | 0.41 |
| 26:BE:43:THR:O | 26:BE:44:ARG:HB3 | 2.21 | 0.41 |
| 28:BG:74:SER:HA | 28:BG:77:ILE:HG12 | 2.02 | 0.41 |
| 29:BH:82:SER:HB3 | 29:BH:146:VAL:HG12 | 2.03 | 0.41 |
| 29:BH:95:GLY:HA2 | 29:BH:117:LEU:CD2 | 2.51 | 0.41 |
| 29:BH:100:ALA:HB2 | 29:BH:115:VAL:CG2 | 2.50 | 0.41 |
| 30:BI:92:LYS:HB3 | 30:BI:95:LYS:HG2 | 2.03 | 0.41 |
| 33:BL:74:THR:HA | 33:BL:107:PHE:O | 2.21 | 0.41 |
| 34:BM:106:ASP:OD2 | 34:BM:106:ASP:C | 2.59 | 0.41 |
| 39:BR:66:HIS:ND1 | 39:BR:94:THR:CG2 | 2.82 | 0.41 |
| 40:BS:36:LEU:CD1 | 40:BS:47:VAL:HG12 | 2.51 | 0.41 |
| 41:BT:1:MET:C | 41:BT:2:ILE:HD12 | 2.41 | 0.41 |
| 43:BV:56:PHE:O | 43:BV:61:LEU:HD11 | 2.19 | 0.41 |
| 1:CA:6:G:H4' | 1:CA:298:A:H4' | 2.03 | 0.41 |
| 1:CA:177:G:C6 | 1:CA:178:C:N4 | 2.89 | 0.41 |
| 1:CA:270:A:H2' | 1:CA:271:C:C6 | 2.56 | 0.41 |
| 1:CA:376:G:N3 | 1:CA:389:A:C2 | 2.89 | 0.41 |
| 1:CA:435:A:C2' | 1:CA:436:C:O5' | 2.69 | 0.41 |
| 1:CA:554:A:H2' | 1:CA:555:U:C6 | 2.55 | 0.41 |
| 1:CA:661:G:C5 | 1:CA:662:U:C5 | 3.08 | 0.41 |
| 1:CA:764:C:C5 | 1:CA:765:G:N7 | 2.89 | 0.41 |
| 1:CA:771:G:C2 | 1:CA:809:G:C2 | 3.08 | 0.41 |
| 1:CA:994:A:N3 | 1:CA:994:A:C2' | 2.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1056:U:H5' | 3:CC:163:ALA:HB3 | 2.02 | 0.41 |
| 1:CA:1138:G:C2 | 1:CA:1140:C:C4 | 3.09 | 0.41 |
| 1:CA:1361:G:C2' | 1:CA:1362:A:H5'' | 2.51 | 0.41 |
| 1:CA:1434:A:N6 | 1:CA:1435:G:N1 | 2.68 | 0.41 |
| 2:CB:72:THR:HG22 | 2:CB:95:ARG:NH1 | 2.36 | 0.41 |
| 3:CC:47:LEU:HD22 | 3:CC:76:VAL:HG22 | 2.03 | 0.41 |
| 4:CD:129:VAL:O | 4:CD:129:VAL:HG13 | 2.19 | 0.41 |
| 5:CE:77:ASN:O | 5:CE:80:THR:HG22 | 2.20 | 0.41 |
| 5:CE:150:PRO:HA | 8:CH:99:LEU:HD21 | 2.02 | 0.41 |
| 6:CF:38:ARG:CG | 6:CF:63:ASN:HB2 | 2.50 | 0.41 |
| 6:CF:47:LEU:CD2 | 6:CF:59:TYR:OH | 2.69 | 0.41 |
| 9:CI:15:SER:OG | 9:CI:70:GLY:HA3 | 2.19 | 0.41 |
| 9:CI:49:ARG:NH2 | 9:CI:53:GLU:HA | 2.35 | 0.41 |
| 13:CM:25:VAL:HG13 | 13:CM:25:VAL:O | 2.20 | 0.41 |
| 17:CQ:15:ASP:HA | 17:CQ:21:ILE:HD12 | 2.02 | 0.41 |
| 22:DA:158:U:C5 | 22:DA:159:G:N7 | 2.88 | 0.41 |
| 22:DA:195:A:C5 | 22:DA:198:C:C5 | 3.08 | 0.41 |
| 22:DA:503:A:C2 | 22:DA:506:G:C5 | 3.09 | 0.41 |
| 22:DA:520:G:H2' | 22:DA:521:U:C6 | 2.56 | 0.41 |
| 22:DA:527:C:OP2 | 22:DA:2779:U:N3 | 2.54 | 0.41 |
| 22:DA:543:G:N1 | 22:DA:551:G:C6 | 2.88 | 0.41 |
| 22:DA:1221:C:H2' | 22:DA:1222:U:O4' | 2.21 | 0.41 |
| 22:DA:1268:A:H2' | 22:DA:1269:A:O4' | 2.20 | 0.41 |
| 22:DA:1417:C:N3 | 22:DA:1581:G:O6 | 2.54 | 0.41 |
| 22:DA:1876:A:N7 | 22:DA:1877:A:C5 | 2.88 | 0.41 |
| 22:DA:2127:G:H1' | 22:DA:2162:G:N7 | 2.36 | 0.41 |
| 22:DA:2409:G:C6 | 22:DA:2410:G:C5 | 3.08 | 0.41 |
| 22:DA:2513:A:C4 | 22:DA:2514:U:C5 | 3.08 | 0.41 |
| 22:DA:2718:G:C2 | 22:DA:2719:G:C1' | 3.03 | 0.41 |
| 22:DA:2746:U:H2' | 22:DA:2747:G:O4' | 2.20 | 0.41 |
| 22:DA:2748:A:N1 | 22:DA:2749:A:C2 | 2.89 | 0.41 |
| 22:DA:2847:U:H2' | 22:DA:2848:G:H5' | 2.02 | 0.41 |
| 22:DA:2892:G:H5'' | 22:DA:2894:G:N2 | 2.36 | 0.41 |
| 25:DD:5:VAL:HG21 | 25:DD:80:TRP:CG | 2.56 | 0.41 |
| 25:DD:104:VAL:HG23 | 25:DD:105:LYS:N | 2.36 | 0.41 |
| 29:DH:53:GLU:C | 29:DH:55:GLU:N | 2.72 | 0.41 |
| 33:DL:78:ARG:CB | 33:DL:113:ALA:HB3 | 2.50 | 0.41 |
| 36:DO:18:LEU:CD1 | 36:DO:23:ALA:HB3 | 2.51 | 0.41 |
| 41:DT:64:LYS:HA | 41:DT:79:ASP:OD1 | 2.21 | 0.41 |
| 48:D0:7:LYS:HE2 | 48:D0:8:PRO:O | 2.21 | 0.41 |
| 50:D2:46:LYS:C | 50:D2:46:LYS:HD3 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:131:A:C2 | 1:AA:132:C:N3 | 2.89 | 0.41 |
| 1:AA:148:G:C2' | 1:AA:149:A:O5' | 2.69 | 0.41 |
| 1:AA:255:G:H4' | 17:AQ:19:LYS:HD3 | 2.03 | 0.41 |
| 1:AA:399:G:H2' | 1:AA:400:C:C6 | 2.56 | 0.41 |
| 1:AA:472:U:C4 | 1:AA:473:U:C4 | 3.09 | 0.41 |
| 1:AA:502:A:C2 | 1:AA:544:G:C2 | 3.09 | 0.41 |
| 1:AA:1501:C:C5 | 1:AA:1504:G:C8 | 3.09 | 0.41 |
| 2:AB:144:LEU:O | 2:AB:145:GLU:C | 2.59 | 0.41 |
| 2:AB:167:ASP:O | 2:AB:170:HIS:CE1 | 2.74 | 0.41 |
| 2:AB:186:ILE:HD11 | 2:AB:204:ASP:HA | 2.02 | 0.41 |
| 6:AF:38:ARG:CZ | 6:AF:61:LEU:HD21 | 2.50 | 0.41 |
| 8:AH:49:PHE:HB3 | 8:AH:61:LEU:CD2 | 2.50 | 0.41 |
| 8:AH:49:PHE:CB | 8:AH:61:LEU:HD23 | 2.51 | 0.41 |
| 11:AK:56:ARG:HA | 11:AK:56:ARG:NE | 2.35 | 0.41 |
| 13:AM:90:ARG:NH1 | 13:AM:95:LEU:HB3 | 2.36 | 0.41 |
| 15:AO:46:HIS:O | 15:AO:47:LYS:HB2 | 2.21 | 0.41 |
| 16:AP:45:GLU:O | 16:AP:46:LYS:C | 2.59 | 0.41 |
| 16:AP:78:VAL:O | 16:AP:78:VAL:CG1 | 2.68 | 0.41 |
| 18:AR:25:ASP:O | 18:AR:27:ALA:N | 2.54 | 0.41 |
| 19:AS:18:LYS:HE3 | 19:AS:33:THR:CG2 | 2.51 | 0.41 |
| 20:AT:67:ILE:CD1 | 20:AT:71:LYS:HG2 | 2.51 | 0.41 |
| 21:AU:53:VAL:O | 21:AU:54:LYS:CB | 2.69 | 0.41 |
| 22:BA:247:G:H4' | 22:BA:386:G:C5 | 2.55 | 0.41 |
| 22:BA:477:A:C6 | 22:BA:478:A:C6 | 3.08 | 0.41 |
| 22:BA:524:G:O2' | 22:BA:525:U:H5' | 2.21 | 0.41 |
| 22:BA:673:C:OP1 | 26:BE:49:ARG:NH2 | 2.53 | 0.41 |
| 22:BA:674:G:O2' | 26:BE:69:ARG:HB3 | 2.21 | 0.41 |
| 22:BA:996:A:C5 | 22:BA:1160:G:C2 | 3.09 | 0.41 |
| 22:BA:1045:C:H3' | 22:BA:1046:A:H5' | 2.01 | 0.41 |
| 22:BA:1073:A:H2' | 22:BA:1074:G:H5'' | 2.02 | 0.41 |
| 22:BA:1171:G:C5 | 22:BA:1172:C:C4 | 3.08 | 0.41 |
| 22:BA:1195:G:O2' | 22:BA:1196:C:H5' | 2.20 | 0.41 |
| 22:BA:1869:G:C2 | 22:BA:1873:G:C6 | 3.08 | 0.41 |
| 22:BA:2648:G:H2' | 22:BA:2649:C:C6 | 2.55 | 0.41 |
| 24:BC:157:SER:O | 24:BC:158:ALA:C | 2.59 | 0.41 |
| 26:BE:149:ILE:CD1 | 26:BE:172:ALA:N | 2.84 | 0.41 |
| 27:BF:107:ALA:C | 27:BF:109:PRO:HD2 | 2.41 | 0.41 |
| 28:BG:146:ALA:O | 28:BG:149:ARG:HB3 | 2.20 | 0.41 |
| 29:BH:30:LEU:C | 29:BH:32:PRO:HD2 | 2.41 | 0.41 |
| 30:BI:18:ALA:O | 30:BI:19:ASN:HB2 | 2.21 | 0.41 |
| 30:BI:29:GLY:C | 30:BI:30:GLN:HG3 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BK:71:ARG:O | 32:BK:73:ASP:N | 2.53 | 0.41 |
| 36:BO:78:VAL:HG23 | 36:BO:79:ALA:N | 2.36 | 0.41 |
| 37:BP:27:GLU:O | 37:BP:27:GLU:HG3 | 2.21 | 0.41 |
| 39:BR:14:VAL:CG1 | 39:BR:15:SER:N | 2.83 | 0.41 |
| 44:BW:47:ALA:HB1 | 44:BW:51:VAL:O | 2.21 | 0.41 |
| 45:BX:4:VAL:HG22 | 45:BX:11:ARG:HB3 | 2.03 | 0.41 |
| 1:CA:280:C:H4' | 1:CA:281:G:OP2 | 2.21 | 0.41 |
| 1:CA:386:C:C4 | 1:CA:387:U:C5 | 3.09 | 0.41 |
| 1:CA:1074:G:H4' | 2:CB:102:THR:O | 2.21 | 0.41 |
| 1:CA:1243:C:H2' | 1:CA:1244:G:C8 | 2.56 | 0.41 |
| 1:CA:1260:G:OP1 | 1:CA:1284:C:O2' | 2.25 | 0.41 |
| 1:CA:1386:G:N3 | 1:CA:1387:G:C8 | 2.88 | 0.41 |
| 1:CA:1423:G:C6 | 1:CA:1424:U:C4 | 3.09 | 0.41 |
| 2:CB:94:HIS:CG | 2:CB:95:ARG:NH2 | 2.89 | 0.41 |
| 2:CB:116:ASP:O | 2:CB:120:GLN:HB3 | 2.21 | 0.41 |
| 2:CB:170:HIS:CE1 | 2:CB:171:ILE:HG13 | 2.56 | 0.41 |
| 4:CD:33:LYS:NZ | 4:CD:33:LYS:HB2 | 2.35 | 0.41 |
| 4:CD:58:LYS:CB | 4:CD:200:ILE:HB | 2.50 | 0.41 |
| 4:CD:126:ASN:HA | 4:CD:142:VAL:HG23 | 2.01 | 0.41 |
| 5:CE:154:ALA:O | 5:CE:156:LYS:N | 2.54 | 0.41 |
| 5:CE:156:LYS:CD | 8:CH:71:VAL:HG13 | 2.51 | 0.41 |
| 6:CF:9:MET:HG3 | 6:CF:86:ARG:HB2 | 2.02 | 0.41 |
| 6:CF:68:GLN:O | 6:CF:72:ASP:HB2 | 2.21 | 0.41 |
| 8:CH:95:VAL:CG2 | 8:CH:128:TYR:HB3 | 2.51 | 0.41 |
| 9:CI:13:LYS:O | 9:CI:14:SER:CB | 2.69 | 0.41 |
| 16:CP:38:PHE:CZ | 16:CP:51:ARG:HB3 | 2.55 | 0.41 |
| 19:CS:36:ARG:NH1 | 19:CS:72:GLY:HA3 | 2.36 | 0.41 |
| 20:CT:11:ALA:O | 20:CT:14:SER:OG | 2.33 | 0.41 |
| 22:DA:126:A:P | 50:D2:19:ARG:HG3 | 2.60 | 0.41 |
| 22:DA:201:C:C5 | 22:DA:202:U:C5 | 3.08 | 0.41 |
| 22:DA:235:U:C4 | 22:DA:430:A:C2 | 3.08 | 0.41 |
| 22:DA:319:G:OP2 | 26:DE:132:LYS:HE3 | 2.21 | 0.41 |
| 22:DA:319:G:C5 | 22:DA:333:G:C2 | 3.09 | 0.41 |
| 22:DA:492:A:H2' | 22:DA:493:G:O4' | 2.20 | 0.41 |
| 22:DA:612:G:O2' | 22:DA:613:A:C8 | 2.73 | 0.41 |
| 22:DA:1032:A:H4' | 52:D4:16:ILE:HD12 | 2.03 | 0.41 |
| 22:DA:1158:C:H5'' | 47:DZ:31:ARG:HG3 | 2.03 | 0.41 |
| 22:DA:1502:A:C2 | 22:DA:1503:A:C5 | 3.09 | 0.41 |
| 22:DA:1602:U:O4 | 58:DA:3711:HOH:O | 2.20 | 0.41 |
| 22:DA:1654:A:OP1 | 35:DN:1:MET:HA | 2.21 | 0.41 |
| 22:DA:1973:G:C4 | 22:DA:1974:C:C5 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:1999:C:O2 | 22:DA:2687:U:O2' | 2.34 | 0.41 |
| 22:DA:2093:G:C2 | 22:DA:2094:A:N7 | 2.89 | 0.41 |
| 22:DA:2134:A:C8 | 22:DA:2158:A:C2 | 3.08 | 0.41 |
| 22:DA:2303:G:N1 | 22:DA:2314:A:C6 | 2.89 | 0.41 |
| 22:DA:2345:G:C4 | 22:DA:2347:C:C5 | 3.09 | 0.41 |
| 22:DA:2393:U:H2' | 22:DA:2394:C:O4' | 2.21 | 0.41 |
| 22:DA:2648:G:C4 | 22:DA:2673:G:C2 | 3.09 | 0.41 |
| 22:DA:2704:C:H2' | 22:DA:2705:A:O4' | 2.21 | 0.41 |
| 22:DA:2784:U:H2' | 22:DA:2785:C:C6 | 2.56 | 0.41 |
| 56:DA:3001:DOL:N9 | 56:DA:3001:DOL:HC41 | 2.36 | 0.41 |
| 23:DB:7:G:O2' | 36:DO:38:GLN:OE1 | 2.35 | 0.41 |
| 29:DH:2:GLN:O | 29:DH:3:VAL:O | 2.38 | 0.41 |
| 31:DJ:39:LYS:HD3 | 31:DJ:39:LYS:HA | 1.91 | 0.41 |
| 31:DJ:84:ILE:O | 31:DJ:85:LYS:C | 2.59 | 0.41 |
| 32:DK:21:CYS:SG | 32:DK:39:ILE:HB | 2.60 | 0.41 |
| 32:DK:66:LYS:NZ | 32:DK:79:PHE:O | 2.43 | 0.41 |
| 32:DK:92:GLU:HB3 | 32:DK:93:GLN:H | 1.70 | 0.41 |
| 33:DL:23:ILE:HD12 | 39:DR:84:ARG:HG2 | 2.02 | 0.41 |
| 34:DM:19:GLY:C | 34:DM:20:LEU:HD22 | 2.41 | 0.41 |
| 41:DT:34:VAL:HG11 | 41:DT:43:ILE:HD13 | 2.02 | 0.41 |
| 42:DU:13:VAL:HB | 42:DU:18:ASP:O | 2.20 | 0.41 |
| 42:DU:86:ARG:NH2 | 42:DU:95:PHE:HB3 | 2.36 | 0.41 |
| 43:DV:32:GLY:O | 43:DV:93:ARG:HB2 | 2.21 | 0.41 |
| 45:DX:40:VAL:CG1 | 45:DX:68:LEU:HD11 | 2.50 | 0.41 |
| 46:DY:20:ASN:HB3 | 46:DY:50:VAL:HG22 | 2.02 | 0.41 |
| 1:AA:76:G:N2 | 1:AA:95:C:C2 | 2.89 | 0.41 |
| 1:AA:113:G:H2' | 1:AA:114:U:H6 | 1.85 | 0.41 |
| 1:AA:263:A:H2' | 1:AA:264:C:C5 | 2.56 | 0.41 |
| 1:AA:515:G:N2 | 1:AA:537:G:C4 | 2.89 | 0.41 |
| 1:AA:592:G:C6 | 1:AA:593:U:N3 | 2.89 | 0.41 |
| 1:AA:597:G:C8 | 1:AA:598:U:C5 | 3.08 | 0.41 |
| 1:AA:644:U:O2' | 1:AA:645:G:H5' | 2.20 | 0.41 |
| 1:AA:686:U:O4 | 1:AA:703:G:O2' | 2.26 | 0.41 |
| 1:AA:741:G:H2' | 1:AA:742:G:O4' | 2.21 | 0.41 |
| 1:AA:747:A:C6 | 1:AA:748:G:C6 | 3.09 | 0.41 |
| 1:AA:990:C:N3 | 1:AA:991:U:C4 | 2.88 | 0.41 |
| 1:AA:1032:G:H3' | 1:AA:1033:G:O4' | 2.21 | 0.41 |
| 1:AA:1217:C:H2' | 1:AA:1218:C:H6 | 1.86 | 0.41 |
| 1:AA:1323:G:O2' | 1:AA:1324:A:H5' | 2.21 | 0.41 |
| 1:AA:1402:C:H2' | 1:AA:1403:C:O4' | 2.21 | 0.41 |
| 2:AB:101:LEU:HD13 | 2:AB:101:LEU:HA | 1.94 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:151:ILE:O | 2:AB:153:ASP:N | 2.53 | 0.41 |
| 2:AB:157:LEU:HA | 2:AB:158:PRO:HD3 | 1.98 | 0.41 |
| 3:AC:22:TRP:CB | 3:AC:59:ARG:HG2 | 2.49 | 0.41 |
| 3:AC:113:ALA:HB1 | 3:AC:200:VAL:CG2 | 2.51 | 0.41 |
| 4:AD:123:ILE:N | 4:AD:123:ILE:CD1 | 2.82 | 0.41 |
| 5:AE:80:THR:HB | 5:AE:122:ASN:OD1 | 2.20 | 0.41 |
| 5:AE:141:ILE:HG22 | 5:AE:142:ASP:N | 2.36 | 0.41 |
| 5:AE:151:GLU:O | 5:AE:153:VAL:N | 2.54 | 0.41 |
| 6:AF:3:HIS:CE1 | 6:AF:65:GLU:CD | 2.94 | 0.41 |
| 7:AG:42:ILE:HG21 | 7:AG:116:MET:HB3 | 2.02 | 0.41 |
| 9:AI:17:ALA:CB | 9:AI:67:VAL:HB | 2.51 | 0.41 |
| 9:AI:57:MET:C | 9:AI:59:GLU:N | 2.74 | 0.41 |
| 9:AI:105:THR:CG2 | 9:AI:106:ARG:N | 2.84 | 0.41 |
| 9:AI:127:PHE:CD2 | 9:AI:127:PHE:C | 2.92 | 0.41 |
| 10:AJ:29:ALA:O | 10:AJ:32:THR:HG23 | 2.21 | 0.41 |
| 11:AK:36:ASP:OD2 | 11:AK:38:GLN:C | 2.59 | 0.41 |
| 11:AK:65:VAL:O | 11:AK:65:VAL:CG2 | 2.68 | 0.41 |
| 12:AL:24:LEU:HB2 | 12:AL:59:ASN:HD22 | 1.84 | 0.41 |
| 12:AL:67:ILE:HG21 | 12:AL:72:HIS:CD2 | 2.56 | 0.41 |
| 14:AN:73:PHE:CD1 | 14:AN:74:LEU:N | 2.89 | 0.41 |
| 15:AO:22:THR:HG22 | 15:AO:23:GLY:N | 2.35 | 0.41 |
| 16:AP:14:ARG:N | 16:AP:15:PRO:CD | 2.84 | 0.41 |
| 16:AP:22:ALA:HA | 16:AP:33:ILE:CG1 | 2.49 | 0.41 |
| 16:AP:49:GLY:O | 16:AP:50:THR:OG1 | 2.31 | 0.41 |
| 16:AP:78:VAL:O | 16:AP:78:VAL:HG13 | 2.20 | 0.41 |
| 19:AS:36:ARG:NE | 19:AS:52:HIS:O | 2.52 | 0.41 |
| 20:AT:67:ILE:HG13 | 20:AT:71:LYS:CG | 2.48 | 0.41 |
| 20:AT:73:ALA:O | 20:AT:74:ARG:C | 2.60 | 0.41 |
| 22:BA:158:U:O2 | 22:BA:158:U:H2' | 2.21 | 0.41 |
| 22:BA:359:G:H2' | 22:BA:360:U:O4' | 2.21 | 0.41 |
| 22:BA:416:U:C4 | 22:BA:417:C:C4 | 3.08 | 0.41 |
| 22:BA:548:G:O2' | 22:BA:549:G:C2 | 2.72 | 0.41 |
| 22:BA:593:U:H2' | 22:BA:594:U:C6 | 2.56 | 0.41 |
| 22:BA:669:G:C6 | 22:BA:801:G:O6 | 2.73 | 0.41 |
| 22:BA:910:A:N3 | 22:BA:2264:C:O2' | 2.42 | 0.41 |
| 22:BA:936:A:H2' | 22:BA:937:C:C6 | 2.56 | 0.41 |
| 22:BA:975:A:C2 | 22:BA:990:A:C8 | 3.09 | 0.41 |
| 22:BA:982:C:H5'' | 22:BA:983:A:P | 2.60 | 0.41 |
| 22:BA:1011:G:H1' | 22:BA:1013:C:O4' | 2.21 | 0.41 |
| 22:BA:1026:G:C5 | 22:BA:1134:A:C5 | 3.08 | 0.41 |
| 22:BA:1095:A:H2' | 22:BA:1096:A:C8 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1266:G:N7 | 40:BS:16:LYS:HE3 | 2.36 | 0.41 |
| 22:BA:1301:A:C2 | 22:BA:1303:G:C6 | 3.08 | 0.41 |
| 22:BA:1340:U:H4' | 22:BA:1341:G:OP2 | 2.20 | 0.41 |
| 22:BA:1501:G:O2' | 22:BA:1502:A:H5' | 2.21 | 0.41 |
| 22:BA:1537:G:H3' | 22:BA:1537:G:N3 | 2.36 | 0.41 |
| 22:BA:1638:C:H4' | 22:BA:2710:C:O2 | 2.21 | 0.41 |
| 22:BA:1707:G:H2' | 22:BA:1708:C:O4' | 2.21 | 0.41 |
| 22:BA:1734:G:C4 | 22:BA:1735:A:C8 | 3.08 | 0.41 |
| 22:BA:1759:A:H2' | 22:BA:1760:C:C6 | 2.55 | 0.41 |
| 22:BA:1792:G:OP1 | 24:BC:204:VAL:O | 2.38 | 0.41 |
| 22:BA:2189:U:C2' | 22:BA:2190:G:C1' | 2.95 | 0.41 |
| 22:BA:2308:G:C5 | 27:BF:77:PHE:CE2 | 3.09 | 0.41 |
| 22:BA:2379:G:H4' | 36:BO:21:LEU:HD11 | 2.03 | 0.41 |
| 22:BA:2458:G:N3 | 22:BA:2490:G:N2 | 2.69 | 0.41 |
| 22:BA:2592:G:C2' | 22:BA:2593:U:H5' | 2.51 | 0.41 |
| 22:BA:2680:U:H2' | 22:BA:2681:C:C6 | 2.56 | 0.41 |
| 22:BA:2740:A:C6 | 22:BA:2764:A:C8 | 3.08 | 0.41 |
| 22:BA:2771:C:H2' | 22:BA:2772:C:C6 | 2.55 | 0.41 |
| 23:BB:116:G:H4' | 36:BO:54:VAL:CG1 | 2.50 | 0.41 |
| 24:BC:77:VAL:HA | 24:BC:114:ASP:O | 2.21 | 0.41 |
| 24:BC:77:VAL:HG22 | 24:BC:78:VAL:N | 2.35 | 0.41 |
| 24:BC:159:GLY:HA2 | 24:BC:198:ALA:HB2 | 2.02 | 0.41 |
| 25:BD:113:SER:O | 25:BD:167:ASN:N | 2.52 | 0.41 |
| 26:BE:61:ARG:NH2 | 26:BE:64:GLY:HA3 | 2.36 | 0.41 |
| 26:BE:171:ASP:OD1 | 26:BE:171:ASP:C | 2.59 | 0.41 |
| 29:BH:90:LEU:HG | 29:BH:92:GLY:C | 2.42 | 0.41 |
| 29:BH:129:GLU:C | 29:BH:130:VAL:HG23 | 2.41 | 0.41 |
| 29:BH:132:PHE:CE2 | 29:BH:142:VAL:CG2 | 3.04 | 0.41 |
| 30:BI:24:VAL:CG2 | 30:BI:28:LEU:CD2 | 2.99 | 0.41 |
| 30:BI:44:ALA:O | 30:BI:45:LYS:CG | 2.67 | 0.41 |
| 30:BI:115:ALA:O | 30:BI:116:ASP:HB2 | 2.20 | 0.41 |
| 31:BJ:120:ARG:O | 31:BJ:123:LYS:HE2 | 2.21 | 0.41 |
| 33:BL:57:LEU:HG | 51:B3:14:PHE:HZ | 1.86 | 0.41 |
| 34:BM:17:ASN:O | 34:BM:38:ARG:HD3 | 2.21 | 0.41 |
| 36:BO:17:LYS:HA | 36:BO:17:LYS:HD3 | 1.82 | 0.41 |
| 37:BP:51:ARG:O | 37:BP:57:SER:HA | 2.21 | 0.41 |
| 37:BP:103:ARG:CG | 37:BP:103:ARG:NH1 | 2.75 | 0.41 |
| 37:BP:113:ARG:O | 37:BP:114:LEU:HG | 2.21 | 0.41 |
| 40:BS:51:LEU:O | 40:BS:54:ALA:HB3 | 2.21 | 0.41 |
| 42:BU:85:PHE:CD1 | 42:BU:85:PHE:N | 2.89 | 0.41 |
| 49:B1:52:ALA:O | 49:B1:53:LYS:OXT | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:B5:21:TYR:O | 53:B5:22:THR:HG23 | 2.20 | 0.41 |
| 53:B5:61:GLY:O | 53:B5:62:THR:C | 2.59 | 0.41 |
| 1:CA:4:U:O2 | 1:CA:4:U:C2' | 2.68 | 0.41 |
| 1:CA:144:G:C6 | 1:CA:145:G:C5 | 3.09 | 0.41 |
| 1:CA:197:A:C5 | 1:CA:221:C:H4' | 2.55 | 0.41 |
| 1:CA:260:G:C6 | 1:CA:261:U:O4 | 2.74 | 0.41 |
| 1:CA:505:G:C2 | 1:CA:506:G:C5 | 3.09 | 0.41 |
| 1:CA:786:G:C2 | 1:CA:787:A:H1' | 2.55 | 0.41 |
| 1:CA:801:U:N3 | 1:CA:802:A:N7 | 2.69 | 0.41 |
| 1:CA:825:A:H2' | 1:CA:826:C:H6 | 1.86 | 0.41 |
| 1:CA:833:G:C5 | 1:CA:834:U:C5 | 3.09 | 0.41 |
| 1:CA:951:G:C5 | 1:CA:952:U:C4 | 3.09 | 0.41 |
| 1:CA:977:A:N6 | 1:CA:1224:U:O4' | 2.54 | 0.41 |
| 1:CA:992:U:O4 | 1:CA:1044:A:C8 | 2.74 | 0.41 |
| 1:CA:1044:A:N7 | 1:CA:1045:C:H1' | 2.36 | 0.41 |
| 1:CA:1126:U:N1 | 1:CA:1281:C:C5 | 2.89 | 0.41 |
| 1:CA:1211:U:HO2' | 1:CA:1212:U:P | 2.36 | 0.41 |
| 1:CA:1243:C:N4 | 1:CA:1244:G:O6 | 2.54 | 0.41 |
| 1:CA:1245:C:C2 | 1:CA:1246:A:C8 | 3.09 | 0.41 |
| 1:CA:1248:A:N3 | 9:CI:72:ILE:HD11 | 2.35 | 0.41 |
| 1:CA:1255:G:N1 | 1:CA:1279:G:N7 | 2.68 | 0.41 |
| 1:CA:1277:C:HO2' | 1:CA:1279:G:C1' | 2.34 | 0.41 |
| 1:CA:1298:U:H4' | 1:CA:1299:A:C4 | 2.55 | 0.41 |
| 1:CA:1346:A:O3' | 1:CA:1347:G:H4' | 2.20 | 0.41 |
| 2:CB:71:GLY:HA3 | 2:CB:164:ILE:HG21 | 2.03 | 0.41 |
| 3:CC:23:PHE:CD2 | 10:CJ:97:ASP:HB2 | 2.56 | 0.41 |
| 3:CC:43:LEU:HD21 | 3:CC:68:ILE:HD11 | 2.02 | 0.41 |
| 4:CD:35:GLU:O | 4:CD:37:ALA:N | 2.49 | 0.41 |
| 4:CD:58:LYS:HE2 | 4:CD:69:GLU:OE1 | 2.21 | 0.41 |
| 4:CD:90:LEU:CD2 | 4:CD:200:ILE:HD11 | 2.50 | 0.41 |
| 5:CE:100:SER:O | 5:CE:102:GLY:N | 2.54 | 0.41 |
| 7:CG:57:SER:HB3 | 7:CG:60:GLU:HB2 | 2.03 | 0.41 |
| 8:CH:95:VAL:HG12 | 8:CH:96:MET:N | 2.36 | 0.41 |
| 10:CJ:52:LEU:HD21 | 10:CJ:59:LYS:HA | 2.02 | 0.41 |
| 10:CJ:71:LEU:O | 10:CJ:72:ARG:HD3 | 2.21 | 0.41 |
| 10:CJ:78:GLU:HG3 | 10:CJ:80:THR:OG1 | 2.20 | 0.41 |
| 11:CK:50:SER:HB3 | 11:CK:65:VAL:CG2 | 2.51 | 0.41 |
| 11:CK:82:LEU:CD2 | 11:CK:105:PHE:HB3 | 2.51 | 0.41 |
| 12:CL:36:ARG:O | 12:CL:54:ARG:N | 2.53 | 0.41 |
| 12:CL:47:SER:O | 12:CL:48:ALA:HB3 | 2.19 | 0.41 |
| 15:CO:58:ARG:O | 15:CO:62:GLN:HB2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:CP:21:VAL:HG23 | 16:CP:36:VAL:CG2 | 2.51 | 0.41 |
| 17:CQ:24:ALA:HA | 17:CQ:43:LYS:HA | 2.01 | 0.41 |
| 17:CQ:46:VAL:HG12 | 17:CQ:47:HIS:N | 2.36 | 0.41 |
| 17:CQ:49:GLU:O | 17:CQ:50:ASN:CG | 2.59 | 0.41 |
| 20:CT:37:ALA:HA | 20:CT:40:GLU:HB3 | 2.03 | 0.41 |
| 20:CT:79:LEU:O | 20:CT:83:ILE:HG23 | 2.20 | 0.41 |
| 21:CU:41:PRO:O | 21:CU:42:THR:C | 2.59 | 0.41 |
| 22:DA:80:G:O2' | 22:DA:346:A:N7 | 2.52 | 0.41 |
| 22:DA:116:C:H4' | 22:DA:127:A:H5' | 2.03 | 0.41 |
| 22:DA:120:U:O4 | 22:DA:177:G:C8 | 2.74 | 0.41 |
| 22:DA:236:C:H2' | 22:DA:237:C:H6 | 1.85 | 0.41 |
| 22:DA:320:A:H4' | 22:DA:322:A:N7 | 2.36 | 0.41 |
| 22:DA:371:A:N3 | 45:DX:61:LYS:NZ | 2.67 | 0.41 |
| 22:DA:532:A:H3' | 38:DQ:28:ARG:CZ | 2.51 | 0.41 |
| 22:DA:542:C:N4 | 22:DA:543:G:O6 | 2.53 | 0.41 |
| 22:DA:561:G:O2' | 38:DQ:45:TYR:OH | 2.28 | 0.41 |
| 22:DA:562:U:H2' | 22:DA:572:A:O4' | 2.21 | 0.41 |
| 22:DA:580:U:H2' | 22:DA:581:C:O4' | 2.21 | 0.41 |
| 22:DA:616:A:C2 | 22:DA:617:G:C1' | 3.04 | 0.41 |
| 22:DA:616:A:N3 | 22:DA:616:A:H2' | 2.36 | 0.41 |
| 22:DA:667:U:C4 | 22:DA:668:A:C5 | 3.08 | 0.41 |
| 22:DA:961:C:C6 | 22:DA:2031:A:C2 | 3.09 | 0.41 |
| 22:DA:971:G:C2 | 22:DA:972:A:H1' | 2.56 | 0.41 |
| 22:DA:1068:G:H2' | 22:DA:1096:A:H5' | 2.03 | 0.41 |
| 22:DA:1361:G:C4 | 22:DA:1362:C:C5 | 3.08 | 0.41 |
| 22:DA:1370:C:N3 | 22:DA:1371:G:C5 | 2.89 | 0.41 |
| 22:DA:1409:U:H2' | 22:DA:1410:G:C8 | 2.56 | 0.41 |
| 22:DA:1652:A:C2 | 22:DA:2006:C:N3 | 2.89 | 0.41 |
| 22:DA:2023:C:O2' | 22:DA:2024:G:H5' | 2.21 | 0.41 |
| 22:DA:2128:G:C4 | 22:DA:2173:A:O2' | 2.72 | 0.41 |
| 22:DA:2290:G:H2' | 22:DA:2291:U:O4' | 2.20 | 0.41 |
| 22:DA:2416:C:H2' | 22:DA:2417:C:C6 | 2.56 | 0.41 |
| 22:DA:2468:A:C2 | 22:DA:2481:G:C2 | 3.09 | 0.41 |
| 22:DA:2624:G:H1' | 48:D0:19:HIS:HE1 | 1.86 | 0.41 |
| 22:DA:2651:C:O2' | 22:DA:2652:C:H5' | 2.20 | 0.41 |
| 23:DB:34:A:C6 | 23:DB:44:G:C4 | 3.09 | 0.41 |
| 23:DB:77:U:C2' | 23:DB:78:A:H5' | 2.51 | 0.41 |
| 24:DC:145:GLU:HG2 | 24:DC:152:GLY:N | 2.36 | 0.41 |
| 24:DC:267:ILE:O | 24:DC:267:ILE:CG2 | 2.69 | 0.41 |
| 25:DD:35:THR:O | 25:DD:36:GLN:HB2 | 2.21 | 0.41 |
| 26:DE:148:ILE:HB | 26:DE:169:VAL:HG13 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DE:149:ILE:CG2 | 26:DE:188:MET:HG2 | 2.51 | 0.41 |
| 27:DF:6:ASP:HA | 27:DF:9:LYS:CD | 2.51 | 0.41 |
| 27:DF:141:ILE:O | 27:DF:141:ILE:HG22 | 2.21 | 0.41 |
| 28:DG:141:ILE:O | 28:DG:145:ALA:N | 2.53 | 0.41 |
| 28:DG:144:VAL:O | 28:DG:144:VAL:CG1 | 2.69 | 0.41 |
| 29:DH:1:MET:HB3 | 29:DH:21:VAL:O | 2.20 | 0.41 |
| 30:DI:22:PRO:CB | 30:DI:23:PRO:HD3 | 2.51 | 0.41 |
| 31:DJ:6:ALA:O | 31:DJ:7:LYS:CB | 2.68 | 0.41 |
| 31:DJ:34:ARG:CZ | 31:DJ:39:LYS:HG3 | 2.50 | 0.41 |
| 32:DK:2:ILE:N | 32:DK:33:ALA:O | 2.52 | 0.41 |
| 32:DK:64:ARG:HD3 | 32:DK:102:PRO:O | 2.21 | 0.41 |
| 32:DK:78:ARG:NH2 | 37:DP:73:VAL:CG1 | 2.84 | 0.41 |
| 33:DL:90:VAL:CG1 | 33:DL:125:LEU:HD22 | 2.51 | 0.41 |
| 34:DM:95:LEU:O | 34:DM:97:GLN:NE2 | 2.54 | 0.41 |
| 34:DM:135:VAL:O | 34:DM:136:MET:HB3 | 2.21 | 0.41 |
| 36:DO:99:TYR:CZ | 36:DO:104:GLN:HG3 | 2.55 | 0.41 |
| 37:DP:63:LYS:O | 37:DP:63:LYS:CG | 2.69 | 0.41 |
| 38:DQ:58:ARG:NH2 | 38:DQ:92:ARG:CZ | 2.84 | 0.41 |
| 39:DR:1:MET:HA | 39:DR:42:ALA:O | 2.21 | 0.41 |
| 39:DR:85:LYS:HG2 | 39:DR:86:GLN:N | 2.35 | 0.41 |
| 40:DS:32:ALA:O | 40:DS:35:ILE:HB | 2.21 | 0.41 |
| 41:DT:44:LYS:O | 41:DT:48:GLN:HG2 | 2.20 | 0.41 |
| 43:DV:63:ILE:CD1 | 43:DV:72:VAL:HG21 | 2.51 | 0.41 |
| 50:D2:44:VAL:O | 50:D2:45:SER:CB | 2.69 | 0.41 |
| 1:AA:596:A:C5 | 1:AA:645:G:C2 | 3.09 | 0.41 |
| 1:AA:628:G:H2' | 1:AA:629:A:O4' | 2.21 | 0.41 |
| 1:AA:655:A:N1 | 1:AA:656:G:C5 | 2.89 | 0.41 |
| 1:AA:947:G:C5 | 1:AA:948:C:C4 | 3.08 | 0.41 |
| 1:AA:1069:C:H2' | 1:AA:1070:U:O5' | 2.21 | 0.41 |
| 1:AA:1360:A:C8 | 14:AN:58:SER:HB3 | 2.56 | 0.41 |
| 1:AA:1476:A:H2' | 1:AA:1477:U:O4' | 2.20 | 0.41 |
| 2:AB:78:GLU:C | 2:AB:80:VAL:H | 2.24 | 0.41 |
| 2:AB:151:ILE:CG2 | 2:AB:152:LYS:N | 2.84 | 0.41 |
| 4:AD:122:ALA:C | 4:AD:123:ILE:HG23 | 2.41 | 0.41 |
| 4:AD:159:LEU:HD13 | 4:AD:175:ALA:HA | 2.02 | 0.41 |
| 5:AE:109:GLY:HA2 | 5:AE:112:ARG:HB3 | 2.03 | 0.41 |
| 8:AH:25:VAL:CG1 | 8:AH:61:LEU:HB2 | 2.50 | 0.41 |
| 10:AJ:29:ALA:HA | 10:AJ:32:THR:CG2 | 2.51 | 0.41 |
| 13:AM:40:ALA:HB3 | 13:AM:43:VAL:CG1 | 2.51 | 0.41 |
| 13:AM:109:ARG:HG3 | 13:AM:109:ARG:O | 2.20 | 0.41 |
| 14:AN:66:GLN:HG3 | 14:AN:79:LEU:HD21 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AT:58:VAL:HG13 | 20:AT:72:ALA:CB | 2.51 | 0.41 |
| 21:AU:14:VAL:HG13 | 21:AU:16:LEU:HD11 | 2.03 | 0.41 |
| 22:BA:22:C:H2' | 22:BA:23:G:O5' | 2.21 | 0.41 |
| 22:BA:784:G:O2' | 22:BA:785:G:H5'' | 2.21 | 0.41 |
| 22:BA:864:G:O2' | 22:BA:865:C:H5' | 2.20 | 0.41 |
| 22:BA:988:A:OP2 | 47:BZ:12:SER:HB3 | 2.21 | 0.41 |
| 22:BA:1353:A:C2' | 22:BA:1354:A:H5' | 2.51 | 0.41 |
| 22:BA:1515:A:H2' | 22:BA:1516:G:O4' | 2.21 | 0.41 |
| 22:BA:1607:C:C4 | 22:BA:1622:G:N7 | 2.88 | 0.41 |
| 22:BA:1789:A:H5'' | 24:BC:219:THR:O | 2.20 | 0.41 |
| 22:BA:2313:C:H5'' | 27:BF:88:LYS:HD3 | 2.03 | 0.41 |
| 22:BA:2345:G:N3 | 22:BA:2381:A:H2' | 2.35 | 0.41 |
| 22:BA:2820:A:C2' | 22:BA:2821:A:OP1 | 2.69 | 0.41 |
| 26:BE:149:ILE:CD1 | 26:BE:172:ALA:CA | 2.96 | 0.41 |
| 29:BH:129:GLU:C | 29:BH:130:VAL:CG2 | 2.90 | 0.41 |
| 30:BI:101:ILE:HD11 | 30:BI:138:LEU:HD13 | 2.03 | 0.41 |
| 37:BP:65:SER:O | 37:BP:66:ASN:C | 2.59 | 0.41 |
| 38:BQ:50:ARG:NH2 | 39:BR:74:ILE:HD12 | 2.36 | 0.41 |
| 39:BR:74:ILE:N | 39:BR:74:ILE:HD13 | 2.35 | 0.41 |
| 53:B5:76:LEU:O | 53:B5:122:GLY:N | 2.54 | 0.41 |
| 53:B5:191:ARG:O | 53:B5:195:ARG:N | 2.54 | 0.41 |
| 1:CA:173:U:H1' | 1:CA:197:A:C5 | 2.56 | 0.41 |
| 1:CA:189:A:N6 | 1:CA:190:A:N1 | 2.69 | 0.41 |
| 1:CA:204:G:H2' | 1:CA:205:A:O4' | 2.21 | 0.41 |
| 1:CA:206:C:H2' | 1:CA:207:C:C4' | 2.51 | 0.41 |
| 1:CA:295:C:C4 | 1:CA:296:U:C4 | 3.09 | 0.41 |
| 1:CA:462:G:N2 | 1:CA:471:U:C2 | 2.89 | 0.41 |
| 1:CA:511:C:C2 | 1:CA:512:U:C6 | 3.09 | 0.41 |
| 1:CA:604:G:C6 | 1:CA:605:U:C4 | 3.09 | 0.41 |
| 1:CA:784:A:H2' | 1:CA:785:G:O4' | 2.20 | 0.41 |
| 1:CA:844:G:OP2 | 1:CA:844:G:N9 | 2.54 | 0.41 |
| 1:CA:994:A:C2 | 1:CA:995:C:C1' | 3.04 | 0.41 |
| 1:CA:1126:U:C5 | 1:CA:1281:C:N4 | 2.88 | 0.41 |
| 1:CA:1262:C:N4 | 1:CA:1263:C:C4 | 2.89 | 0.41 |
| 1:CA:1271:A:H5' | 1:CA:1314:C:OP1 | 2.20 | 0.41 |
| 1:CA:1388:C:C2 | 1:CA:1389:C:C5 | 3.09 | 0.41 |
| 1:CA:1462:C:H2' | 1:CA:1463:U:C6 | 2.56 | 0.41 |
| 1:CA:1527:U:H2' | 1:CA:1528:U:C6 | 2.56 | 0.41 |
| 2:CB:221:VAL:O | 2:CB:221:VAL:CG1 | 2.69 | 0.41 |
| 3:CC:40:ARG:NH1 | 3:CC:55:ILE:HG13 | 2.36 | 0.41 |
| 5:CE:16:ILE:CD1 | 5:CE:38:VAL:HG23 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:CG:75:VAL:CG2 | 7:CG:144:MET:HG2 | 2.51 | 0.41 |
| 7:CG:88:PRO:HD2 | 7:CG:151:PHE:O | 2.21 | 0.41 |
| 7:CG:130:ASN:HA | 7:CG:135:VAL:HG11 | 2.02 | 0.41 |
| 9:CI:21:ILE:O | 9:CI:21:ILE:HG22 | 2.20 | 0.41 |
| 17:CQ:12:VAL:CG1 | 17:CQ:21:ILE:HD11 | 2.51 | 0.41 |
| 18:CR:25:ASP:O | 18:CR:27:ALA:N | 2.53 | 0.41 |
| 22:DA:184:C:H2' | 22:DA:185:G:C8 | 2.56 | 0.41 |
| 22:DA:218:A:C6 | 22:DA:219:A:C5 | 3.08 | 0.41 |
| 22:DA:222:A:N1 | 22:DA:233:A:H5'' | 2.35 | 0.41 |
| 22:DA:349:U:H2' | 22:DA:350:G:H8 | 1.86 | 0.41 |
| 22:DA:362:A:N7 | 22:DA:363:G:N7 | 2.69 | 0.41 |
| 22:DA:420:C:C2 | 22:DA:421:C:C5 | 3.09 | 0.41 |
| 22:DA:543:G:C2 | 22:DA:551:G:C6 | 3.09 | 0.41 |
| 22:DA:586:A:OP2 | 22:DA:586:A:C8 | 2.74 | 0.41 |
| 22:DA:630:G:C5' | 22:DA:631:A:OP2 | 2.69 | 0.41 |
| 22:DA:642:U:H1' | 22:DA:644:A:N7 | 2.36 | 0.41 |
| 22:DA:647:G:C4 | 22:DA:648:G:C8 | 3.09 | 0.41 |
| 22:DA:822:G:O6 | 22:DA:943:A:H2 | 2.04 | 0.41 |
| 22:DA:1203:U:C4 | 22:DA:1204:A:C5 | 3.09 | 0.41 |
| 22:DA:1334:G:C6 | 22:DA:1335:C:N3 | 2.89 | 0.41 |
| 22:DA:1352:U:H5 | 22:DA:1377:G:C6 | 2.39 | 0.41 |
| 22:DA:1437:C:N3 | 22:DA:1438:U:C4 | 2.89 | 0.41 |
| 22:DA:1567:G:N7 | 24:DC:83:TYR:CD1 | 2.89 | 0.41 |
| 22:DA:1751:U:O4' | 22:DA:2860:A:C2 | 2.74 | 0.41 |
| 22:DA:1866:A:C2 | 22:DA:1876:A:C5 | 3.09 | 0.41 |
| 22:DA:1926:U:H2' | 22:DA:1928:A:C8 | 2.55 | 0.41 |
| 22:DA:2050:C:C4 | 22:DA:2051:A:C6 | 3.08 | 0.41 |
| 22:DA:2083:G:N7 | 22:DA:2084:C:C5 | 2.89 | 0.41 |
| 22:DA:2177:C:H2' | 22:DA:2178:C:C6 | 2.56 | 0.41 |
| 22:DA:2267:A:H5'' | 22:DA:2268:A:C5' | 2.51 | 0.41 |
| 22:DA:2271:G:H2' | 22:DA:2272:U:C6 | 2.56 | 0.41 |
| 22:DA:2327:A:H2' | 22:DA:2328:A:C8 | 2.55 | 0.41 |
| 22:DA:2366:A:H2' | 22:DA:2367:G:H5' | 2.02 | 0.41 |
| 22:DA:2516:A:C2' | 22:DA:2517:C:O5' | 2.69 | 0.41 |
| 22:DA:2659:G:C4 | 22:DA:2661:G:OP2 | 2.74 | 0.41 |
| 22:DA:2741:A:C2' | 22:DA:2742:G:H5' | 2.51 | 0.41 |
| 22:DA:2831:G:N7 | 25:DD:59:ARG:NH1 | 2.67 | 0.41 |
| 22:DA:2893:A:O4' | 22:DA:2894:G:C2 | 2.74 | 0.41 |
| 24:DC:24:LEU:HD11 | 24:DC:90:ASN:HD21 | 1.86 | 0.41 |
| 24:DC:145:GLU:HA | 24:DC:152:GLY:HA2 | 2.03 | 0.41 |
| 24:DC:175:ARG:O | 24:DC:175:ARG:HG3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DD:56:LYS:C | 25:DD:58:ASN:N | 2.75 | 0.41 |
| 30:DI:57:VAL:HG22 | 30:DI:58:VAL:N | 2.36 | 0.41 |
| 31:DJ:102:GLU:O | 31:DJ:106:LYS:HB2 | 2.21 | 0.41 |
| 41:DT:11:LEU:CD2 | 41:DT:34:VAL:HG12 | 2.51 | 0.41 |
| 41:DT:30:ILE:HD13 | 41:DT:32:LEU:HG | 2.02 | 0.41 |
| 41:DT:30:ILE:HG23 | 41:DT:32:LEU:HG | 2.03 | 0.41 |
| 1:AA:257:G:C2 | 1:AA:258:G:C5 | 3.09 | 0.40 |
| 1:AA:508:U:H1' | 1:AA:509:A:N7 | 2.36 | 0.40 |
| 1:AA:972:C:H4' | 10:AJ:59:LYS:HE3 | 2.02 | 0.40 |
| 1:AA:1143:G:C5 | 1:AA:1144:G:N7 | 2.89 | 0.40 |
| 1:AA:1190:G:P | 3:AC:5:VAL:HG12 | 2.61 | 0.40 |
| 1:AA:1191:A:OP1 | 3:AC:4:LYS:HD3 | 2.21 | 0.40 |
| 1:AA:1322:C:O2' | 1:AA:1323:G:P | 2.79 | 0.40 |
| 1:AA:1501:C:C4 | 1:AA:1504:G:C5 | 3.09 | 0.40 |
| 3:AC:16:LYS:HG3 | 3:AC:17:PRO:HD2 | 2.02 | 0.40 |
| 3:AC:85:GLU:C | 3:AC:87:LEU:N | 2.72 | 0.40 |
| 5:AE:50:TYR:O | 5:AE:63:ALA:CB | 2.69 | 0.40 |
| 5:AE:98:PRO:O | 5:AE:99:ALA:HB3 | 2.20 | 0.40 |
| 6:AF:54:LEU:O | 6:AF:54:LEU:HD13 | 2.21 | 0.40 |
| 6:AF:64:VAL:CG1 | 6:AF:65:GLU:N | 2.84 | 0.40 |
| 8:AH:46:ILE:HG22 | 8:AH:63:LEU:HA | 2.02 | 0.40 |
| 10:AJ:36:VAL:HA | 10:AJ:75:ASP:O | 2.21 | 0.40 |
| 11:AK:70:CYS:O | 11:AK:74:VAL:HG22 | 2.21 | 0.40 |
| 16:AP:51:ARG:HH11 | 16:AP:51:ARG:HB3 | 1.86 | 0.40 |
| 16:AP:61:VAL:HG22 | 16:AP:67:ILE:HD11 | 2.02 | 0.40 |
| 21:AU:25:LYS:O | 21:AU:27:GLY:N | 2.54 | 0.40 |
| 22:BA:63:A:C2 | 22:BA:64:A:C8 | 3.09 | 0.40 |
| 22:BA:404:A:C2' | 22:BA:405:U:OP2 | 2.69 | 0.40 |
| 22:BA:499:U:C4 | 22:BA:500:G:C6 | 3.10 | 0.40 |
| 22:BA:528:A:C2 | 22:BA:2043:C:C4' | 3.01 | 0.40 |
| 22:BA:585:G:H5'' | 22:BA:586:A:P | 2.61 | 0.40 |
| 22:BA:725:G:C6 | 22:BA:726:G:N1 | 2.88 | 0.40 |
| 22:BA:1179:G:C8 | 22:BA:1180:U:O4' | 2.74 | 0.40 |
| 22:BA:1196:C:H1' | 22:BA:1226:A:C4 | 2.57 | 0.40 |
| 22:BA:1378:A:C2' | 58:BA:3753:HOH:O | 2.69 | 0.40 |
| 22:BA:1414:C:C5 | 22:BA:1415:U:H5 | 2.39 | 0.40 |
| 22:BA:1478:G:H1 | 22:BA:1513:U:H3 | 1.69 | 0.40 |
| 22:BA:1846:G:C2 | 22:BA:1895:C:C2 | 3.09 | 0.40 |
| 22:BA:1851:U:O2' | 22:BA:1852:U:H5' | 2.21 | 0.40 |
| 22:BA:1900:A:O2' | 22:BA:1901:A:OP1 | 2.29 | 0.40 |
| 22:BA:1913:A:OP2 | 22:BA:1913:A:H2' | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2694:G:C5 | 22:BA:2695:U:C4 | 3.09 | 0.40 |
| 25:BD:113:SER:O | 25:BD:167:ASN:HA | 2.22 | 0.40 |
| 26:BE:31:VAL:HG21 | 26:BE:104:ALA:CB | 2.51 | 0.40 |
| 29:BH:1:MET:HE3 | 29:BH:26:ALA:HB3 | 2.02 | 0.40 |
| 29:BH:88:GLY:C | 29:BH:125:THR:OG1 | 2.59 | 0.40 |
| 29:BH:97:ARG:NH1 | 1:CA:369:G:C2' | 2.84 | 0.40 |
| 36:BO:117:PHE:CD1 | 36:BO:117:PHE:O | 2.74 | 0.40 |
| 42:BU:26:LYS:HA | 42:BU:26:LYS:CE | 2.51 | 0.40 |
| 42:BU:39:ILE:O | 42:BU:40:ASN:C | 2.58 | 0.40 |
| 43:BV:26:PHE:CZ | 43:BV:42:LEU:HD12 | 2.57 | 0.40 |
| 46:BY:54:LYS:HA | 46:BY:57:LEU:HD23 | 2.02 | 0.40 |
| 53:B5:94:TYR:O | 53:B5:95:VAL:HG23 | 2.20 | 0.40 |
| 1:CA:246:A:N3 | 1:CA:279:A:N6 | 2.68 | 0.40 |
| 1:CA:249:U:C2 | 1:CA:276:G:N1 | 2.89 | 0.40 |
| 1:CA:407:U:C2 | 1:CA:408:A:C8 | 3.09 | 0.40 |
| 1:CA:552:U:H4' | 12:CL:83:ARG:CG | 2.51 | 0.40 |
| 1:CA:603:U:H2' | 1:CA:604:G:C8 | 2.56 | 0.40 |
| 1:CA:811:C:C5 | 1:CA:812:G:C5 | 3.10 | 0.40 |
| 1:CA:875:U:O3' | 8:CH:15:ARG:NH1 | 2.53 | 0.40 |
| 1:CA:1014:A:N3 | 19:CS:34:TRP:CZ2 | 2.89 | 0.40 |
| 1:CA:1084:G:H5' | 1:CA:1102:A:OP2 | 2.21 | 0.40 |
| 1:CA:1126:U:C6 | 1:CA:1281:C:C4 | 3.08 | 0.40 |
| 1:CA:1262:C:N4 | 1:CA:1263:C:N4 | 2.68 | 0.40 |
| 2:CB:47:VAL:HB | 2:CB:48:PRO:CD | 2.51 | 0.40 |
| 5:CE:102:GLY:C | 5:CE:104:GLY:N | 2.72 | 0.40 |
| 5:CE:155:ALA:C | 5:CE:156:LYS:HG3 | 2.41 | 0.40 |
| 6:CF:29:ILE:HG21 | 6:CF:64:VAL:CG1 | 2.51 | 0.40 |
| 9:CI:83:ILE:O | 9:CI:87:LEU:N | 2.53 | 0.40 |
| 13:CM:71:ARG:HA | 13:CM:74:SER:HB3 | 2.02 | 0.40 |
| 19:CS:64:ASP:O | 19:CS:67:VAL:HG23 | 2.21 | 0.40 |
| 22:DA:225:C:H2' | 22:DA:226:A:O4' | 2.20 | 0.40 |
| 22:DA:416:U:H2' | 22:DA:417:C:C6 | 2.56 | 0.40 |
| 22:DA:443:A:C8 | 26:DE:40:ARG:CG | 3.04 | 0.40 |
| 22:DA:444:C:OP2 | 22:DA:444:C:H4' | 2.22 | 0.40 |
| 22:DA:567:U:H4' | 22:DA:808:G:OP1 | 2.22 | 0.40 |
| 22:DA:585:G:C6 | 22:DA:1251:C:C5 | 3.09 | 0.40 |
| 22:DA:638:G:O6 | 22:DA:650:C:N3 | 2.54 | 0.40 |
| 22:DA:783:A:C4 | 22:DA:785:G:H1' | 2.56 | 0.40 |
| 22:DA:919:U:C4 | 22:DA:920:A:C5 | 3.10 | 0.40 |
| 22:DA:1205:A:C2 | 26:DE:165:HIS:HB2 | 2.56 | 0.40 |
| 22:DA:1401:G:C5 | 22:DA:1402:U:C5 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1401:G:C6 | 22:DA:1402:U:C4 | 3.09 | 0.40 |
| 22:DA:1468:U:H2' | 22:DA:1522:A:N6 | 2.36 | 0.40 |
| 22:DA:1545:A:H2' | 22:DA:1546:G:O4' | 2.21 | 0.40 |
| 22:DA:1676:A:N6 | 22:DA:1677:A:C6 | 2.89 | 0.40 |
| 22:DA:1773:A:C2 | 22:DA:1978:A:C2 | 3.09 | 0.40 |
| 22:DA:2066:C:O2' | 22:DA:2067:G:H5' | 2.20 | 0.40 |
| 22:DA:2093:G:C2 | 22:DA:2094:A:C8 | 3.08 | 0.40 |
| 22:DA:2145:C:H5'' | 22:DA:2146:C:OP1 | 2.21 | 0.40 |
| 22:DA:2250:G:C8 | 22:DA:2250:G:O5' | 2.74 | 0.40 |
| 22:DA:2262:U:H4' | 22:DA:2328:A:C2 | 2.56 | 0.40 |
| 22:DA:2326:C:H1' | 22:DA:2327:A:OP1 | 2.21 | 0.40 |
| 22:DA:2702:G:C5 | 22:DA:2703:C:C5 | 3.09 | 0.40 |
| 22:DA:2825:G:C2' | 22:DA:2826:A:H5' | 2.50 | 0.40 |
| 23:DB:55:U:H4' | 27:DF:25:VAL:HG12 | 2.03 | 0.40 |
| 24:DC:45:ASN:C | 24:DC:47:GLY:H | 2.25 | 0.40 |
| 25:DD:33:ARG:NH2 | 25:DD:74:GLU:O | 2.54 | 0.40 |
| 27:DF:73:SER:HB2 | 27:DF:81:GLN:HB2 | 2.03 | 0.40 |
| 30:DI:28:LEU:HD13 | 30:DI:38:PHE:CE2 | 2.56 | 0.40 |
| 31:DJ:110:PRO:O | 31:DJ:115:GLY:HA3 | 2.21 | 0.40 |
| 32:DK:9:ASN:O | 32:DK:83:ALA:HA | 2.20 | 0.40 |
| 34:DM:63:ILE:CG2 | 34:DM:64:TRP:N | 2.84 | 0.40 |
| 35:DN:103:ARG:HB2 | 35:DN:110:MET:HE3 | 2.03 | 0.40 |
| 36:DO:79:ALA:CB | 36:DO:113:ALA:HB3 | 2.50 | 0.40 |
| 41:DT:62:VAL:CG1 | 41:DT:63:VAL:N | 2.84 | 0.40 |
| 44:DW:47:ALA:HB2 | 44:DW:59:LEU:HD22 | 2.04 | 0.40 |
| 1:AA:126:G:H2' | 1:AA:127:G:O4' | 2.22 | 0.40 |
| 1:AA:246:A:H4' | 1:AA:247:G:OP1 | 2.21 | 0.40 |
| 1:AA:451:A:C5' | 16:AP:70:ARG:HH22 | 2.34 | 0.40 |
| 1:AA:606:G:H1' | 1:AA:633:G:C2 | 2.56 | 0.40 |
| 1:AA:751:U:H4' | 15:AO:24:SER:HA | 2.01 | 0.40 |
| 1:AA:1008:U:H2' | 1:AA:1009:U:C6 | 2.56 | 0.40 |
| 1:AA:1256:A:N6 | 1:AA:1277:C:C2 | 2.90 | 0.40 |
| 1:AA:1356:G:H2' | 1:AA:1357:A:C8 | 2.57 | 0.40 |
| 2:AB:118:GLU:HB3 | 2:AB:141:LEU:HD11 | 2.02 | 0.40 |
| 2:AB:148:LEU:HD22 | 2:AB:148:LEU:HA | 1.92 | 0.40 |
| 4:AD:28:ILE:O | 4:AD:29:ASP:C | 2.60 | 0.40 |
| 4:AD:60:LYS:NZ | 4:AD:194:ASP:O | 2.54 | 0.40 |
| 5:AE:50:TYR:CE2 | 5:AE:134:ILE:HD11 | 2.56 | 0.40 |
| 5:AE:105:ILE:HG13 | 5:AE:105:ILE:O | 2.21 | 0.40 |
| 6:AF:76:THR:O | 6:AF:79:ARG:N | 2.51 | 0.40 |
| 6:AF:98:GLU:O | 6:AF:99:ALA:C | 2.59 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AI:52:LEU:HA | 9:AI:55:VAL:HG23 | 2.03 | 0.40 |
| 12:AL:110:ARG:NH1 | 12:AL:113:ALA:HB3 | 2.36 | 0.40 |
| 17:AQ:8:LEU:N | 17:AQ:8:LEU:HD13 | 2.36 | 0.40 |
| 17:AQ:81:LYS:N | 17:AQ:81:LYS:HE2 | 2.36 | 0.40 |
| 19:AS:52:HIS:CD2 | 19:AS:54:GLY:N | 2.89 | 0.40 |
| 21:AU:25:LYS:C | 21:AU:27:GLY:N | 2.75 | 0.40 |
| 22:BA:467:G:H2' | 22:BA:468:G:O4' | 2.22 | 0.40 |
| 22:BA:531:C:C5 | 22:BA:2035:G:C2 | 3.10 | 0.40 |
| 22:BA:792:A:N3 | 22:BA:2072:C:O2' | 2.35 | 0.40 |
| 22:BA:1330:C:O2' | 22:BA:1331:G:H5' | 2.20 | 0.40 |
| 22:BA:1334:G:C6 | 22:BA:1335:C:C4 | 3.10 | 0.40 |
| 22:BA:1356:G:C2 | 22:BA:1357:C:C2 | 3.09 | 0.40 |
| 22:BA:1922:G:C2 | 22:BA:1923:U:C6 | 3.09 | 0.40 |
| 22:BA:2030:A:C2 | 22:BA:2499:C:H5'' | 2.56 | 0.40 |
| 22:BA:2247:A:C2' | 22:BA:2248:C:O5' | 2.70 | 0.40 |
| 22:BA:2286:G:H4' | 22:BA:2287:A:O4' | 2.20 | 0.40 |
| 22:BA:2492:U:H2' | 22:BA:2493:U:H6 | 1.87 | 0.40 |
| 22:BA:2665:A:C2 | 22:BA:2666:C:C2 | 3.09 | 0.40 |
| 24:BC:24:LEU:HD12 | 24:BC:24:LEU:HA | 1.85 | 0.40 |
| 24:BC:53:HIS:CD2 | 24:BC:219:THR:HA | 2.56 | 0.40 |
| 24:BC:141:VAL:HG13 | 24:BC:191:THR:C | 2.42 | 0.40 |
| 24:BC:199:GLU:O | 24:BC:200:HIS:C | 2.59 | 0.40 |
| 26:BE:37:ALA:O | 26:BE:40:ARG:HB2 | 2.21 | 0.40 |
| 26:BE:61:ARG:HD2 | 26:BE:63:LYS:O | 2.22 | 0.40 |
| 30:BI:100:LYS:HD2 | 30:BI:139:VAL:HG21 | 2.02 | 0.40 |
| 30:BI:133:ALA:O | 30:BI:138:LEU:HD12 | 2.21 | 0.40 |
| 31:BJ:37:ARG:O | 31:BJ:37:ARG:HG3 | 2.20 | 0.40 |
| 32:BK:122:VAL:OXT | 32:BK:122:VAL:HG12 | 2.22 | 0.40 |
| 42:BU:22:ARG:CZ | 42:BU:73:PHE:CE2 | 3.04 | 0.40 |
| 47:BZ:56:LYS:HE3 | 47:BZ:58:GLU:OE1 | 2.21 | 0.40 |
| 49:B1:38:LYS:HB2 | 49:B1:49:TYR:CD2 | 2.56 | 0.40 |
| 53:B5:23:ILE:O | 53:B5:23:ILE:HG22 | 2.22 | 0.40 |
| 53:B5:74:ARG:HB3 | 53:B5:93:ASP:OD1 | 2.22 | 0.40 |
| 1:CA:68:G:C6 | 1:CA:69:G:H1' | 2.56 | 0.40 |
| 1:CA:173:U:H3' | 1:CA:174:A:H5' | 2.01 | 0.40 |
| 1:CA:542:G:C2 | 1:CA:543:U:C5 | 3.10 | 0.40 |
| 1:CA:583:A:C8 | 1:CA:584:G:C8 | 3.09 | 0.40 |
| 1:CA:1092:A:N6 | 1:CA:1093:A:N1 | 2.70 | 0.40 |
| 1:CA:1169:A:H2' | 1:CA:1170:A:C8 | 2.55 | 0.40 |
| 1:CA:1192:C:C5 | 1:CA:1193:G:C8 | 3.09 | 0.40 |
| 1:CA:1261:A:H2' | 1:CA:1262:C:H5' | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:57:LEU:HD21 | 2:CB:67:ILE:HD11 | 2.03 | 0.40 |
| 3:CC:20:SER:HB2 | 14:CN:92:GLU:O | 2.20 | 0.40 |
| 3:CC:71:ALA:HA | 3:CC:106:VAL:HB | 2.02 | 0.40 |
| 5:CE:20:ARG:O | 5:CE:20:ARG:HG2 | 2.21 | 0.40 |
| 5:CE:41:ASP:OD2 | 5:CE:45:ARG:HB2 | 2.21 | 0.40 |
| 6:CF:38:ARG:HG2 | 6:CF:63:ASN:CB | 2.50 | 0.40 |
| 10:CJ:6:ILE:HB | 10:CJ:76:ILE:O | 2.22 | 0.40 |
| 11:CK:124:PRO:HB2 | 11:CK:126:LYS:HE3 | 2.04 | 0.40 |
| 13:CM:27:LYS:CD | 13:CM:27:LYS:O | 2.69 | 0.40 |
| 13:CM:109:ARG:HG3 | 13:CM:109:ARG:O | 2.20 | 0.40 |
| 16:CP:3:THR:CG2 | 16:CP:5:ARG:HG2 | 2.52 | 0.40 |
| 19:CS:36:ARG:NE | 19:CS:52:HIS:O | 2.49 | 0.40 |
| 19:CS:40:ILE:HG22 | 19:CS:67:VAL:HA | 2.02 | 0.40 |
| 19:CS:63:THR:HG22 | 19:CS:64:ASP:H | 1.86 | 0.40 |
| 19:CS:67:VAL:O | 19:CS:67:VAL:CG1 | 2.69 | 0.40 |
| 20:CT:27:MET:HG3 | 20:CT:28:MET:N | 2.36 | 0.40 |
| 22:DA:30:G:C5 | 22:DA:31:C:C4 | 3.10 | 0.40 |
| 22:DA:120:U:H1' | 22:DA:149:A:N7 | 2.36 | 0.40 |
| 22:DA:662:G:C2 | 22:DA:663:G:C8 | 3.10 | 0.40 |
| 22:DA:843:G:H2' | 22:DA:844:A:C8 | 2.56 | 0.40 |
| 22:DA:962:G:C5 | 22:DA:963:U:C5 | 3.09 | 0.40 |
| 22:DA:1000:A:C6 | 22:DA:1001:A:C6 | 3.09 | 0.40 |
| 22:DA:1063:G:C8 | 22:DA:1064:C:C6 | 3.09 | 0.40 |
| 22:DA:1131:G:N7 | 22:DA:2025:C:H4' | 2.36 | 0.40 |
| 22:DA:1317:G:N7 | 22:DA:1318:U:C4 | 2.89 | 0.40 |
| 22:DA:1354:A:C8 | 22:DA:1355:G:C8 | 3.09 | 0.40 |
| 22:DA:1355:G:C6 | 22:DA:1356:G:N7 | 2.89 | 0.40 |
| 22:DA:1357:C:O2' | 22:DA:1358:G:H5' | 2.22 | 0.40 |
| 22:DA:1567:G:O2' | 24:DC:63:ARG:NH1 | 2.54 | 0.40 |
| 22:DA:1765:U:O2' | 22:DA:1766:G:H5' | 2.21 | 0.40 |
| 22:DA:1959:G:H2' | 22:DA:1960:A:O4' | 2.21 | 0.40 |
| 22:DA:2013:A:N6 | 22:DA:2014:A:N1 | 2.69 | 0.40 |
| 22:DA:2282:G:C5 | 22:DA:2425:A:N1 | 2.90 | 0.40 |
| 22:DA:2662:A:C4 | 22:DA:2663:G:H1' | 2.56 | 0.40 |
| 22:DA:2786:U:H4' | 25:DD:67:HIS:HA | 2.04 | 0.40 |
| 23:DB:7:G:C5' | 36:DO:29:HIS:CE1 | 3.04 | 0.40 |
| 23:DB:8:C:O2' | 36:DO:40:ILE:HD13 | 2.22 | 0.40 |
| 25:DD:34:VAL:HG22 | 25:DD:50:VAL:HG12 | 2.02 | 0.40 |
| 28:DG:95:ARG:HG3 | 28:DG:106:SER:HB2 | 2.03 | 0.40 |
| 29:DH:96:THR:O | 29:DH:98:ASP:N | 2.54 | 0.40 |
| 30:DI:24:VAL:CG1 | 30:DI:28:LEU:HB3 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:DI:103:ARG:O | 30:DI:107:GLN:N | 2.53 | 0.40 |
| 31:DJ:56:VAL:HB | 31:DJ:124:VAL:HG12 | 2.02 | 0.40 |
| 31:DJ:102:GLU:HG3 | 31:DJ:124:VAL:HG21 | 2.04 | 0.40 |
| 32:DK:39:ILE:O | 32:DK:39:ILE:HG13 | 2.21 | 0.40 |
| 32:DK:91:SER:O | 32:DK:92:GLU:O | 2.39 | 0.40 |
| 33:DL:77:ILE:CG2 | 33:DL:81:ASP:OD2 | 2.69 | 0.40 |
| 35:DN:47:VAL:O | 35:DN:47:VAL:HG12 | 2.22 | 0.40 |
| 36:DO:64:TYR:O | 36:DO:67:ASN:ND2 | 2.45 | 0.40 |
| 40:DS:20:VAL:HG23 | 40:DS:39:THR:HG21 | 2.02 | 0.40 |
| 41:DT:4:GLU:O | 41:DT:8:LEU:N | 2.54 | 0.40 |
| 44:DW:37:ILE:HG22 | 44:DW:38:VAL:HG23 | 2.03 | 0.40 |
| 1:AA:110:C:C4 | 1:AA:111:G:C5 | 3.09 | 0.40 |
| 1:AA:141:G:C2 | 1:AA:142:G:H1' | 2.56 | 0.40 |
| 1:AA:346:G:P | 32:BK:105:ARG:HH12 | 2.44 | 0.40 |
| 1:AA:849:G:N3 | 1:AA:849:G:H2' | 2.35 | 0.40 |
| 1:AA:924:C:H2' | 1:AA:925:G:H8 | 1.86 | 0.40 |
| 1:AA:1076:U:C2 | 1:AA:1082:A:C2 | 3.09 | 0.40 |
| 1:AA:1112:C:O2' | 3:AC:179:ARG:HG3 | 2.21 | 0.40 |
| 1:AA:1141:C:O2' | 1:AA:1142:G:P | 2.79 | 0.40 |
| 1:AA:1538:C:C2' | 1:AA:1539:C:H5' | 2.51 | 0.40 |
| 2:AB:68:LEU:C | 2:AB:68:LEU:CD2 | 2.89 | 0.40 |
| 4:AD:170:TRP:HB2 | 4:AD:184:ARG:O | 2.22 | 0.40 |
| 16:AP:36:VAL:O | 16:AP:36:VAL:HG13 | 2.21 | 0.40 |
| 16:AP:52:LEU:O | 16:AP:54:LEU:N | 2.53 | 0.40 |
| 18:AR:55:LEU:HD22 | 18:AR:55:LEU:HA | 1.94 | 0.40 |
| 21:AU:47:ARG:HA | 21:AU:47:ARG:HE | 1.86 | 0.40 |
| 22:BA:27:G:C2 | 22:BA:512:G:N3 | 2.89 | 0.40 |
| 22:BA:146:A:H2' | 22:BA:147:C:C6 | 2.56 | 0.40 |
| 22:BA:221:A:C4 | 22:BA:266:G:N7 | 2.89 | 0.40 |
| 22:BA:253:C:OP2 | 51:B3:5:LYS:CE | 2.68 | 0.40 |
| 22:BA:372:G:N2 | 22:BA:400:G:H2' | 2.36 | 0.40 |
| 22:BA:489:G:O4' | 22:BA:1284:A:C8 | 2.74 | 0.40 |
| 22:BA:974:G:C8 | 22:BA:989:G:C2 | 3.09 | 0.40 |
| 22:BA:1018:U:O3' | 22:BA:1120:G:N2 | 2.53 | 0.40 |
| 22:BA:1046:A:H3' | 22:BA:1047:G:H5' | 2.03 | 0.40 |
| 22:BA:1122:G:N3 | 22:BA:1122:G:H2' | 2.36 | 0.40 |
| 22:BA:1142:A:C4 | 22:BA:1144:A:C8 | 3.09 | 0.40 |
| 22:BA:1438:U:C4 | 22:BA:1552:A:C2 | 3.10 | 0.40 |
| 22:BA:1735:A:H2' | 22:BA:1736:U:H5' | 2.03 | 0.40 |
| 22:BA:1927:A:N1 | 22:BA:1928:A:C2 | 2.89 | 0.40 |
| 22:BA:1959:G:H2' | 22:BA:1960:A:O5' | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:2001:C:N3 | 22:BA:2002:G:C8 | 2.90 | 0.40 |
| 22:BA:2720:U:C2 | 22:BA:2872:A:C6 | 3.10 | 0.40 |
| 24:BC:107:PRO:HB3 | 24:BC:142:HIS:CE1 | 2.57 | 0.40 |
| 24:BC:172:VAL:HG23 | 24:BC:174:LEU:CD1 | 2.50 | 0.40 |
| 27:BF:134:GLU:HG2 | 27:BF:136:ILE:CD1 | 2.51 | 0.40 |
| 27:BF:136:ILE:HD11 | 27:BF:149:VAL:HG12 | 2.04 | 0.40 |
| 30:BI:24:VAL:HG22 | 30:BI:25:GLY:N | 2.37 | 0.40 |
| 38:BQ:50:ARG:O | 38:BQ:54:LYS:HE3 | 2.21 | 0.40 |
| 39:BR:86:GLN:CG | 39:BR:87:GLN:N | 2.84 | 0.40 |
| 39:BR:98:ILE:HG21 | 39:BR:101:ILE:HD11 | 2.02 | 0.40 |
| 40:BS:38:TYR:CD1 | 48:B0:28:LEU:HD11 | 2.56 | 0.40 |
| 42:BU:18:ASP:O | 42:BU:20:GLY:N | 2.54 | 0.40 |
| 42:BU:54:GLN:N | 42:BU:55:PRO:HD2 | 2.37 | 0.40 |
| 44:BW:23:VAL:HG22 | 44:BW:38:VAL:CG1 | 2.51 | 0.40 |
| 44:BW:28:GLY:O | 44:BW:66:LYS:HG2 | 2.20 | 0.40 |
| 44:BW:51:VAL:CG2 | 44:BW:81:SER:HA | 2.51 | 0.40 |
| 48:B0:55:ILE:HG22 | 48:B0:56:ALA:H | 1.86 | 0.40 |
| 51:B3:32:ILE:O | 51:B3:32:ILE:HG22 | 2.21 | 0.40 |
| 1:CA:41:G:H2' | 1:CA:42:G:C8 | 2.57 | 0.40 |
| 1:CA:72:A:N6 | 1:CA:99:C:H1' | 2.36 | 0.40 |
| 1:CA:149:A:C2 | 1:CA:150:U:C2 | 3.10 | 0.40 |
| 1:CA:155:A:C2 | 1:CA:167:A:C4 | 3.09 | 0.40 |
| 1:CA:484:G:C8 | 1:CA:486:U:O4' | 2.75 | 0.40 |
| 1:CA:541:G:C4 | 1:CA:542:G:C8 | 3.09 | 0.40 |
| 1:CA:780:A:C2 | 1:CA:803:G:N1 | 2.89 | 0.40 |
| 1:CA:1007:U:C3' | 1:CA:1008:U:H5' | 2.51 | 0.40 |
| 1:CA:1216:A:H2' | 1:CA:1217:C:C6 | 2.56 | 0.40 |
| 1:CA:1250:A:N3 | 1:CA:1287:A:C6 | 2.89 | 0.40 |
| 2:CB:23:TRP:CZ2 | 2:CB:25:PRO:HA | 2.57 | 0.40 |
| 2:CB:72:THR:HA | 2:CB:93:ASN:O | 2.21 | 0.40 |
| 2:CB:72:THR:CG2 | 2:CB:95:ARG:NH1 | 2.84 | 0.40 |
| 3:CC:9:GLY:HA2 | 3:CC:12:LEU:HG | 2.02 | 0.40 |
| 4:CD:22:LYS:O | 4:CD:24:GLY:N | 2.55 | 0.40 |
| 6:CF:93:LYS:N | 6:CF:93:LYS:HD3 | 2.37 | 0.40 |
| 10:CJ:84:VAL:HA | 10:CJ:87:LEU:HD12 | 2.04 | 0.40 |
| 15:CO:67:LEU:O | 15:CO:68:ASP:C | 2.60 | 0.40 |
| 15:CO:89:ARG:NH1 | 22:DA:714:U:C5 | 2.89 | 0.40 |
| 19:CS:6:LYS:HB2 | 19:CS:7:LYS:HE2 | 2.02 | 0.40 |
| 22:DA:372:G:P | 45:DX:62:LYS:HZ2 | 2.45 | 0.40 |
| 22:DA:465:G:C6 | 22:DA:466:A:N6 | 2.89 | 0.40 |
| 22:DA:498:G:C2 | 22:DA:499:U:C5 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:517:C:O2' | 40:DS:18:ARG:NH1 | 2.55 | 0.40 |
| 22:DA:634:C:P | 33:DL:70:LYS:HE2 | 2.61 | 0.40 |
| 22:DA:647:G:C6 | 22:DA:648:G:C5 | 3.09 | 0.40 |
| 22:DA:711:G:C2 | 22:DA:721:A:C2 | 3.09 | 0.40 |
| 22:DA:927:A:H2' | 22:DA:928:A:O4' | 2.21 | 0.40 |
| 22:DA:959:A:H2' | 22:DA:960:A:C8 | 2.56 | 0.40 |
| 22:DA:978:G:C2 | 22:DA:986:C:C2 | 3.09 | 0.40 |
| 22:DA:1121:C:H2' | 22:DA:1122:G:O5' | 2.22 | 0.40 |
| 22:DA:1308:A:H2' | 22:DA:1309:G:O4' | 2.21 | 0.40 |
| 22:DA:1373:A:N6 | 22:DA:1374:G:N3 | 2.69 | 0.40 |
| 22:DA:1607:C:O2 | 22:DA:1621:U:N3 | 2.53 | 0.40 |
| 22:DA:1668:A:N3 | 22:DA:1674:G:C8 | 2.89 | 0.40 |
| 22:DA:1800:C:OP1 | 24:DC:258:ARG:NH2 | 2.54 | 0.40 |
| 22:DA:1809:A:N6 | 22:DA:1810:A:C6 | 2.89 | 0.40 |
| 22:DA:1914:C:O2 | 22:DA:1914:C:O4' | 2.37 | 0.40 |
| 22:DA:2201:G:C6 | 22:DA:2223:G:C2 | 3.09 | 0.40 |
| 22:DA:2323:G:H2' | 22:DA:2324:U:O4' | 2.21 | 0.40 |
| 22:DA:2345:G:OP2 | 49:D1:46:HIS:NE2 | 2.51 | 0.40 |
| 22:DA:2439:A:H4' | 22:DA:2440:C:H5'' | 2.03 | 0.40 |
| 22:DA:2574:G:N2 | 22:DA:2575:C:H1' | 2.36 | 0.40 |
| 22:DA:2785:C:H2' | 22:DA:2786:U:O4' | 2.21 | 0.40 |
| 22:DA:2854:G:N2 | 22:DA:2864:G:C4 | 2.89 | 0.40 |
| 22:DA:2885:G:O6 | 48:D0:29:SER:HB3 | 2.21 | 0.40 |
| 26:DE:24:ASN:O | 26:DE:28:VAL:HG23 | 2.21 | 0.40 |
| 26:DE:47:LYS:O | 26:DE:83:VAL:CB | 2.70 | 0.40 |
| 27:DF:36:LEU:HD23 | 27:DF:57:LEU:HD22 | 2.03 | 0.40 |
| 31:DJ:13:ARG:HG2 | 31:DJ:51:GLY:O | 2.20 | 0.40 |
| 31:DJ:74:TYR:CD1 | 31:DJ:92:MET:HG3 | 2.56 | 0.40 |
| 37:DP:103:ARG:HB3 | 37:DP:108:ALA:CB | 2.50 | 0.40 |
| 41:DT:38:ALA:C | 41:DT:39:THR:HG22 | 2.41 | 0.40 |
| 41:DT:67:VAL:HG12 | 41:DT:68:LYS:N | 2.37 | 0.40 |
| 43:DV:75:GLN:CB | 43:DV:92:VAL:HG23 | 2.52 | 0.40 |
| 1:AA:69:G:C3' | 1:AA:70:U:H6 | 2.35 | 0.40 |
| 1:AA:110:C:C4 | 1:AA:111:G:C6 | 3.10 | 0.40 |
| 1:AA:126:G:O2' | 1:AA:635:A:H4' | 2.22 | 0.40 |
| 1:AA:295:C:H2' | 1:AA:296:U:O4' | 2.22 | 0.40 |
| 1:AA:300:A:H1' | 1:AA:565:U:O2 | 2.21 | 0.40 |
| 1:AA:374:A:C5 | 1:AA:375:U:C5 | 3.09 | 0.40 |
| 1:AA:457:G:H5' | 1:AA:458:U:OP2 | 2.21 | 0.40 |
| 1:AA:1080:A:O3' | 5:AE:21:VAL:HG21 | 2.21 | 0.40 |
| 1:AA:1081:A:OP1 | 5:AE:21:VAL:CG2 | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1102:A:H2' | 1:AA:1103:C:C6 | 2.56 | 0.40 |
| 1:AA:1154:G:H2' | 1:AA:1154:G:N3 | 2.36 | 0.40 |
| 1:AA:1213:A:C5 | 1:AA:1215:G:C5 | 3.10 | 0.40 |
| 1:AA:1272:G:H2' | 1:AA:1273:C:O4' | 2.22 | 0.40 |
| 1:AA:1379:G:N1 | 1:AA:1380:U:C4 | 2.89 | 0.40 |
| 3:AC:26:THR:O | 3:AC:27:LYS:C | 2.60 | 0.40 |
| 8:AH:7:ILE:N | 8:AH:7:ILE:CD1 | 2.85 | 0.40 |
| 8:AH:15:ARG:HB2 | 8:AH:75:ILE:CG2 | 2.51 | 0.40 |
| 10:AJ:52:LEU:HD23 | 10:AJ:62:ARG:HG2 | 2.03 | 0.40 |
| 11:AK:72:ASP:O | 11:AK:73:ALA:HB2 | 2.22 | 0.40 |
| 15:AO:87:LEU:N | 15:AO:87:LEU:HD23 | 2.36 | 0.40 |
| 19:AS:3:ARG:O | 19:AS:4:SER:CB | 2.69 | 0.40 |
| 22:BA:26:G:C2' | 22:BA:27:G:O5' | 2.70 | 0.40 |
| 22:BA:364:C:H2' | 22:BA:365:U:C6 | 2.57 | 0.40 |
| 22:BA:372:G:H5'' | 45:BX:61:LYS:HD2 | 2.03 | 0.40 |
| 22:BA:511:U:O4 | 22:BA:512:G:N1 | 2.55 | 0.40 |
| 22:BA:743:A:O3' | 58:BA:3654:HOH:O | 2.22 | 0.40 |
| 22:BA:1003:G:C2 | 22:BA:1004:U:C4 | 3.08 | 0.40 |
| 22:BA:1046:A:OP2 | 22:BA:1046:A:H4' | 2.21 | 0.40 |
| 22:BA:1139:G:O3' | 31:BJ:26:GLY:HA3 | 2.22 | 0.40 |
| 22:BA:1180:U:H2' | 22:BA:1181:U:H5' | 2.02 | 0.40 |
| 22:BA:1482:G:N3 | 22:BA:1483:G:C8 | 2.89 | 0.40 |
| 22:BA:1502:A:C2 | 22:BA:1503:A:C4 | 3.09 | 0.40 |
| 22:BA:1647:U:H3' | 22:BA:1647:U:P | 2.62 | 0.40 |
| 22:BA:1801:A:OP2 | 24:BC:150:LYS:NZ | 2.54 | 0.40 |
| 22:BA:1958:C:H2' | 22:BA:1959:G:H5' | 2.03 | 0.40 |
| 22:BA:2137:U:C5 | 22:BA:2138:G:N7 | 2.89 | 0.40 |
| 22:BA:2393:U:O3' | 33:BL:62:PRO:HA | 2.22 | 0.40 |
| 22:BA:2533:U:C2' | 22:BA:2534:A:H5' | 2.51 | 0.40 |
| 22:BA:2560:A:C6 | 22:BA:2561:U:C4 | 3.09 | 0.40 |
| 24:BC:36:LYS:O | 24:BC:37:ASN:HB3 | 2.22 | 0.40 |
| 26:BE:136:GLN:O | 26:BE:137:LYS:C | 2.60 | 0.40 |
| 30:BI:28:LEU:HG | 30:BI:35:ILE:CD1 | 2.51 | 0.40 |
| 31:BJ:20:ALA:O | 31:BJ:23:LYS:HG2 | 2.21 | 0.40 |
| 32:BK:25:LEU:HD12 | 32:BK:38:ILE:HG22 | 2.02 | 0.40 |
| 35:BN:1:MET:O | 35:BN:2:ARG:HB2 | 2.21 | 0.40 |
| 42:BU:94:ARG:HB3 | 42:BU:103:ILE:HD12 | 2.04 | 0.40 |
| 53:B5:76:LEU:O | 53:B5:121:MET:HA | 2.22 | 0.40 |
| 1:CA:228:A:H2' | 1:CA:229:U:O4' | 2.21 | 0.40 |
| 1:CA:666:G:C6 | 1:CA:741:G:C5 | 3.10 | 0.40 |
| 1:CA:815:A:C2 | 1:CA:1529:G:C4 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1220:G:H1' | 19:CS:52:HIS:CD2 | 2.56 | 0.40 |
| 1:CA:1299:A:O2' | 1:CA:1301:U:O4' | 2.39 | 0.40 |
| 1:CA:1522:U:O2' | 1:CA:1523:G:H5' | 2.21 | 0.40 |
| 2:CB:57:LEU:CD2 | 2:CB:67:ILE:HD11 | 2.51 | 0.40 |
| 2:CB:221:VAL:O | 2:CB:221:VAL:HG12 | 2.20 | 0.40 |
| 4:CD:59:GLN:OE1 | 4:CD:59:GLN:CA | 2.65 | 0.40 |
| 4:CD:148:LYS:H | 4:CD:148:LYS:CE | 2.34 | 0.40 |
| 5:CE:23:LYS:O | 5:CE:24:THR:CB | 2.69 | 0.40 |
| 5:CE:80:THR:OG1 | 5:CE:81:LEU:N | 2.54 | 0.40 |
| 6:CF:36:ILE:O | 6:CF:36:ILE:CG1 | 2.69 | 0.40 |
| 6:CF:86:ARG:HD3 | 18:CR:64:TYR:CE1 | 2.56 | 0.40 |
| 9:CI:51:PRO:HG2 | 9:CI:83:ILE:HD12 | 2.04 | 0.40 |
| 9:CI:57:MET:HA | 9:CI:60:LYS:HB3 | 2.04 | 0.40 |
| 21:CU:41:PRO:O | 21:CU:44:GLU:N | 2.54 | 0.40 |
| 22:DA:83:A:H2 | 22:DA:103:A:N7 | 2.18 | 0.40 |
| 22:DA:192:C:C4 | 22:DA:193:U:C2 | 3.09 | 0.40 |
| 22:DA:207:A:C2 | 22:DA:208:C:C1' | 3.04 | 0.40 |
| 22:DA:582:A:C6 | 22:DA:583:G:C6 | 3.09 | 0.40 |
| 22:DA:637:A:P | 33:DL:112:LEU:HB3 | 2.60 | 0.40 |
| 22:DA:773:U:C5' | 22:DA:774:G:OP2 | 2.69 | 0.40 |
| 22:DA:927:A:H2' | 22:DA:928:A:C8 | 2.56 | 0.40 |
| 22:DA:1372:U:H2' | 22:DA:1373:A:C8 | 2.57 | 0.40 |
| 22:DA:1601:G:C5 | 22:DA:1602:U:C5 | 3.10 | 0.40 |
| 22:DA:1649:G:C6 | 22:DA:2009:A:N6 | 2.89 | 0.40 |
| 22:DA:1670:C:C4 | 22:DA:1671:U:N3 | 2.90 | 0.40 |
| 22:DA:1693:U:O4 | 22:DA:1976:U:O2' | 2.39 | 0.40 |
| 22:DA:2010:G:H5'' | 40:DS:42:LYS:HB2 | 2.01 | 0.40 |
| 22:DA:2067:G:C6 | 22:DA:2444:G:N1 | 2.90 | 0.40 |
| 22:DA:2285:C:C5 | 49:D1:6:ARG:NH1 | 2.89 | 0.40 |
| 22:DA:2320:U:H5' | 22:DA:2321:U:C5 | 2.57 | 0.40 |
| 22:DA:2679:A:H2' | 22:DA:2680:U:O4' | 2.22 | 0.40 |
| 23:DB:14:U:O2 | 23:DB:14:U:H2' | 2.21 | 0.40 |
| 23:DB:110:C:H2' | 23:DB:111:U:O4' | 2.21 | 0.40 |
| 24:DC:121:ASP:O | 24:DC:122:ALA:C | 2.60 | 0.40 |
| 28:DG:91:GLY:O | 28:DG:94:TYR:CG | 2.74 | 0.40 |
| 28:DG:123:ALA:HB2 | 28:DG:133:LEU:HA | 2.03 | 0.40 |
| 30:DI:73:THR:HG21 | 30:DI:113:LYS:HE3 | 2.02 | 0.40 |
| 31:DJ:80:HIS:C | 31:DJ:82:GLY:N | 2.74 | 0.40 |
| 35:DN:44:LEU:O | 35:DN:48:VAL:HG23 | 2.21 | 0.40 |
| 38:DQ:76:TYR:OH | 38:DQ:92:ARG:NH1 | 2.55 | 0.40 |
| 42:DU:7:ARG:HG3 | 42:DU:8:ASP:H | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 46:DY:28:LEU:CD1 | 46:DY:46:VAL:HG21 | 2.51 | 0.40 |
| 1:AA:34:C:H2' | 1:AA:35:G:C8 | 2.56 | 0.40 |
| 1:AA:345:C:O2' | 32:BK:116:ILE:CD1 | 2.67 | 0.40 |
| 1:AA:451:A:H4' | 1:AA:452:A:O5' | 2.22 | 0.40 |
| 1:AA:582:C:N3 | 1:AA:583:A:C8 | 2.90 | 0.40 |
| 1:AA:599:C:C2 | 1:AA:600:A:C8 | 3.09 | 0.40 |
| 1:AA:669:G:O2' | 1:AA:670:G:H5' | 2.21 | 0.40 |
| 1:AA:836:G:C5 | 1:AA:851:G:C6 | 3.10 | 0.40 |
| 1:AA:1124:G:P | 10:AJ:38:GLY:HA3 | 2.62 | 0.40 |
| 1:AA:1253:G:N1 | 1:AA:1285:A:N6 | 2.69 | 0.40 |
| 1:AA:1304:G:C6 | 1:AA:1305:G:C2 | 3.09 | 0.40 |
| 1:AA:1493:A:O2' | 1:AA:1494:G:P | 2.79 | 0.40 |
| 1:AA:1539:C:O3' | 21:AU:18:ARG:HB3 | 2.21 | 0.40 |
| 2:AB:66:LYS:HB2 | 2:AB:159:ASP:OD2 | 2.21 | 0.40 |
| 2:AB:84:ALA:O | 2:AB:89:GLN:OE1 | 2.40 | 0.40 |
| 2:AB:118:GLU:O | 2:AB:120:GLN:N | 2.55 | 0.40 |
| 4:AD:99:ASP:OD2 | 4:AD:115:ARG:CZ | 2.68 | 0.40 |
| 5:AE:116:GLU:HG2 | 5:AE:117:VAL:N | 2.37 | 0.40 |
| 6:AF:3:HIS:CE1 | 6:AF:65:GLU:OE2 | 2.74 | 0.40 |
| 7:AG:66:LEU:O | 7:AG:70:ARG:HD3 | 2.22 | 0.40 |
| 16:AP:39:PHE:CD1 | 16:AP:39:PHE:C | 2.95 | 0.40 |
| 17:AQ:48:ASP:OD2 | 17:AQ:48:ASP:O | 2.39 | 0.40 |
| 20:AT:54:MET:HG3 | 20:AT:55:GLN:N | 2.36 | 0.40 |
| 22:BA:162:U:H4' | 22:BA:163:C:OP1 | 2.21 | 0.40 |
| 22:BA:184:C:H2' | 22:BA:185:G:C8 | 2.55 | 0.40 |
| 22:BA:565:C:H4' | 22:BA:1253:A:N6 | 2.37 | 0.40 |
| 22:BA:567:U:C2' | 22:BA:568:U:O5' | 2.70 | 0.40 |
| 22:BA:582:A:H2' | 22:BA:583:G:C8 | 2.57 | 0.40 |
| 22:BA:988:A:H4' | 22:BA:1155:A:N1 | 2.37 | 0.40 |
| 22:BA:1000:A:C6 | 22:BA:1001:A:C6 | 3.10 | 0.40 |
| 22:BA:1039:A:H2' | 22:BA:1040:A:O4' | 2.22 | 0.40 |
| 22:BA:1070:A:N1 | 22:BA:1097:U:O2' | 2.47 | 0.40 |
| 22:BA:1075:C:N3 | 22:BA:1076:C:N4 | 2.70 | 0.40 |
| 22:BA:1177:G:H2' | 22:BA:1178:C:O4' | 2.22 | 0.40 |
| 22:BA:1482:G:C2 | 22:BA:1483:G:C8 | 3.10 | 0.40 |
| 22:BA:1829:A:H2' | 22:BA:1830:C:O4' | 2.21 | 0.40 |
| 22:BA:1883:U:O4 | 22:BA:1884:G:C6 | 2.75 | 0.40 |
| 22:BA:1920:C:O2 | 22:BA:1920:C:H2' | 2.20 | 0.40 |
| 22:BA:2564:A:C5 | 22:BA:2565:A:C6 | 3.10 | 0.40 |
| 22:BA:2580:U:C5 | 22:BA:2581:G:C6 | 3.09 | 0.40 |
| 23:BB:65:U:O4 | 23:BB:108:A:H1' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BC:221:ARG:NH2 | 58:BC:403:HOH:O | 2.54 | 0.40 |
| 24:BC:245:VAL:HA | 24:BC:250:VAL:O | 2.21 | 0.40 |
| 25:BD:2:ILE:HG23 | 25:BD:88:GLU:OE1 | 2.21 | 0.40 |
| 25:BD:186:LEU:HD21 | 37:BP:4:ILE:HG21 | 2.03 | 0.40 |
| 27:BF:48:LYS:HA | 27:BF:51:ASP:HB2 | 2.03 | 0.40 |
| 27:BF:49:LEU:HD21 | 27:BF:148:ARG:NH2 | 2.37 | 0.40 |
| 28:BG:19:ILE:CD1 | 28:BG:45:HIS:HB2 | 2.51 | 0.40 |
| 29:BH:66:ASN:OD1 | 29:BH:138:VAL:HG11 | 2.21 | 0.40 |
| 29:BH:120:GLY:HA2 | 29:BH:122:LEU:HA | 2.04 | 0.40 |
| 30:BI:115:ALA:O | 30:BI:116:ASP:CB | 2.69 | 0.40 |
| 31:BJ:44:TYR:CD2 | 31:BJ:44:TYR:C | 2.94 | 0.40 |
| 35:BN:72:ASP:O | 35:BN:76:VAL:HG12 | 2.21 | 0.40 |
| 36:BO:87:ILE:O | 36:BO:88:LYS:O | 2.40 | 0.40 |
| 39:BR:20:VAL:HG21 | 39:BR:22:LEU:HD21 | 2.04 | 0.40 |
| 43:BV:14:LYS:HD2 | 43:BV:18:ARG:NH1 | 2.37 | 0.40 |
| 46:BY:57:LEU:O | 46:BY:57:LEU:CG | 2.69 | 0.40 |
| 1:CA:9:G:OP2 | 5:CE:126:LYS:CE | 2.70 | 0.40 |
| 1:CA:17:U:H4' | 1:CA:1080:A:O4' | 2.21 | 0.40 |
| 1:CA:59:A:N3 | 1:CA:59:A:H2' | 2.37 | 0.40 |
| 1:CA:299:G:C6 | 1:CA:300:A:C6 | 3.10 | 0.40 |
| 1:CA:582:C:O2' | 1:CA:583:A:H5' | 2.21 | 0.40 |
| 1:CA:613:C:H2' | 1:CA:614:C:C6 | 2.56 | 0.40 |
| 1:CA:840:C:H3' | 1:CA:841:C:C5' | 2.50 | 0.40 |
| 1:CA:1000:A:C5 | 1:CA:1001:C:C2 | 3.09 | 0.40 |
| 1:CA:1082:A:OP1 | 5:CE:23:LYS:NZ | 2.54 | 0.40 |
| 1:CA:1126:U:C6 | 1:CA:1281:C:C5 | 3.10 | 0.40 |
| 3:CC:66:VAL:O | 3:CC:66:VAL:HG12 | 2.21 | 0.40 |
| 3:CC:77:ILE:HA | 3:CC:84:VAL:HG22 | 2.01 | 0.40 |
| 4:CD:125:VAL:HG23 | 4:CD:130:VAL:CG2 | 2.51 | 0.40 |
| 4:CD:145:ILE:HD13 | 4:CD:178:MET:HB3 | 2.03 | 0.40 |
| 4:CD:162:ALA:HA | 4:CD:165:ARG:HG3 | 2.03 | 0.40 |
| 5:CE:42:GLY:O | 5:CE:119:GLY:HA3 | 2.22 | 0.40 |
| 5:CE:80:THR:HG1 | 5:CE:122:ASN:ND2 | 2.16 | 0.40 |
| 6:CF:3:HIS:O | 6:CF:92:THR:HA | 2.22 | 0.40 |
| 6:CF:4:TYR:CE2 | 6:CF:71:ILE:HG12 | 2.57 | 0.40 |
| 6:CF:71:ILE:CD1 | 6:CF:71:ILE:N | 2.85 | 0.40 |
| 8:CH:18:GLN:HG2 | 8:CH:63:LEU:HD13 | 2.03 | 0.40 |
| 9:CI:129:LYS:O | 9:CI:130:ARG:CD | 2.70 | 0.40 |
| 13:CM:90:ARG:HD2 | 13:CM:97:VAL:HA | 2.03 | 0.40 |
| 17:CQ:55:ILE:HD13 | 17:CQ:55:ILE:C | 2.42 | 0.40 |
| 22:DA:77:G:C2 | 22:DA:78:U:C2 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:118:A:O4' | 22:DA:178:G:O2' | 2.38 | 0.40 |
| 22:DA:119:A:H5' | 58:DA:3218:HOH:O | 2.21 | 0.40 |
| 22:DA:269:C:O2 | 22:DA:269:C:C2' | 2.69 | 0.40 |
| 22:DA:312:G:C2 | 22:DA:313:G:C8 | 3.09 | 0.40 |
| 22:DA:432:A:H2' | 22:DA:433:C:O4' | 2.21 | 0.40 |
| 22:DA:505:A:O2' | 22:DA:509:C:O2' | 2.23 | 0.40 |
| 22:DA:753:A:H2' | 22:DA:754:U:H6 | 1.84 | 0.40 |
| 22:DA:909:A:N6 | 22:DA:912:C:O2 | 2.54 | 0.40 |
| 22:DA:1040:A:H2' | 22:DA:1041:G:O4' | 2.21 | 0.40 |
| 22:DA:1213:A:N3 | 22:DA:1238:G:O2' | 2.39 | 0.40 |
| 22:DA:1343:G:N3 | 22:DA:1597:A:N1 | 2.69 | 0.40 |
| 22:DA:1359:A:C2 | 22:DA:1360:G:H1' | 2.56 | 0.40 |
| 22:DA:1429:G:H1' | 22:DA:1568:G:N3 | 2.37 | 0.40 |
| 22:DA:1802:A:N1 | 22:DA:1803:A:C2 | 2.90 | 0.40 |
| 22:DA:2115:G:N3 | 22:DA:2117:A:C8 | 2.89 | 0.40 |
| 22:DA:2125:G:H5' | 22:DA:2126:A:OP2 | 2.21 | 0.40 |
| 22:DA:2245:U:O2' | 22:DA:2435:A:H3' | 2.22 | 0.40 |
| 22:DA:2449:U:H4' | 22:DA:2450:A:OP1 | 2.22 | 0.40 |
| 22:DA:2452:C:C4' | 56:DA:3001:DOL:H461 | 2.52 | 0.40 |
| 22:DA:2553:G:H2' | 22:DA:2554:U:C4' | 2.52 | 0.40 |
| 22:DA:2842:G:C6 | 22:DA:2876:G:C6 | 3.10 | 0.40 |
| 23:DB:27:C:C5 | 23:DB:28:C:C5 | 3.10 | 0.40 |
| 23:DB:29:A:N3 | 23:DB:56:G:C2 | 2.89 | 0.40 |
| 23:DB:90:C:H5' | 34:DM:18:ARG:HA | 2.04 | 0.40 |
| 26:DE:58:LYS:CD | 26:DE:60:TRP:O | 2.70 | 0.40 |
| 26:DE:91:ASP:O | 26:DE:91:ASP:CG | 2.59 | 0.40 |
| 28:DG:155:GLU:OE1 | 28:DG:158:LYS:HG3 | 2.21 | 0.40 |
| 30:DI:12:GLN:NE2 | 30:DI:55:ILE:O | 2.54 | 0.40 |
| 30:DI:57:VAL:HG23 | 30:DI:71:THR:CA | 2.52 | 0.40 |
| 39:DR:39:LEU:C | 39:DR:49:ILE:HG23 | 2.42 | 0.40 |
| 39:DR:96:VAL:O | 39:DR:96:VAL:HG23 | 2.21 | 0.40 |
| 40:DS:14:ALA:HB1 | 40:DS:18:ARG:CZ | 2.52 | 0.40 |
| 40:DS:47:VAL:HB | 40:DS:103:ILE:HG21 | 2.03 | 0.40 |
| 42:DU:96:PHE:CZ | 42:DU:103:ILE:CG1 | 3.03 | 0.40 |
| 45:DX:5:CYS:O | 45:DX:9:GLY:HA2 | 2.22 | 0.40 |
| 49:D1:10:LYS:O | 49:D1:51:GLU:HG2 | 2.22 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:CA:204:G:OP1 | 22:DA:289:G:O2'[3_545] | 2.12 | 0.08 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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 | 216/218 (99%) | 126 (58%) | 45 (21%) | 45 (21%) | 0 | 0 |
| 2 | CB | 216/218 (99%) | 140 (65%) | 51 (24%) | 25 (12%) | 0 | 1 |
| 3 | AC | 204/206 (99%) | 148 (72%) | 35 (17%) | 21 (10%) | 0 | 1 |
| 3 | CC | 204/206 (99%) | 154 (76%) | 39 (19%) | 11 (5%) | 2 | 5 |
| 4 | AD | 203/205 (99%) | 137 (68%) | 39 (19%) | 27 (13%) | 0 | 0 |
| 4 | CD | 203/205 (99%) | 152 (75%) | 32 (16%) | 19 (9%) | 0 | 1 |
| 5 | AE | 148/150 (99%) | 102 (69%) | 27 (18%) | 19 (13%) | 0 | 1 |
| 5 | CE | 148/150 (99%) | 100 (68%) | 33 (22%) | 15 (10%) | 0 | 1 |
| 6 | AF | 98/100 (98%) | 73 (74%) | 15 (15%) | 10 (10%) | 0 | 1 |
| 6 | CF | 98/100 (98%) | 68 (69%) | 15 (15%) | 15 (15%) | 0 | 0 |
| 7 | AG | 149/151 (99%) | 107 (72%) | 29 (20%) | 13 (9%) | 1 | 1 |
| 7 | CG | 149/151 (99%) | 119 (80%) | 22 (15%) | 8 (5%) | 2 | 5 |
| 8 | AH | 127/129 (98%) | 90 (71%) | 28 (22%) | 9 (7%) | 1 | 2 |
| 8 | CH | 127/129 (98%) | 98 (77%) | 19 (15%) | 10 (8%) | 1 | 2 |
| 9 | AI | 125/127 (98%) | 87 (70%) | 24 (19%) | 14 (11%) | 0 | 1 |
| 9 | CI | 125/127 (98%) | 89 (71%) | 18 (14%) | 18 (14%) | 0 | 0 |
| 10 | AJ | 96/98 (98%) | 64 (67%) | 11 (12%) | 21 (22%) | 0 | 0 |
| 10 | CJ | 96/98 (98%) | 73 (76%) | 11 (12%) | 12 (12%) | 0 | 1 |
| 11 | AK | 115/117 (98%) | 81 (70%) | 17 (15%) | 17 (15%) | 0 | 0 |
| 11 | CK | 115/117 (98%) | 82 (71%) | 24 (21%) | 9 (8%) | 1 | 2 |
| 12 | AL | 121/123 (98%) | 91 (75%) | 21 (17%) | 9 (7%) | 1 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 12 | CL | 121/123 (98%) | 92 (76%) | 18 (15%) | 11 (9%) | 1 | 1 |
| 13 | AM | 112/114 (98%) | 81 (72%) | 21 (19%) | 10 (9%) | 1 | 1 |
| 13 | CM | 112/114 (98%) | 80 (71%) | 18 (16%) | 14 (12%) | 0 | 1 |
| 14 | AN | 92/100 (92%) | 61 (66%) | 21 (23%) | 10 (11%) | 0 | 1 |
| 14 | CN | 92/100 (92%) | 58 (63%) | 20 (22%) | 14 (15%) | 0 | 0 |
| 15 | AO | 86/88 (98%) | 65 (76%) | 14 (16%) | 7 (8%) | 1 | 2 |
| 15 | CO | 86/88 (98%) | 64 (74%) | 17 (20%) | 5 (6%) | 1 | 4 |
| 16 | AP | 80/82 (98%) | 55 (69%) | 15 (19%) | 10 (12%) | 0 | 1 |
| 16 | CP | 80/82 (98%) | 59 (74%) | 13 (16%) | 8 (10%) | 0 | 1 |
| 17 | AQ | 78/80 (98%) | 53 (68%) | 18 (23%) | 7 (9%) | 1 | 1 |
| 17 | CQ | 78/80 (98%) | 56 (72%) | 15 (19%) | 7 (9%) | 1 | 1 |
| 18 | AR | 53/55 (96%) | 42 (79%) | 11 (21%) | 0 | 100 | 100 |
| 18 | CR | 53/55 (96%) | 37 (70%) | 12 (23%) | 4 (8%) | 1 | 2 |
| 19 | AS | 77/79 (98%) | 57 (74%) | 11 (14%) | 9 (12%) | 0 | 1 |
| 19 | CS | 77/79 (98%) | 55 (71%) | 11 (14%) | 11 (14%) | 0 | 0 |
| 20 | AT | 83/85 (98%) | 59 (71%) | 19 (23%) | 5 (6%) | 1 | 4 |
| 20 | CT | 83/85 (98%) | 62 (75%) | 12 (14%) | 9 (11%) | 0 | 1 |
| 21 | AU | 49/51 (96%) | 26 (53%) | 8 (16%) | 15 (31%) | 0 | 0 |
| 21 | CU | 49/51 (96%) | 21 (43%) | 16 (33%) | 12 (24%) | 0 | 0 |
| 24 | BC | 269/271 (99%) | 218 (81%) | 39 (14%) | 12 (4%) | 2 | 8 |
| 24 | DC | 269/271 (99%) | 196 (73%) | 48 (18%) | 25 (9%) | 0 | 1 |
| 25 | BD | 207/209 (99%) | 180 (87%) | 21 (10%) | 6 (3%) | 4 | 15 |
| 25 | DD | 207/209 (99%) | 153 (74%) | 43 (21%) | 11 (5%) | 2 | 6 |
| 26 | BE | 199/201 (99%) | 165 (83%) | 30 (15%) | 4 (2%) | 7 | 24 |
| 26 | DE | 199/201 (99%) | 154 (77%) | 27 (14%) | 18 (9%) | 1 | 1 |
| 27 | BF | 175/177 (99%) | 142 (81%) | 24 (14%) | 9 (5%) | 2 | 6 |
| 27 | DF | 175/177 (99%) | 135 (77%) | 27 (15%) | 13 (7%) | 1 | 2 |
| 28 | BG | 174/176 (99%) | 148 (85%) | 16 (9%) | 10 (6%) | 1 | 5 |
| 28 | DG | 174/176 (99%) | 127 (73%) | 36 (21%) | 11 (6%) | 1 | 3 |
| 29 | BH | 147/149 (99%) | 89 (60%) | 37 (25%) | 21 (14%) | 0 | 0 |
| 29 | DH | 147/149 (99%) | 100 (68%) | 32 (22%) | 15 (10%) | 0 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 30 | BI | 139/141 (99%) | 78 (56%) | 37 (27%) | 24 (17%) | 0 | 0 |
| 30 | DI | 139/141 (99%) | 82 (59%) | 38 (27%) | 19 (14%) | 0 | 0 |
| 31 | BJ | 140/142 (99%) | 125 (89%) | 14 (10%) | 1 (1%) | 22 | 53 |
| 31 | DJ | 140/142 (99%) | 104 (74%) | 23 (16%) | 13 (9%) | 0 | 1 |
| 32 | BK | 120/122 (98%) | 97 (81%) | 14 (12%) | 9 (8%) | 1 | 2 |
| 32 | DK | 120/122 (98%) | 95 (79%) | 15 (12%) | 10 (8%) | 1 | 2 |
| 33 | BL | 141/143 (99%) | 112 (79%) | 21 (15%) | 8 (6%) | 1 | 5 |
| 33 | DL | 141/143 (99%) | 98 (70%) | 31 (22%) | 12 (8%) | 1 | 1 |
| 34 | BM | 134/136 (98%) | 120 (90%) | 11 (8%) | 3 (2%) | 6 | 22 |
| 34 | DM | 134/136 (98%) | 112 (84%) | 17 (13%) | 5 (4%) | 3 | 11 |
| 35 | BN | 118/120 (98%) | 95 (80%) | 21 (18%) | 2 (2%) | 9 | 29 |
| 35 | DN | 118/120 (98%) | 90 (76%) | 18 (15%) | 10 (8%) | 1 | 1 |
| 36 | BO | 114/116 (98%) | 96 (84%) | 14 (12%) | 4 (4%) | 3 | 12 |
| 36 | DO | 114/116 (98%) | 82 (72%) | 24 (21%) | 8 (7%) | 1 | 3 |
| 37 | BP | 112/114 (98%) | 99 (88%) | 8 (7%) | 5 (4%) | 2 | 8 |
| 37 | DP | 112/114 (98%) | 88 (79%) | 18 (16%) | 6 (5%) | 2 | 5 |
| 38 | BQ | 115/117 (98%) | 102 (89%) | 12 (10%) | 1 (1%) | 17 | 46 |
| 38 | DQ | 115/117 (98%) | 92 (80%) | 22 (19%) | 1 (1%) | 17 | 46 |
| 39 | BR | 101/103 (98%) | 81 (80%) | 10 (10%) | 10 (10%) | 0 | 1 |
| 39 | DR | 101/103 (98%) | 72 (71%) | 23 (23%) | 6 (6%) | 1 | 4 |
| 40 | BS | 108/110 (98%) | 94 (87%) | 10 (9%) | 4 (4%) | 3 | 11 |
| 40 | DS | 108/110 (98%) | 83 (77%) | 17 (16%) | 8 (7%) | 1 | 2 |
| 41 | BT | 91/93 (98%) | 74 (81%) | 9 (10%) | 8 (9%) | 1 | 1 |
| 41 | DT | 91/93 (98%) | 53 (58%) | 28 (31%) | 10 (11%) | 0 | 1 |
| 42 | BU | 100/102 (98%) | 77 (77%) | 19 (19%) | 4 (4%) | 3 | 9 |
| 42 | DU | 100/102 (98%) | 69 (69%) | 19 (19%) | 12 (12%) | 0 | 1 |
| 43 | BV | 92/94 (98%) | 84 (91%) | 7 (8%) | 1 (1%) | 14 | 41 |
| 43 | DV | 92/94 (98%) | 76 (83%) | 14 (15%) | 2 (2%) | 6 | 22 |
| 44 | BW | 74/76 (97%) | 68 (92%) | 4 (5%) | 2 (3%) | 5 | 17 |
| 44 | DW | 73/76 (96%) | 61 (84%) | 12 (16%) | 0 | 100 | 100 |
| 45 | BX | 75/77 (97%) | 68 (91%) | 6 (8%) | 1 (1%) | 12 | 36 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 45 | DX | 75/77 (97%) | 58 (77%) | 12 (16%) | 5 (7%) | 1 | 3 |
| 46 | BY | 61/63 (97%) | 43 (70%) | 10 (16%) | 8 (13%) | 0 | 1 |
| 46 | DY | 61/63 (97%) | 44 (72%) | 12 (20%) | 5 (8%) | 1 | 2 |
| 47 | BZ | 56/58 (97%) | 54 (96%) | 2 (4%) | 0 | 100 | 100 |
| 47 | DZ | 56/58 (97%) | 41 (73%) | 10 (18%) | 5 (9%) | 1 | 1 |
| 48 | B0 | 54/56 (96%) | 46 (85%) | 4 (7%) | 4 (7%) | 1 | 2 |
| 48 | D0 | 54/56 (96%) | 37 (68%) | 12 (22%) | 5 (9%) | 0 | 1 |
| 49 | B1 | 48/50 (96%) | 40 (83%) | 4 (8%) | 4 (8%) | 1 | 2 |
| 49 | D1 | 48/50 (96%) | 36 (75%) | 8 (17%) | 4 (8%) | 1 | 2 |
| 50 | B2 | 44/46 (96%) | 37 (84%) | 5 (11%) | 2 (4%) | 2 | 8 |
| 50 | D2 | 44/46 (96%) | 34 (77%) | 6 (14%) | 4 (9%) | 1 | 1 |
| 51 | B3 | 62/64 (97%) | 56 (90%) | 5 (8%) | 1 (2%) | 9 | 31 |
| 51 | D3 | 62/64 (97%) | 52 (84%) | 6 (10%) | 4 (6%) | 1 | 3 |
| 52 | B4 | 36/38 (95%) | 31 (86%) | 4 (11%) | 1 (3%) | 5 | 17 |
| 52 | D4 | 36/38 (95%) | 32 (89%) | 2 (6%) | 2 (6%) | 2 | 5 |
| 53 | B5 | 183/228 (80%) | 87 (48%) | 53 (29%) | 43 (24%) | 0 | 0 |
| 54 | B6 | 2/8 (25%) | 2 (100%) | 0 | 0 | 100 | 100 |
| 54 | D6 | 2/8 (25%) | 0 | 2 (100%) | 0 | 100 | 100 |
| All | All | 11422/11688 (98%) | 8528 (75%) | 1918 (17%) | 976 (8%) | 1 | 1 |

All (976) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 16 | PHE |
| 2 | AB | 20 | THR |
| 2 | AB | 22 | TYR |
| 2 | AB | 25 | PRO |
| 2 | AB | 34 | ALA |
| 2 | AB | 43 | LEU |
| 2 | AB | 64 | LYS |
| 2 | AB | 73 | LYS |
| 2 | AB | 74 | ARG |
| 2 | AB | 75 | ALA |
| 2 | AB | 76 | ALA |
| 2 | AB | 88 | ASP |
| 2 | AB | 107 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 120 | GLN |
| 2 | AB | 126 | PHE |
| 2 | AB | 134 | ALA |
| 2 | AB | 148 | LEU |
| 2 | AB | 152 | LYS |
| 2 | AB | 155 | GLY |
| 2 | AB | 182 | PRO |
| 2 | AB | 193 | PRO |
| 2 | AB | 194 | ASP |
| 2 | AB | 201 | PRO |
| 3 | AC | 12 | LEU |
| 3 | AC | 18 | TRP |
| 3 | AC | 26 | THR |
| 3 | AC | 80 | LYS |
| 3 | AC | 127 | ARG |
| 3 | AC | 140 | ASN |
| 3 | AC | 141 | ALA |
| 3 | AC | 146 | ALA |
| 3 | AC | 166 | GLU |
| 4 | AD | 23 | SER |
| 4 | AD | 25 | VAL |
| 4 | AD | 29 | ASP |
| 4 | AD | 33 | LYS |
| 4 | AD | 34 | ILE |
| 4 | AD | 35 | GLU |
| 4 | AD | 47 | ARG |
| 4 | AD | 85 | ASN |
| 4 | AD | 126 | ASN |
| 4 | AD | 153 | SER |
| 4 | AD | 168 | PRO |
| 4 | AD | 192 | SER |
| 5 | AE | 69 | ARG |
| 5 | AE | 70 | ASN |
| 5 | AE | 100 | SER |
| 5 | AE | 137 | VAL |
| 5 | AE | 158 | GLY |
| 6 | AF | 91 | ARG |
| 6 | AF | 92 | THR |
| 6 | AF | 99 | ALA |
| 7 | AG | 9 | GLN |
| 7 | AG | 14 | PRO |
| 7 | AG | 15 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AG | 56 | LYS |
| 7 | AG | 57 | SER |
| 7 | AG | 81 | GLY |
| 8 | AH | 67 | GLN |
| 9 | AI | 41 | ARG |
| 9 | AI | 44 | ALA |
| 9 | AI | 58 | VAL |
| 9 | AI | 59 | GLU |
| 9 | AI | 116 | VAL |
| 10 | AJ | 34 | ALA |
| 10 | AJ | 35 | GLN |
| 10 | AJ | 57 | VAL |
| 10 | AJ | 74 | VAL |
| 10 | AJ | 93 | ALA |
| 10 | AJ | 101 | SER |
| 11 | AK | 27 | PHE |
| 11 | AK | 39 | GLY |
| 11 | AK | 41 | ALA |
| 11 | AK | 52 | PHE |
| 11 | AK | 55 | SER |
| 11 | AK | 56 | ARG |
| 11 | AK | 73 | ALA |
| 11 | AK | 103 | ALA |
| 11 | AK | 126 | LYS |
| 12 | AL | 24 | LEU |
| 12 | AL | 26 | ALA |
| 12 | AL | 44 | LYS |
| 12 | AL | 89 | ASP |
| 13 | AM | 5 | ALA |
| 13 | AM | 12 | HIS |
| 13 | AM | 107 | ARG |
| 13 | AM | 114 | LYS |
| 14 | AN | 34 | VAL |
| 14 | AN | 42 | TRP |
| 14 | AN | 47 | LYS |
| 14 | AN | 52 | PRO |
| 14 | AN | 62 | ASN |
| 14 | AN | 92 | GLU |
| 15 | AO | 3 | LEU |
| 15 | AO | 17 | ARG |
| 16 | AP | 43 | ALA |
| 16 | AP | 46 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | AP | 80 | LYS |
| 17 | AQ | 13 | VAL |
| 17 | AQ | 18 | GLU |
| 17 | AQ | 51 | ASN |
| 17 | AQ | 82 | ALA |
| 19 | AS | 23 | VAL |
| 19 | AS | 65 | GLU |
| 20 | AT | 4 | ILE |
| 20 | AT | 5 | LYS |
| 20 | AT | 6 | SER |
| 21 | AU | 9 | ASN |
| 21 | AU | 12 | PHE |
| 21 | AU | 23 | CYS |
| 21 | AU | 24 | GLU |
| 21 | AU | 35 | ARG |
| 21 | AU | 36 | GLU |
| 21 | AU | 37 | PHE |
| 21 | AU | 40 | LYS |
| 24 | BC | 71 | LYS |
| 24 | BC | 122 | ALA |
| 24 | BC | 168 | ASP |
| 24 | BC | 196 | GLY |
| 24 | BC | 253 | LYS |
| 25 | BD | 104 | VAL |
| 25 | BD | 152 | PRO |
| 26 | BE | 11 | ALA |
| 26 | BE | 86 | ALA |
| 27 | BF | 3 | LYS |
| 27 | BF | 41 | GLY |
| 27 | BF | 175 | PHE |
| 28 | BG | 39 | ASP |
| 28 | BG | 110 | SER |
| 28 | BG | 119 | ALA |
| 28 | BG | 175 | LYS |
| 29 | BH | 10 | ALA |
| 29 | BH | 34 | GLY |
| 29 | BH | 53 | GLU |
| 29 | BH | 87 | GLU |
| 29 | BH | 90 | LEU |
| 29 | BH | 118 | PRO |
| 29 | BH | 121 | VAL |
| 29 | BH | 140 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BI | 19 | ASN |
| 30 | BI | 45 | LYS |
| 30 | BI | 63 | ALA |
| 30 | BI | 75 | PRO |
| 30 | BI | 83 | ALA |
| 30 | BI | 86 | ILE |
| 30 | BI | 113 | LYS |
| 30 | BI | 117 | MET |
| 32 | BK | 35 | VAL |
| 33 | BL | 15 | ALA |
| 33 | BL | 69 | ARG |
| 33 | BL | 94 | THR |
| 34 | BM | 69 | PRO |
| 37 | BP | 94 | LYS |
| 37 | BP | 114 | LEU |
| 38 | BQ | 25 | TYR |
| 39 | BR | 49 | ILE |
| 39 | BR | 51 | VAL |
| 39 | BR | 53 | PHE |
| 39 | BR | 55 | ASP |
| 40 | BS | 64 | ALA |
| 41 | BT | 2 | ILE |
| 41 | BT | 89 | GLU |
| 45 | BX | 3 | ARG |
| 46 | BY | 22 | LEU |
| 46 | BY | 24 | GLU |
| 46 | BY | 35 | GLY |
| 46 | BY | 36 | GLN |
| 46 | BY | 58 | ASN |
| 46 | BY | 62 | GLY |
| 48 | B0 | 56 | ALA |
| 49 | B1 | 17 | THR |
| 50 | B2 | 44 | VAL |
| 53 | B5 | 53 | ARG |
| 53 | B5 | 60 | ARG |
| 53 | B5 | 86 | GLU |
| 53 | B5 | 126 | SER |
| 53 | B5 | 134 | PRO |
| 53 | B5 | 141 | PRO |
| 53 | B5 | 167 | ASP |
| 53 | B5 | 173 | HIS |
| 53 | B5 | 175 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | B5 | 183 | PRO |
| 53 | B5 | 184 | GLU |
| 53 | B5 | 185 | LYS |
| 53 | B5 | 203 | GLU |
| 53 | B5 | 214 | TYR |
| 53 | B5 | 215 | VAL |
| 53 | B5 | 221 | PRO |
| 2 | CB | 16 | PHE |
| 2 | CB | 35 | ARG |
| 2 | CB | 36 | ASN |
| 2 | CB | 74 | ARG |
| 2 | CB | 87 | CYS |
| 2 | CB | 88 | ASP |
| 2 | CB | 120 | GLN |
| 2 | CB | 126 | PHE |
| 2 | CB | 141 | LEU |
| 2 | CB | 168 | HIS |
| 2 | CB | 193 | PRO |
| 2 | CB | 194 | ASP |
| 2 | CB | 207 | ILE |
| 2 | CB | 220 | THR |
| 3 | CC | 66 | VAL |
| 3 | CC | 82 | GLU |
| 3 | CC | 127 | ARG |
| 3 | CC | 146 | ALA |
| 4 | CD | 28 | ILE |
| 4 | CD | 30 | THR |
| 4 | CD | 32 | CYS |
| 4 | CD | 33 | LYS |
| 4 | CD | 35 | GLU |
| 4 | CD | 42 | GLY |
| 5 | CE | 51 | GLY |
| 5 | CE | 100 | SER |
| 5 | CE | 101 | GLU |
| 5 | CE | 102 | GLY |
| 5 | CE | 103 | THR |
| 5 | CE | 123 | VAL |
| 5 | CE | 158 | GLY |
| 6 | CF | 33 | GLU |
| 6 | CF | 55 | HIS |
| 6 | CF | 56 | LYS |
| 6 | CF | 65 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | CF | 92 | THR |
| 6 | CF | 93 | LYS |
| 6 | CF | 98 | GLU |
| 6 | CF | 99 | ALA |
| 7 | CG | 3 | ARG |
| 7 | CG | 56 | LYS |
| 7 | CG | 130 | ASN |
| 7 | CG | 146 | GLU |
| 9 | CI | 26 | GLY |
| 9 | CI | 41 | ARG |
| 9 | CI | 53 | GLU |
| 9 | CI | 72 | ILE |
| 9 | CI | 91 | ASP |
| 9 | CI | 120 | LYS |
| 10 | CJ | 91 | ASP |
| 11 | CK | 52 | PHE |
| 11 | CK | 93 | ARG |
| 11 | CK | 127 | ARG |
| 12 | CL | 4 | VAL |
| 12 | CL | 43 | LYS |
| 12 | CL | 44 | LYS |
| 12 | CL | 48 | ALA |
| 12 | CL | 58 | THR |
| 12 | CL | 89 | ASP |
| 13 | CM | 7 | ILE |
| 13 | CM | 11 | ASP |
| 13 | CM | 41 | GLU |
| 13 | CM | 99 | GLY |
| 14 | CN | 29 | ALA |
| 14 | CN | 52 | PRO |
| 14 | CN | 53 | ARG |
| 14 | CN | 59 | ARG |
| 14 | CN | 81 | ARG |
| 14 | CN | 92 | GLU |
| 15 | CO | 14 | GLU |
| 15 | CO | 18 | ASP |
| 17 | CQ | 51 | ASN |
| 17 | CQ | 70 | THR |
| 17 | CQ | 76 | VAL |
| 18 | CR | 21 | ILE |
| 19 | CS | 5 | LEU |
| 20 | CT | 4 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CT | 6 | SER |
| 20 | CT | 68 | HIS |
| 21 | CU | 12 | PHE |
| 21 | CU | 13 | ASP |
| 21 | CU | 24 | GLU |
| 21 | CU | 36 | GLU |
| 21 | CU | 37 | PHE |
| 21 | CU | 40 | LYS |
| 21 | CU | 52 | ALA |
| 24 | DC | 10 | SER |
| 24 | DC | 19 | VAL |
| 24 | DC | 29 | PRO |
| 24 | DC | 35 | GLU |
| 24 | DC | 58 | HIS |
| 24 | DC | 71 | LYS |
| 24 | DC | 238 | ARG |
| 24 | DC | 239 | ASN |
| 24 | DC | 251 | GLN |
| 25 | DD | 36 | GLN |
| 25 | DD | 57 | ALA |
| 25 | DD | 98 | VAL |
| 25 | DD | 105 | LYS |
| 25 | DD | 151 | THR |
| 25 | DD | 152 | PRO |
| 26 | DE | 6 | LYS |
| 26 | DE | 62 | GLN |
| 26 | DE | 145 | ASP |
| 27 | DF | 9 | LYS |
| 27 | DF | 122 | PHE |
| 27 | DF | 123 | ASP |
| 27 | DF | 175 | PHE |
| 28 | DG | 92 | VAL |
| 28 | DG | 119 | ALA |
| 28 | DG | 127 | THR |
| 28 | DG | 159 | GLY |
| 28 | DG | 175 | LYS |
| 29 | DH | 3 | VAL |
| 29 | DH | 10 | ALA |
| 29 | DH | 33 | GLN |
| 29 | DH | 35 | LYS |
| 29 | DH | 41 | LYS |
| 29 | DH | 53 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | DH | 54 | LEU |
| 29 | DH | 83 | LYS |
| 29 | DH | 109 | GLU |
| 30 | DI | 3 | LYS |
| 30 | DI | 7 | ALA |
| 30 | DI | 19 | ASN |
| 30 | DI | 101 | ILE |
| 30 | DI | 102 | SER |
| 30 | DI | 115 | ALA |
| 31 | DJ | 6 | ALA |
| 31 | DJ | 11 | VAL |
| 31 | DJ | 42 | ALA |
| 31 | DJ | 81 | ILE |
| 31 | DJ | 94 | ALA |
| 32 | DK | 35 | VAL |
| 32 | DK | 92 | GLU |
| 32 | DK | 108 | ARG |
| 32 | DK | 120 | PRO |
| 33 | DL | 39 | LYS |
| 33 | DL | 40 | SER |
| 33 | DL | 111 | ILE |
| 35 | DN | 70 | THR |
| 35 | DN | 88 | ALA |
| 35 | DN | 107 | ASN |
| 36 | DO | 12 | THR |
| 36 | DO | 34 | HIS |
| 36 | DO | 57 | ALA |
| 36 | DO | 115 | LEU |
| 37 | DP | 66 | ASN |
| 39 | DR | 102 | SER |
| 40 | DS | 29 | VAL |
| 40 | DS | 62 | ASP |
| 40 | DS | 66 | ILE |
| 40 | DS | 67 | ASP |
| 40 | DS | 72 | THR |
| 41 | DT | 21 | SER |
| 41 | DT | 22 | THR |
| 41 | DT | 28 | ASN |
| 41 | DT | 39 | THR |
| 41 | DT | 66 | LYS |
| 41 | DT | 78 | SER |
| 42 | DU | 37 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DU | 89 | ASP |
| 43 | DV | 24 | ASN |
| 45 | DX | 62 | LYS |
| 47 | DZ | 4 | THR |
| 47 | DZ | 52 | SER |
| 47 | DZ | 53 | PHE |
| 48 | D0 | 56 | ALA |
| 49 | D1 | 16 | GLY |
| 50 | D2 | 44 | VAL |
| 50 | D2 | 45 | SER |
| 52 | D4 | 23 | ILE |
| 2 | AB | 35 | ARG |
| 2 | AB | 41 | ILE |
| 2 | AB | 68 | LEU |
| 2 | AB | 80 | VAL |
| 2 | AB | 83 | ALA |
| 2 | AB | 119 | THR |
| 2 | AB | 137 | ARG |
| 2 | AB | 150 | GLY |
| 2 | AB | 156 | GLY |
| 2 | AB | 188 | ASP |
| 2 | AB | 202 | GLY |
| 2 | AB | 210 | VAL |
| 2 | AB | 212 | LEU |
| 2 | AB | 220 | THR |
| 3 | AC | 15 | VAL |
| 3 | AC | 17 | PRO |
| 3 | AC | 30 | ALA |
| 3 | AC | 61 | ALA |
| 3 | AC | 88 | ARG |
| 3 | AC | 160 | ALA |
| 3 | AC | 168 | TYR |
| 4 | AD | 17 | THR |
| 4 | AD | 24 | GLY |
| 4 | AD | 121 | LYS |
| 4 | AD | 191 | LEU |
| 5 | AE | 12 | GLN |
| 5 | AE | 45 | ARG |
| 5 | AE | 101 | GLU |
| 5 | AE | 109 | GLY |
| 5 | AE | 110 | ALA |
| 5 | AE | 122 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 138 | ARG |
| 7 | AG | 77 | SER |
| 7 | AG | 100 | ALA |
| 7 | AG | 130 | ASN |
| 8 | AH | 88 | ARG |
| 9 | AI | 13 | LYS |
| 9 | AI | 120 | LYS |
| 10 | AJ | 17 | LEU |
| 10 | AJ | 32 | THR |
| 10 | AJ | 36 | VAL |
| 10 | AJ | 38 | GLY |
| 10 | AJ | 41 | PRO |
| 10 | AJ | 81 | GLU |
| 10 | AJ | 91 | ASP |
| 11 | AK | 17 | SER |
| 11 | AK | 36 | ASP |
| 11 | AK | 108 | THR |
| 12 | AL | 25 | GLU |
| 12 | AL | 58 | THR |
| 12 | AL | 118 | GLY |
| 13 | AM | 4 | ILE |
| 13 | AM | 65 | VAL |
| 14 | AN | 23 | LYS |
| 14 | AN | 28 | LYS |
| 15 | AO | 88 | ARG |
| 16 | AP | 11 | ALA |
| 17 | AQ | 70 | THR |
| 19 | AS | 6 | LYS |
| 19 | AS | 64 | ASP |
| 21 | AU | 27 | GLY |
| 21 | AU | 38 | TYR |
| 21 | AU | 39 | GLU |
| 24 | BC | 271 | ARG |
| 25 | BD | 86 | GLU |
| 25 | BD | 102 | ALA |
| 25 | BD | 105 | LYS |
| 26 | BE | 49 | ARG |
| 27 | BF | 42 | GLU |
| 27 | BF | 172 | ALA |
| 27 | BF | 176 | PRO |
| 28 | BG | 38 | ASN |
| 28 | BG | 100 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | BH | 3 | VAL |
| 29 | BH | 11 | ASN |
| 29 | BH | 14 | SER |
| 29 | BH | 15 | LEU |
| 29 | BH | 66 | ASN |
| 29 | BH | 119 | ASN |
| 30 | BI | 10 | LYS |
| 30 | BI | 39 | CYS |
| 30 | BI | 58 | VAL |
| 30 | BI | 102 | SER |
| 30 | BI | 116 | ASP |
| 30 | BI | 138 | LEU |
| 32 | BK | 108 | ARG |
| 32 | BK | 110 | GLU |
| 33 | BL | 88 | GLY |
| 35 | BN | 70 | THR |
| 35 | BN | 118 | ARG |
| 36 | BO | 87 | ILE |
| 36 | BO | 88 | LYS |
| 37 | BP | 16 | ASP |
| 37 | BP | 35 | GLY |
| 37 | BP | 105 | GLY |
| 39 | BR | 29 | THR |
| 39 | BR | 57 | GLY |
| 40 | BS | 63 | GLY |
| 41 | BT | 17 | SER |
| 41 | BT | 52 | GLU |
| 41 | BT | 71 | GLY |
| 41 | BT | 72 | GLN |
| 42 | BU | 8 | ASP |
| 42 | BU | 19 | LYS |
| 42 | BU | 52 | LEU |
| 43 | BV | 66 | ASP |
| 46 | BY | 23 | ARG |
| 49 | B1 | 5 | ILE |
| 49 | B1 | 52 | ALA |
| 51 | B3 | 28 | ASN |
| 53 | B5 | 37 | LYS |
| 53 | B5 | 41 | THR |
| 53 | B5 | 62 | THR |
| 53 | B5 | 69 | LEU |
| 53 | B5 | 90 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | B5 | 136 | GLY |
| 53 | B5 | 209 | PHE |
| 53 | B5 | 213 | VAL |
| 53 | B5 | 216 | THR |
| 53 | B5 | 217 | THR |
| 53 | B5 | 223 | VAL |
| 2 | CB | 22 | TYR |
| 2 | CB | 124 | GLY |
| 3 | CC | 140 | ASN |
| 3 | CC | 141 | ALA |
| 4 | CD | 29 | ASP |
| 4 | CD | 36 | GLN |
| 4 | CD | 153 | SER |
| 4 | CD | 174 | ASP |
| 4 | CD | 175 | ALA |
| 5 | CE | 122 | ASN |
| 6 | CF | 91 | ARG |
| 6 | CF | 94 | HIS |
| 7 | CG | 84 | THR |
| 7 | CG | 114 | LYS |
| 8 | CH | 22 | LYS |
| 8 | CH | 54 | ASP |
| 9 | CI | 57 | MET |
| 9 | CI | 123 | ARG |
| 10 | CJ | 38 | GLY |
| 10 | CJ | 41 | PRO |
| 10 | CJ | 57 | VAL |
| 10 | CJ | 90 | LEU |
| 10 | CJ | 93 | ALA |
| 11 | CK | 78 | GLY |
| 11 | CK | 126 | LYS |
| 12 | CL | 22 | PRO |
| 12 | CL | 26 | ALA |
| 12 | CL | 76 | GLU |
| 13 | CM | 44 | LYS |
| 13 | CM | 94 | GLY |
| 14 | CN | 22 | ALA |
| 14 | CN | 32 | SER |
| 15 | CO | 21 | ASP |
| 16 | CP | 77 | GLU |
| 17 | CQ | 18 | GLU |
| 17 | CQ | 80 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | CR | 25 | ASP |
| 18 | CR | 47 | THR |
| 19 | CS | 6 | LYS |
| 19 | CS | 32 | ARG |
| 19 | CS | 45 | ILE |
| 19 | CS | 67 | VAL |
| 21 | CU | 9 | ASN |
| 21 | CU | 10 | GLU |
| 24 | DC | 25 | HIS |
| 24 | DC | 122 | ALA |
| 24 | DC | 205 | LEU |
| 24 | DC | 218 | PRO |
| 24 | DC | 240 | PHE |
| 24 | DC | 255 | LYS |
| 25 | DD | 40 | LEU |
| 26 | DE | 18 | THR |
| 26 | DE | 48 | THR |
| 26 | DE | 82 | GLY |
| 26 | DE | 86 | ALA |
| 26 | DE | 122 | GLU |
| 26 | DE | 126 | VAL |
| 26 | DE | 129 | PRO |
| 27 | DF | 148 | ARG |
| 28 | DG | 20 | ASN |
| 28 | DG | 28 | GLY |
| 29 | DH | 31 | VAL |
| 29 | DH | 77 | THR |
| 29 | DH | 118 | PRO |
| 30 | DI | 9 | VAL |
| 30 | DI | 93 | PRO |
| 30 | DI | 106 | LEU |
| 30 | DI | 134 | ARG |
| 31 | DJ | 25 | LEU |
| 31 | DJ | 127 | GLY |
| 33 | DL | 16 | GLY |
| 33 | DL | 36 | LYS |
| 33 | DL | 42 | SER |
| 34 | DM | 23 | GLY |
| 35 | DN | 104 | ALA |
| 36 | DO | 116 | GLN |
| 37 | DP | 36 | SER |
| 37 | DP | 94 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | DQ | 87 | SER |
| 39 | DR | 53 | PHE |
| 41 | DT | 18 | GLU |
| 41 | DT | 90 | GLY |
| 42 | DU | 53 | ASN |
| 42 | DU | 57 | GLY |
| 42 | DU | 98 | SER |
| 42 | DU | 99 | ASN |
| 45 | DX | 7 | VAL |
| 46 | DY | 57 | LEU |
| 48 | D0 | 55 | ILE |
| 51 | D3 | 26 | HIS |
| 2 | AB | 203 | ASN |
| 3 | AC | 54 | ARG |
| 3 | AC | 86 | LYS |
| 4 | AD | 32 | CYS |
| 4 | AD | 167 | LYS |
| 4 | AD | 169 | THR |
| 5 | AE | 88 | VAL |
| 5 | AE | 147 | MET |
| 6 | AF | 6 | ILE |
| 6 | AF | 42 | TRP |
| 6 | AF | 68 | GLN |
| 6 | AF | 69 | GLU |
| 7 | AG | 59 | LEU |
| 7 | AG | 85 | TYR |
| 8 | AH | 21 | ASN |
| 8 | AH | 50 | LYS |
| 9 | AI | 67 | VAL |
| 9 | AI | 88 | MET |
| 10 | AJ | 58 | ASN |
| 10 | AJ | 61 | ALA |
| 10 | AJ | 92 | LEU |
| 11 | AK | 128 | ARG |
| 12 | AL | 102 | LEU |
| 13 | AM | 10 | PRO |
| 13 | AM | 67 | GLY |
| 15 | AO | 73 | LYS |
| 16 | AP | 10 | GLY |
| 16 | AP | 49 | GLY |
| 16 | AP | 50 | THR |
| 16 | AP | 57 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | AQ | 12 | VAL |
| 20 | AT | 68 | HIS |
| 20 | AT | 69 | LYS |
| 21 | AU | 8 | GLU |
| 24 | BC | 29 | PRO |
| 26 | BE | 44 | ARG |
| 29 | BH | 9 | VAL |
| 29 | BH | 30 | LEU |
| 29 | BH | 85 | GLY |
| 29 | BH | 93 | SER |
| 29 | BH | 105 | ALA |
| 30 | BI | 4 | LYS |
| 30 | BI | 8 | TYR |
| 30 | BI | 20 | PRO |
| 30 | BI | 60 | THR |
| 30 | BI | 101 | ILE |
| 32 | BK | 109 | SER |
| 32 | BK | 119 | ALA |
| 34 | BM | 6 | ARG |
| 39 | BR | 31 | GLU |
| 39 | BR | 50 | GLY |
| 48 | B0 | 55 | ILE |
| 52 | B4 | 37 | GLN |
| 53 | B5 | 27 | ALA |
| 53 | B5 | 79 | ALA |
| 53 | B5 | 133 | GLY |
| 53 | B5 | 208 | THR |
| 53 | B5 | 219 | MET |
| 2 | CB | 19 | GLN |
| 2 | CB | 130 | THR |
| 3 | CC | 37 | PHE |
| 3 | CC | 156 | ARG |
| 3 | CC | 174 | PRO |
| 4 | CD | 4 | TYR |
| 4 | CD | 10 | LYS |
| 4 | CD | 154 | ARG |
| 4 | CD | 168 | PRO |
| 5 | CE | 12 | GLN |
| 5 | CE | 45 | ARG |
| 5 | CE | 138 | ARG |
| 5 | CE | 143 | GLY |
| 5 | CE | 155 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | CF | 85 | ILE |
| 7 | CG | 126 | ASP |
| 7 | CG | 140 | ASP |
| 8 | CH | 3 | MET |
| 8 | CH | 66 | PHE |
| 8 | CH | 96 | MET |
| 8 | CH | 114 | ARG |
| 9 | CI | 12 | ARG |
| 10 | CJ | 79 | PRO |
| 11 | CK | 120 | GLY |
| 12 | CL | 23 | ALA |
| 13 | CM | 12 | HIS |
| 13 | CM | 82 | ASP |
| 13 | CM | 114 | LYS |
| 14 | CN | 11 | VAL |
| 14 | CN | 21 | PHE |
| 14 | CN | 62 | ASN |
| 15 | CO | 46 | HIS |
| 16 | CP | 24 | SER |
| 16 | CP | 31 | ARG |
| 17 | CQ | 20 | SER |
| 19 | CS | 66 | MET |
| 19 | CS | 73 | GLU |
| 20 | CT | 7 | ALA |
| 21 | CU | 35 | ARG |
| 24 | DC | 26 | LYS |
| 24 | DC | 143 | ASN |
| 25 | DD | 102 | ALA |
| 26 | DE | 61 | ARG |
| 26 | DE | 149 | ILE |
| 28 | DG | 8 | PRO |
| 29 | DH | 16 | GLY |
| 29 | DH | 40 | THR |
| 31 | DJ | 8 | PRO |
| 31 | DJ | 10 | THR |
| 32 | DK | 105 | ARG |
| 33 | DL | 9 | ALA |
| 33 | DL | 53 | GLY |
| 33 | DL | 69 | ARG |
| 34 | DM | 3 | GLN |
| 34 | DM | 57 | VAL |
| 34 | DM | 58 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DM | 69 | PRO |
| 35 | DN | 86 | ARG |
| 35 | DN | 118 | ARG |
| 36 | DO | 3 | LYS |
| 36 | DO | 63 | LYS |
| 37 | DP | 80 | VAL |
| 40 | DS | 40 | ASN |
| 42 | DU | 41 | LEU |
| 42 | DU | 58 | ILE |
| 45 | DX | 26 | LYS |
| 46 | DY | 37 | LEU |
| 47 | DZ | 29 | LEU |
| 47 | DZ | 30 | ARG |
| 48 | D0 | 52 | ARG |
| 49 | D1 | 27 | LYS |
| 52 | D4 | 20 | ASP |
| 4 | AD | 26 | ARG |
| 4 | AD | 28 | ILE |
| 4 | AD | 36 | GLN |
| 4 | AD | 160 | GLU |
| 4 | AD | 193 | ALA |
| 5 | AE | 24 | THR |
| 5 | AE | 26 | LYS |
| 6 | AF | 62 | MET |
| 7 | AG | 5 | ARG |
| 8 | AH | 66 | PHE |
| 9 | AI | 9 | THR |
| 10 | AJ | 42 | LEU |
| 10 | AJ | 75 | ASP |
| 11 | AK | 14 | LYS |
| 11 | AK | 119 | ASN |
| 13 | AM | 64 | VAL |
| 14 | AN | 44 | ALA |
| 15 | AO | 20 | ASN |
| 15 | AO | 46 | HIS |
| 16 | AP | 53 | ASP |
| 16 | AP | 79 | ASN |
| 17 | AQ | 16 | LYS |
| 19 | AS | 4 | SER |
| 19 | AS | 29 | LYS |
| 19 | AS | 43 | ASN |
| 21 | AU | 10 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AU | 26 | ALA |
| 24 | BC | 121 | ASP |
| 24 | BC | 124 | ILE |
| 24 | BC | 265 | LYS |
| 27 | BF | 10 | ASP |
| 28 | BG | 12 | PRO |
| 28 | BG | 80 | THR |
| 29 | BH | 83 | LYS |
| 30 | BI | 9 | VAL |
| 30 | BI | 84 | ALA |
| 30 | BI | 98 | VAL |
| 31 | BJ | 81 | ILE |
| 33 | BL | 68 | SER |
| 36 | BO | 50 | ALA |
| 39 | BR | 43 | ASN |
| 39 | BR | 52 | PRO |
| 41 | BT | 18 | GLU |
| 42 | BU | 100 | SER |
| 44 | BW | 11 | ARG |
| 46 | BY | 46 | VAL |
| 49 | B1 | 51 | GLU |
| 53 | B5 | 65 | LEU |
| 53 | B5 | 66 | PRO |
| 53 | B5 | 106 | ASP |
| 2 | CB | 108 | ARG |
| 2 | CB | 136 | MET |
| 2 | CB | 142 | GLU |
| 2 | CB | 149 | GLY |
| 4 | CD | 47 | ARG |
| 4 | CD | 192 | SER |
| 5 | CE | 150 | PRO |
| 9 | CI | 9 | THR |
| 10 | CJ | 35 | GLN |
| 10 | CJ | 36 | VAL |
| 10 | CJ | 92 | LEU |
| 10 | CJ | 95 | GLY |
| 12 | CL | 24 | LEU |
| 13 | CM | 14 | HIS |
| 14 | CN | 23 | LYS |
| 14 | CN | 31 | ILE |
| 16 | CP | 44 | SER |
| 19 | CS | 31 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | CS | 69 | HIS |
| 20 | CT | 67 | ILE |
| 21 | CU | 11 | PRO |
| 24 | DC | 121 | ASP |
| 24 | DC | 203 | ARG |
| 25 | DD | 70 | LYS |
| 25 | DD | 194 | PRO |
| 26 | DE | 125 | SER |
| 26 | DE | 127 | GLU |
| 26 | DE | 153 | LEU |
| 27 | DF | 174 | ASP |
| 28 | DG | 46 | ALA |
| 29 | DH | 9 | VAL |
| 30 | DI | 10 | LYS |
| 30 | DI | 65 | ARG |
| 30 | DI | 84 | ALA |
| 32 | DK | 93 | GLN |
| 33 | DL | 29 | LYS |
| 33 | DL | 30 | THR |
| 35 | DN | 59 | SER |
| 35 | DN | 61 | ALA |
| 35 | DN | 85 | PRO |
| 37 | DP | 114 | LEU |
| 39 | DR | 7 | SER |
| 39 | DR | 82 | HIS |
| 40 | DS | 63 | GLY |
| 40 | DS | 64 | ALA |
| 42 | DU | 7 | ARG |
| 42 | DU | 52 | LEU |
| 43 | DV | 84 | PRO |
| 50 | D2 | 8 | SER |
| 51 | D3 | 7 | VAL |
| 2 | AB | 13 | GLY |
| 2 | AB | 161 | LEU |
| 3 | AC | 66 | VAL |
| 3 | AC | 159 | GLY |
| 4 | AD | 151 | LYS |
| 5 | AE | 78 | ASN |
| 6 | AF | 54 | LEU |
| 6 | AF | 98 | GLU |
| 8 | AH | 57 | PRO |
| 10 | AJ | 16 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | AJ | 33 | GLY |
| 11 | AK | 16 | VAL |
| 15 | AO | 49 | ASP |
| 19 | AS | 9 | PRO |
| 21 | AU | 52 | ALA |
| 27 | BF | 177 | PHE |
| 28 | BG | 14 | GLY |
| 32 | BK | 91 | SER |
| 32 | BK | 93 | GLN |
| 33 | BL | 29 | LYS |
| 33 | BL | 86 | GLU |
| 33 | BL | 92 | LEU |
| 41 | BT | 25 | GLU |
| 44 | BW | 57 | HIS |
| 48 | B0 | 34 | SER |
| 50 | B2 | 42 | LEU |
| 53 | B5 | 148 | PHE |
| 53 | B5 | 171 | ALA |
| 53 | B5 | 180 | SER |
| 53 | B5 | 201 | LYS |
| 53 | B5 | 210 | LEU |
| 2 | CB | 166 | ALA |
| 2 | CB | 203 | ASN |
| 3 | CC | 160 | ALA |
| 4 | CD | 34 | ILE |
| 6 | CF | 39 | LEU |
| 8 | CH | 21 | ASN |
| 8 | CH | 57 | PRO |
| 8 | CH | 67 | GLN |
| 8 | CH | 97 | ALA |
| 9 | CI | 14 | SER |
| 9 | CI | 55 | VAL |
| 9 | CI | 58 | VAL |
| 9 | CI | 128 | SER |
| 11 | CK | 15 | GLN |
| 13 | CM | 37 | ALA |
| 13 | CM | 66 | GLU |
| 16 | CP | 46 | LYS |
| 17 | CQ | 5 | ILE |
| 20 | CT | 5 | LYS |
| 20 | CT | 20 | HIS |
| 20 | CT | 56 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | CU | 16 | LEU |
| 24 | DC | 34 | LEU |
| 24 | DC | 46 | ASN |
| 24 | DC | 85 | PRO |
| 24 | DC | 247 | PRO |
| 24 | DC | 260 | ASN |
| 25 | DD | 195 | GLY |
| 26 | DE | 80 | SER |
| 27 | DF | 27 | GLN |
| 27 | DF | 79 | ILE |
| 27 | DF | 118 | SER |
| 27 | DF | 176 | PRO |
| 30 | DI | 20 | PRO |
| 30 | DI | 22 | PRO |
| 31 | DJ | 95 | ARG |
| 32 | DK | 110 | GLU |
| 35 | DN | 3 | HIS |
| 41 | DT | 77 | ARG |
| 48 | D0 | 24 | ALA |
| 48 | D0 | 43 | ILE |
| 49 | D1 | 51 | GLU |
| 2 | AB | 21 | ARG |
| 2 | AB | 48 | PRO |
| 2 | AB | 183 | VAL |
| 3 | AC | 147 | LYS |
| 4 | AD | 198 | HIS |
| 8 | AH | 14 | ILE |
| 8 | AH | 96 | MET |
| 9 | AI | 43 | THR |
| 9 | AI | 51 | PRO |
| 11 | AK | 89 | PRO |
| 12 | AL | 22 | PRO |
| 19 | AS | 76 | PRO |
| 24 | BC | 97 | LYS |
| 24 | BC | 234 | GLY |
| 25 | BD | 40 | LEU |
| 29 | BH | 120 | GLY |
| 30 | BI | 7 | ALA |
| 30 | BI | 23 | PRO |
| 32 | BK | 118 | LEU |
| 36 | BO | 61 | GLN |
| 40 | BS | 29 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | B5 | 36 | ALA |
| 53 | B5 | 218 | THR |
| 2 | CB | 68 | LEU |
| 5 | CE | 24 | THR |
| 6 | CF | 13 | ASP |
| 6 | CF | 18 | VAL |
| 9 | CI | 32 | GLN |
| 9 | CI | 129 | LYS |
| 10 | CJ | 75 | ASP |
| 13 | CM | 96 | PRO |
| 18 | CR | 71 | THR |
| 26 | DE | 161 | ALA |
| 28 | DG | 12 | PRO |
| 30 | DI | 61 | VAL |
| 36 | DO | 90 | VAL |
| 45 | DX | 44 | LYS |
| 49 | D1 | 5 | ILE |
| 51 | D3 | 47 | LYS |
| 4 | AD | 173 | VAL |
| 5 | AE | 105 | ILE |
| 5 | AE | 149 | SER |
| 8 | AH | 25 | VAL |
| 10 | AJ | 43 | PRO |
| 28 | BG | 79 | VAL |
| 32 | BK | 72 | PRO |
| 48 | B0 | 54 | VAL |
| 53 | B5 | 51 | ASP |
| 9 | CI | 50 | GLN |
| 13 | CM | 25 | VAL |
| 14 | CN | 34 | VAL |
| 15 | CO | 36 | ILE |
| 30 | DI | 13 | VAL |
| 30 | DI | 52 | GLY |
| 31 | DJ | 82 | GLY |
| 32 | DK | 72 | PRO |
| 42 | DU | 54 | GLN |
| 50 | D2 | 38 | GLY |
| 2 | AB | 124 | GLY |
| 9 | AI | 24 | GLY |
| 13 | AM | 16 | VAL |
| 19 | CS | 30 | PRO |
| 19 | CS | 76 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | DC | 228 | VAL |
| 27 | DF | 85 | ILE |
| 28 | DG | 17 | VAL |
| 32 | DK | 48 | PRO |
| 33 | DL | 87 | GLY |
| 45 | DX | 51 | VAL |
| 46 | DY | 11 | VAL |
| 9 | AI | 72 | ILE |
| 14 | AN | 91 | GLY |
| 27 | BF | 85 | ILE |
| 40 | BS | 66 | ILE |
| 6 | CF | 64 | VAL |
| 11 | CK | 92 | GLY |
| 16 | CP | 14 | ARG |
| 16 | CP | 42 | ILE |
| 20 | CT | 65 | GLY |
| 31 | DJ | 64 | VAL |
| 37 | DP | 84 | ILE |
| 42 | DU | 25 | VAL |
| 2 | AB | 224 | GLY |
| 7 | AG | 80 | VAL |
| 34 | BM | 26 | VAL |
| 4 | CD | 167 | LYS |
| 9 | CI | 104 | VAL |
| 11 | CK | 89 | PRO |
| 26 | DE | 83 | VAL |
| 27 | DF | 31 | VAL |
| 27 | DF | 44 | ILE |
| 30 | DI | 98 | VAL |
| 32 | DK | 119 | ALA |
| 39 | DR | 101 | ILE |
| 41 | DT | 47 | VAL |
| 46 | DY | 46 | VAL |
| 51 | D3 | 32 | ILE |
| 3 | CC | 64 | ILE |
| 16 | CP | 15 | PRO |
| 31 | DJ | 136 | GLN |
| 39 | DR | 30 | GLY |
| 46 | DY | 35 | GLY |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AB | 180/180 (100%) | 132 (73%) | 48 (27%) | 0 | 1 |
| 2 | CB | 180/180 (100%) | 130 (72%) | 50 (28%) | 0 | 1 |
| 3 | AC | 170/170 (100%) | 135 (79%) | 35 (21%) | 1 | 3 |
| 3 | CC | 170/170 (100%) | 144 (85%) | 26 (15%) | 2 | 8 |
| 4 | AD | 172/172 (100%) | 139 (81%) | 33 (19%) | 1 | 4 |
| 4 | CD | 172/172 (100%) | 143 (83%) | 29 (17%) | 2 | 6 |
| 5 | AE | 113/113 (100%) | 84 (74%) | 29 (26%) | 0 | 1 |
| 5 | CE | 113/113 (100%) | 86 (76%) | 27 (24%) | 0 | 2 |
| 6 | AF | 87/87 (100%) | 69 (79%) | 18 (21%) | 1 | 3 |
| 6 | CF | 87/87 (100%) | 61 (70%) | 26 (30%) | 0 | 1 |
| 7 | AG | 124/124 (100%) | 101 (82%) | 23 (18%) | 1 | 5 |
| 7 | CG | 124/124 (100%) | 99 (80%) | 25 (20%) | 1 | 4 |
| 8 | AH | 104/104 (100%) | 84 (81%) | 20 (19%) | 1 | 4 |
| 8 | CH | 104/104 (100%) | 82 (79%) | 22 (21%) | 1 | 3 |
| 9 | AI | 105/105 (100%) | 77 (73%) | 28 (27%) | 0 | 1 |
| 9 | CI | 105/105 (100%) | 88 (84%) | 17 (16%) | 2 | 7 |
| 10 | AJ | 86/86 (100%) | 67 (78%) | 19 (22%) | 1 | 3 |
| 10 | CJ | 86/86 (100%) | 68 (79%) | 18 (21%) | 1 | 3 |
| 11 | AK | 90/90 (100%) | 76 (84%) | 14 (16%) | 2 | 8 |
| 11 | CK | 90/90 (100%) | 71 (79%) | 19 (21%) | 1 | 3 |
| 12 | AL | 103/103 (100%) | 89 (86%) | 14 (14%) | 3 | 11 |
| 12 | CL | 103/103 (100%) | 82 (80%) | 21 (20%) | 1 | 4 |
| 13 | AM | 92/92 (100%) | 74 (80%) | 18 (20%) | 1 | 4 |
| 13 | CM | 92/92 (100%) | 75 (82%) | 17 (18%) | 1 | 5 |
| 14 | AN | 79/83 (95%) | 64 (81%) | 15 (19%) | 1 | 4 |
| 14 | CN | 79/83 (95%) | 70 (89%) | 9 (11%) | 5 | 18 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 15 | AO | 75/76 (99%) | 63 (84%) | 12 (16%) | 2 | 7 |
| 15 | CO | 75/76 (99%) | 65 (87%) | 10 (13%) | 4 | 12 |
| 16 | AP | 65/65 (100%) | 50 (77%) | 15 (23%) | 1 | 2 |
| 16 | CP | 65/65 (100%) | 54 (83%) | 11 (17%) | 2 | 6 |
| 17 | AQ | 74/74 (100%) | 50 (68%) | 24 (32%) | 0 | 0 |
| 17 | CQ | 74/74 (100%) | 51 (69%) | 23 (31%) | 0 | 0 |
| 18 | AR | 48/48 (100%) | 38 (79%) | 10 (21%) | 1 | 3 |
| 18 | CR | 48/48 (100%) | 38 (79%) | 10 (21%) | 1 | 3 |
| 19 | AS | 70/70 (100%) | 55 (79%) | 15 (21%) | 1 | 3 |
| 19 | CS | 70/70 (100%) | 58 (83%) | 12 (17%) | 2 | 6 |
| 20 | AT | 65/65 (100%) | 51 (78%) | 14 (22%) | 1 | 3 |
| 20 | CT | 65/65 (100%) | 57 (88%) | 8 (12%) | 4 | 15 |
| 21 | AU | 44/44 (100%) | 29 (66%) | 15 (34%) | 0 | 0 |
| 21 | CU | 44/44 (100%) | 29 (66%) | 15 (34%) | 0 | 0 |
| 24 | BC | 216/216 (100%) | 189 (88%) | 27 (12%) | 4 | 14 |
| 24 | DC | 216/216 (100%) | 197 (91%) | 19 (9%) | 10 | 29 |
| 25 | BD | 164/164 (100%) | 148 (90%) | 16 (10%) | 8 | 24 |
| 25 | DD | 164/164 (100%) | 145 (88%) | 19 (12%) | 5 | 17 |
| 26 | BE | 165/165 (100%) | 136 (82%) | 29 (18%) | 2 | 5 |
| 26 | DE | 165/165 (100%) | 137 (83%) | 28 (17%) | 2 | 6 |
| 27 | BF | 148/148 (100%) | 116 (78%) | 32 (22%) | 1 | 3 |
| 27 | DF | 148/148 (100%) | 119 (80%) | 29 (20%) | 1 | 4 |
| 28 | BG | 137/137 (100%) | 118 (86%) | 19 (14%) | 3 | 11 |
| 28 | DG | 137/137 (100%) | 114 (83%) | 23 (17%) | 2 | 6 |
| 29 | BH | 114/114 (100%) | 88 (77%) | 26 (23%) | 1 | 2 |
| 29 | DH | 114/114 (100%) | 88 (77%) | 26 (23%) | 1 | 2 |
| 30 | BI | 109/109 (100%) | 82 (75%) | 27 (25%) | 0 | 2 |
| 30 | DI | 109/109 (100%) | 80 (73%) | 29 (27%) | 0 | 1 |
| 31 | BJ | 116/116 (100%) | 105 (90%) | 11 (10%) | 8 | 25 |
| 31 | DJ | 116/116 (100%) | 94 (81%) | 22 (19%) | 1 | 4 |
| 32 | BK | 103/103 (100%) | 89 (86%) | 14 (14%) | 3 | 11 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 32 | DK | 103/103 (100%) | 90 (87%) | 13 (13%) | 4 | 14 |
| 33 | BL | 102/102 (100%) | 91 (89%) | 11 (11%) | 6 | 19 |
| 33 | DL | 102/102 (100%) | 86 (84%) | 16 (16%) | 2 | 8 |
| 34 | BM | 109/109 (100%) | 99 (91%) | 10 (9%) | 9 | 27 |
| 34 | DM | 109/109 (100%) | 95 (87%) | 14 (13%) | 4 | 13 |
| 35 | BN | 100/100 (100%) | 94 (94%) | 6 (6%) | 19 | 48 |
| 35 | DN | 100/100 (100%) | 76 (76%) | 24 (24%) | 0 | 2 |
| 36 | BO | 86/86 (100%) | 65 (76%) | 21 (24%) | 0 | 2 |
| 36 | DO | 86/86 (100%) | 70 (81%) | 16 (19%) | 1 | 5 |
| 37 | BP | 99/99 (100%) | 81 (82%) | 18 (18%) | 1 | 5 |
| 37 | DP | 99/99 (100%) | 90 (91%) | 9 (9%) | 9 | 27 |
| 38 | BQ | 89/89 (100%) | 78 (88%) | 11 (12%) | 4 | 14 |
| 38 | DQ | 89/89 (100%) | 78 (88%) | 11 (12%) | 4 | 14 |
| 39 | BR | 84/84 (100%) | 74 (88%) | 10 (12%) | 5 | 16 |
| 39 | DR | 84/84 (100%) | 76 (90%) | 8 (10%) | 8 | 25 |
| 40 | BS | 93/93 (100%) | 76 (82%) | 17 (18%) | 1 | 5 |
| 40 | DS | 93/93 (100%) | 83 (89%) | 10 (11%) | 6 | 19 |
| 41 | BT | 80/80 (100%) | 68 (85%) | 12 (15%) | 3 | 9 |
| 41 | DT | 80/80 (100%) | 66 (82%) | 14 (18%) | 2 | 6 |
| 42 | BU | 83/83 (100%) | 72 (87%) | 11 (13%) | 4 | 12 |
| 42 | DU | 83/83 (100%) | 68 (82%) | 15 (18%) | 1 | 5 |
| 43 | BV | 78/78 (100%) | 63 (81%) | 15 (19%) | 1 | 4 |
| 43 | DV | 78/78 (100%) | 65 (83%) | 13 (17%) | 2 | 6 |
| 44 | BW | 57/58 (98%) | 47 (82%) | 10 (18%) | 2 | 6 |
| 44 | DW | 56/58 (97%) | 50 (89%) | 6 (11%) | 6 | 20 |
| 45 | BX | 67/67 (100%) | 61 (91%) | 6 (9%) | 9 | 28 |
| 45 | DX | 67/67 (100%) | 58 (87%) | 9 (13%) | 4 | 12 |
| 46 | BY | 55/55 (100%) | 50 (91%) | 5 (9%) | 9 | 27 |
| 46 | DY | 55/55 (100%) | 43 (78%) | 12 (22%) | 1 | 3 |
| 47 | BZ | 48/48 (100%) | 41 (85%) | 7 (15%) | 3 | 9 |
| 47 | DZ | 48/48 (100%) | 38 (79%) | 10 (21%) | 1 | 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-------------|-----|
| 48 | B0 | 47/47 (100%) | 42 (89%) | 5 (11%) | 6 | 20 |
| 48 | D0 | 47/47 (100%) | 43 (92%) | 4 (8%) | 10 | 31 |
| 49 | B1 | 45/45 (100%) | 42 (93%) | 3 (7%) | 16 | 43 |
| 49 | D1 | 45/45 (100%) | 39 (87%) | 6 (13%) | 4 | 12 |
| 50 | B2 | 38/38 (100%) | 34 (90%) | 4 (10%) | 7 | 20 |
| 50 | D2 | 38/38 (100%) | 31 (82%) | 7 (18%) | 1 | 5 |
| 51 | B3 | 51/51 (100%) | 45 (88%) | 6 (12%) | 5 | 16 |
| 51 | D3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 8 | 24 |
| 52 | B4 | 34/34 (100%) | 32 (94%) | 2 (6%) | 19 | 49 |
| 52 | D4 | 34/34 (100%) | 26 (76%) | 8 (24%) | 1 | 2 |
| 53 | B5 | 61/180 (34%) | 48 (79%) | 13 (21%) | 1 | 3 |
| 54 | B6 | 2/2 (100%) | 2 (100%) | 0 | 100 | 100 |
| 54 | D6 | 2/2 (100%) | 2 (100%) | 0 | 100 | 100 |
| All | All | 9390/9522 (99%) | 7747 (82%) | 1643 (18%) | 2 | 6 |

All (1643) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 9 | MET |
| 2 | AB | 14 | VAL |
| 2 | AB | 15 | HIS |
| 2 | AB | 20 | THR |
| 2 | AB | 21 | ARG |
| 2 | AB | 22 | TYR |
| 2 | AB | 27 | MET |
| 2 | AB | 31 | ILE |
| 2 | AB | 32 | PHE |
| 2 | AB | 39 | HIS |
| 2 | AB | 41 | ILE |
| 2 | AB | 43 | LEU |
| 2 | AB | 46 | THR |
| 2 | AB | 50 | PHE |
| 2 | AB | 64 | LYS |
| 2 | AB | 66 | LYS |
| 2 | AB | 68 | LEU |
| 2 | AB | 85 | LEU |
| 2 | AB | 87 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 88 | ASP |
| 2 | AB | 95 | ARG |
| 2 | AB | 100 | MET |
| 2 | AB | 101 | LEU |
| 2 | AB | 102 | THR |
| 2 | AB | 107 | VAL |
| 2 | AB | 108 | ARG |
| 2 | AB | 114 | LEU |
| 2 | AB | 122 | GLN |
| 2 | AB | 123 | ASP |
| 2 | AB | 126 | PHE |
| 2 | AB | 129 | LEU |
| 2 | AB | 130 | THR |
| 2 | AB | 132 | LYS |
| 2 | AB | 135 | LEU |
| 2 | AB | 148 | LEU |
| 2 | AB | 153 | ASP |
| 2 | AB | 157 | LEU |
| 2 | AB | 161 | LEU |
| 2 | AB | 164 | ILE |
| 2 | AB | 182 | PRO |
| 2 | AB | 188 | ASP |
| 2 | AB | 197 | ASP |
| 2 | AB | 207 | ILE |
| 2 | AB | 208 | ARG |
| 2 | AB | 210 | VAL |
| 2 | AB | 213 | TYR |
| 2 | AB | 220 | THR |
| 2 | AB | 225 | ARG |
| 3 | AC | 3 | GLN |
| 3 | AC | 14 | ILE |
| 3 | AC | 15 | VAL |
| 3 | AC | 18 | TRP |
| 3 | AC | 19 | ASN |
| 3 | AC | 21 | THR |
| 3 | AC | 27 | LYS |
| 3 | AC | 28 | GLU |
| 3 | AC | 29 | PHE |
| 3 | AC | 33 | LEU |
| 3 | AC | 37 | PHE |
| 3 | AC | 38 | LYS |
| 3 | AC | 43 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 52 | VAL |
| 3 | AC | 53 | SER |
| 3 | AC | 55 | ILE |
| 3 | AC | 57 | ILE |
| 3 | AC | 59 | ARG |
| 3 | AC | 64 | ILE |
| 3 | AC | 75 | ILE |
| 3 | AC | 86 | LYS |
| 3 | AC | 103 | ILE |
| 3 | AC | 107 | ARG |
| 3 | AC | 127 | ARG |
| 3 | AC | 131 | ARG |
| 3 | AC | 144 | LEU |
| 3 | AC | 167 | TRP |
| 3 | AC | 168 | TYR |
| 3 | AC | 185 | ASN |
| 3 | AC | 186 | THR |
| 3 | AC | 192 | THR |
| 3 | AC | 193 | TYR |
| 3 | AC | 196 | ILE |
| 3 | AC | 200 | VAL |
| 3 | AC | 207 | ILE |
| 4 | AD | 5 | LEU |
| 4 | AD | 13 | ARG |
| 4 | AD | 23 | SER |
| 4 | AD | 31 | LYS |
| 4 | AD | 32 | CYS |
| 4 | AD | 33 | LYS |
| 4 | AD | 34 | ILE |
| 4 | AD | 35 | GLU |
| 4 | AD | 44 | ARG |
| 4 | AD | 45 | LYS |
| 4 | AD | 56 | ARG |
| 4 | AD | 58 | LYS |
| 4 | AD | 63 | ARG |
| 4 | AD | 73 | ARG |
| 4 | AD | 83 | LYS |
| 4 | AD | 90 | LEU |
| 4 | AD | 93 | LEU |
| 4 | AD | 94 | LEU |
| 4 | AD | 104 | ARG |
| 4 | AD | 111 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AD | 121 | LYS |
| 4 | AD | 123 | ILE |
| 4 | AD | 132 | ILE |
| 4 | AD | 153 | SER |
| 4 | AD | 161 | LEU |
| 4 | AD | 163 | GLU |
| 4 | AD | 171 | LEU |
| 4 | AD | 173 | VAL |
| 4 | AD | 190 | ASP |
| 4 | AD | 195 | ILE |
| 4 | AD | 198 | HIS |
| 4 | AD | 205 | SER |
| 4 | AD | 206 | LYS |
| 5 | AE | 10 | GLU |
| 5 | AE | 14 | LYS |
| 5 | AE | 15 | LEU |
| 5 | AE | 16 | ILE |
| 5 | AE | 18 | VAL |
| 5 | AE | 21 | VAL |
| 5 | AE | 25 | VAL |
| 5 | AE | 32 | SER |
| 5 | AE | 36 | LEU |
| 5 | AE | 37 | THR |
| 5 | AE | 38 | VAL |
| 5 | AE | 60 | ILE |
| 5 | AE | 68 | ARG |
| 5 | AE | 78 | ASN |
| 5 | AE | 81 | LEU |
| 5 | AE | 83 | HIS |
| 5 | AE | 85 | VAL |
| 5 | AE | 94 | VAL |
| 5 | AE | 115 | LEU |
| 5 | AE | 120 | VAL |
| 5 | AE | 124 | LEU |
| 5 | AE | 134 | ILE |
| 5 | AE | 136 | VAL |
| 5 | AE | 137 | VAL |
| 5 | AE | 140 | THR |
| 5 | AE | 142 | ASP |
| 5 | AE | 149 | SER |
| 5 | AE | 153 | VAL |
| 5 | AE | 159 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | AF | 7 | VAL |
| 6 | AF | 9 | MET |
| 6 | AF | 14 | GLN |
| 6 | AF | 15 | SER |
| 6 | AF | 17 | GLN |
| 6 | AF | 24 | ARG |
| 6 | AF | 36 | ILE |
| 6 | AF | 51 | ILE |
| 6 | AF | 54 | LEU |
| 6 | AF | 55 | HIS |
| 6 | AF | 68 | GLN |
| 6 | AF | 69 | GLU |
| 6 | AF | 73 | GLU |
| 6 | AF | 75 | GLU |
| 6 | AF | 84 | VAL |
| 6 | AF | 86 | ARG |
| 6 | AF | 96 | VAL |
| 6 | AF | 98 | GLU |
| 7 | AG | 4 | ARG |
| 7 | AG | 7 | ILE |
| 7 | AG | 22 | LEU |
| 7 | AG | 23 | LEU |
| 7 | AG | 32 | VAL |
| 7 | AG | 36 | LYS |
| 7 | AG | 37 | SER |
| 7 | AG | 38 | THR |
| 7 | AG | 40 | GLU |
| 7 | AG | 48 | GLU |
| 7 | AG | 50 | LEU |
| 7 | AG | 52 | GLN |
| 7 | AG | 58 | GLU |
| 7 | AG | 59 | LEU |
| 7 | AG | 63 | GLU |
| 7 | AG | 70 | ARG |
| 7 | AG | 78 | ARG |
| 7 | AG | 90 | GLU |
| 7 | AG | 106 | GLU |
| 7 | AG | 115 | SER |
| 7 | AG | 135 | VAL |
| 7 | AG | 136 | LYS |
| 7 | AG | 143 | ARG |
| 8 | AH | 2 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | AH | 3 | MET |
| 8 | AH | 22 | LYS |
| 8 | AH | 25 | VAL |
| 8 | AH | 26 | THR |
| 8 | AH | 32 | LEU |
| 8 | AH | 36 | ILE |
| 8 | AH | 38 | ASN |
| 8 | AH | 39 | VAL |
| 8 | AH | 42 | GLU |
| 8 | AH | 47 | GLU |
| 8 | AH | 59 | LEU |
| 8 | AH | 77 | ARG |
| 8 | AH | 83 | LEU |
| 8 | AH | 87 | LYS |
| 8 | AH | 104 | VAL |
| 8 | AH | 108 | LYS |
| 8 | AH | 117 | ARG |
| 8 | AH | 121 | LEU |
| 8 | AH | 129 | VAL |
| 9 | AI | 12 | ARG |
| 9 | AI | 30 | ILE |
| 9 | AI | 33 | ARG |
| 9 | AI | 36 | GLU |
| 9 | AI | 43 | THR |
| 9 | AI | 46 | MET |
| 9 | AI | 48 | VAL |
| 9 | AI | 49 | ARG |
| 9 | AI | 55 | VAL |
| 9 | AI | 56 | ASP |
| 9 | AI | 57 | MET |
| 9 | AI | 60 | LYS |
| 9 | AI | 61 | LEU |
| 9 | AI | 63 | LEU |
| 9 | AI | 65 | ILE |
| 9 | AI | 68 | LYS |
| 9 | AI | 85 | ARG |
| 9 | AI | 88 | MET |
| 9 | AI | 89 | GLU |
| 9 | AI | 90 | TYR |
| 9 | AI | 91 | ASP |
| 9 | AI | 94 | LEU |
| 9 | AI | 100 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AI | 106 | ARG |
| 9 | AI | 115 | LYS |
| 9 | AI | 127 | PHE |
| 9 | AI | 129 | LYS |
| 9 | AI | 130 | ARG |
| 10 | AJ | 5 | ARG |
| 10 | AJ | 6 | ILE |
| 10 | AJ | 8 | ILE |
| 10 | AJ | 27 | GLU |
| 10 | AJ | 30 | LYS |
| 10 | AJ | 40 | ILE |
| 10 | AJ | 42 | LEU |
| 10 | AJ | 45 | ARG |
| 10 | AJ | 48 | ARG |
| 10 | AJ | 49 | PHE |
| 10 | AJ | 50 | THR |
| 10 | AJ | 52 | LEU |
| 10 | AJ | 59 | LYS |
| 10 | AJ | 66 | GLU |
| 10 | AJ | 73 | LEU |
| 10 | AJ | 84 | VAL |
| 10 | AJ | 87 | LEU |
| 10 | AJ | 91 | ASP |
| 10 | AJ | 98 | VAL |
| 11 | AK | 31 | ILE |
| 11 | AK | 33 | THR |
| 11 | AK | 34 | ILE |
| 11 | AK | 52 | PHE |
| 11 | AK | 56 | ARG |
| 11 | AK | 58 | SER |
| 11 | AK | 65 | VAL |
| 11 | AK | 81 | ASN |
| 11 | AK | 96 | THR |
| 11 | AK | 100 | LEU |
| 11 | AK | 101 | ASN |
| 11 | AK | 107 | ILE |
| 11 | AK | 126 | LYS |
| 11 | AK | 128 | ARG |
| 12 | AL | 7 | LEU |
| 12 | AL | 10 | LYS |
| 12 | AL | 29 | GLN |
| 12 | AL | 33 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | AL | 36 | ARG |
| 12 | AL | 44 | LYS |
| 12 | AL | 58 | THR |
| 12 | AL | 62 | GLU |
| 12 | AL | 74 | LEU |
| 12 | AL | 89 | ASP |
| 12 | AL | 102 | LEU |
| 12 | AL | 105 | SER |
| 12 | AL | 115 | SER |
| 12 | AL | 121 | ARG |
| 13 | AM | 4 | ILE |
| 13 | AM | 7 | ILE |
| 13 | AM | 11 | ASP |
| 13 | AM | 13 | LYS |
| 13 | AM | 16 | VAL |
| 13 | AM | 25 | VAL |
| 13 | AM | 27 | LYS |
| 13 | AM | 44 | LYS |
| 13 | AM | 50 | GLU |
| 13 | AM | 59 | GLU |
| 13 | AM | 71 | ARG |
| 13 | AM | 72 | GLU |
| 13 | AM | 80 | LEU |
| 13 | AM | 82 | ASP |
| 13 | AM | 87 | ARG |
| 13 | AM | 91 | HIS |
| 13 | AM | 104 | THR |
| 13 | AM | 108 | THR |
| 14 | AN | 5 | SER |
| 14 | AN | 7 | LYS |
| 14 | AN | 12 | LYS |
| 14 | AN | 14 | VAL |
| 14 | AN | 26 | GLU |
| 14 | AN | 28 | LYS |
| 14 | AN | 46 | LEU |
| 14 | AN | 49 | GLN |
| 14 | AN | 50 | THR |
| 14 | AN | 51 | LEU |
| 14 | AN | 59 | ARG |
| 14 | AN | 84 | VAL |
| 14 | AN | 85 | ARG |
| 14 | AN | 97 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | AN | 98 | LYS |
| 15 | AO | 8 | THR |
| 15 | AO | 13 | SER |
| 15 | AO | 17 | ARG |
| 15 | AO | 22 | THR |
| 15 | AO | 35 | GLN |
| 15 | AO | 39 | LEU |
| 15 | AO | 40 | GLN |
| 15 | AO | 59 | MET |
| 15 | AO | 67 | LEU |
| 15 | AO | 85 | LEU |
| 15 | AO | 87 | LEU |
| 15 | AO | 88 | ARG |
| 16 | AP | 1 | MET |
| 16 | AP | 2 | VAL |
| 16 | AP | 3 | THR |
| 16 | AP | 5 | ARG |
| 16 | AP | 8 | ARG |
| 16 | AP | 19 | VAL |
| 16 | AP | 29 | ASN |
| 16 | AP | 33 | ILE |
| 16 | AP | 46 | LYS |
| 16 | AP | 51 | ARG |
| 16 | AP | 55 | ASP |
| 16 | AP | 56 | ARG |
| 16 | AP | 66 | THR |
| 16 | AP | 76 | LYS |
| 16 | AP | 80 | LYS |
| 17 | AQ | 4 | LYS |
| 17 | AQ | 6 | ARG |
| 17 | AQ | 7 | THR |
| 17 | AQ | 8 | LEU |
| 17 | AQ | 13 | VAL |
| 17 | AQ | 14 | SER |
| 17 | AQ | 16 | LYS |
| 17 | AQ | 17 | MET |
| 17 | AQ | 21 | ILE |
| 17 | AQ | 29 | VAL |
| 17 | AQ | 30 | LYS |
| 17 | AQ | 33 | ILE |
| 17 | AQ | 38 | ILE |
| 17 | AQ | 48 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | AQ | 52 | GLU |
| 17 | AQ | 55 | ILE |
| 17 | AQ | 61 | ILE |
| 17 | AQ | 69 | LYS |
| 17 | AQ | 74 | THR |
| 17 | AQ | 75 | LEU |
| 17 | AQ | 76 | VAL |
| 17 | AQ | 77 | ARG |
| 17 | AQ | 81 | LYS |
| 17 | AQ | 83 | VAL |
| 18 | AR | 21 | ILE |
| 18 | AR | 29 | LEU |
| 18 | AR | 30 | LYS |
| 18 | AR | 31 | ASN |
| 18 | AR | 33 | ILE |
| 18 | AR | 34 | THR |
| 18 | AR | 43 | ARG |
| 18 | AR | 55 | LEU |
| 18 | AR | 57 | ARG |
| 18 | AR | 71 | THR |
| 19 | AS | 6 | LYS |
| 19 | AS | 7 | LYS |
| 19 | AS | 21 | LYS |
| 19 | AS | 24 | GLU |
| 19 | AS | 27 | ASP |
| 19 | AS | 29 | LYS |
| 19 | AS | 32 | ARG |
| 19 | AS | 37 | ARG |
| 19 | AS | 41 | PHE |
| 19 | AS | 45 | ILE |
| 19 | AS | 55 | ARG |
| 19 | AS | 56 | GLN |
| 19 | AS | 58 | VAL |
| 19 | AS | 63 | THR |
| 19 | AS | 65 | GLU |
| 20 | AT | 3 | ASN |
| 20 | AT | 5 | LYS |
| 20 | AT | 6 | SER |
| 20 | AT | 10 | ARG |
| 20 | AT | 12 | ILE |
| 20 | AT | 24 | ARG |
| 20 | AT | 34 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AT | 36 | TYR |
| 20 | AT | 54 | MET |
| 20 | AT | 66 | LEU |
| 20 | AT | 67 | ILE |
| 20 | AT | 69 | LYS |
| 20 | AT | 70 | ASN |
| 20 | AT | 74 | ARG |
| 21 | AU | 5 | LYS |
| 21 | AU | 10 | GLU |
| 21 | AU | 12 | PHE |
| 21 | AU | 18 | ARG |
| 21 | AU | 20 | LYS |
| 21 | AU | 23 | CYS |
| 21 | AU | 25 | LYS |
| 21 | AU | 28 | VAL |
| 21 | AU | 34 | ARG |
| 21 | AU | 37 | PHE |
| 21 | AU | 42 | THR |
| 21 | AU | 46 | LYS |
| 21 | AU | 47 | ARG |
| 21 | AU | 49 | LYS |
| 21 | AU | 54 | LYS |
| 24 | BC | 18 | LYS |
| 24 | BC | 20 | VAL |
| 24 | BC | 23 | GLU |
| 24 | BC | 24 | LEU |
| 24 | BC | 51 | THR |
| 24 | BC | 64 | ILE |
| 24 | BC | 86 | ASN |
| 24 | BC | 90 | ASN |
| 24 | BC | 97 | LYS |
| 24 | BC | 105 | LEU |
| 24 | BC | 111 | LYS |
| 24 | BC | 117 | GLN |
| 24 | BC | 121 | ASP |
| 24 | BC | 140 | THR |
| 24 | BC | 156 | ARG |
| 24 | BC | 162 | VAL |
| 24 | BC | 164 | ILE |
| 24 | BC | 174 | LEU |
| 24 | BC | 177 | ARG |
| 24 | BC | 197 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | BC | 213 | TRP |
| 24 | BC | 216 | VAL |
| 24 | BC | 220 | VAL |
| 24 | BC | 228 | VAL |
| 24 | BC | 242 | LYS |
| 24 | BC | 245 | VAL |
| 24 | BC | 265 | LYS |
| 25 | BD | 1 | MET |
| 25 | BD | 4 | LEU |
| 25 | BD | 14 | ILE |
| 25 | BD | 18 | ASP |
| 25 | BD | 25 | THR |
| 25 | BD | 42 | ASN |
| 25 | BD | 83 | ARG |
| 25 | BD | 95 | SER |
| 25 | BD | 97 | SER |
| 25 | BD | 121 | THR |
| 25 | BD | 129 | THR |
| 25 | BD | 133 | THR |
| 25 | BD | 145 | SER |
| 25 | BD | 174 | SER |
| 25 | BD | 186 | LEU |
| 25 | BD | 197 | THR |
| 26 | BE | 4 | VAL |
| 26 | BE | 5 | LEU |
| 26 | BE | 12 | LEU |
| 26 | BE | 16 | GLU |
| 26 | BE | 30 | GLN |
| 26 | BE | 40 | ARG |
| 26 | BE | 44 | ARG |
| 26 | BE | 55 | SER |
| 26 | BE | 63 | LYS |
| 26 | BE | 74 | LYS |
| 26 | BE | 77 | ILE |
| 26 | BE | 79 | ARG |
| 26 | BE | 93 | SER |
| 26 | BE | 108 | ILE |
| 26 | BE | 111 | GLU |
| 26 | BE | 116 | ASP |
| 26 | BE | 120 | VAL |
| 26 | BE | 122 | GLU |
| 26 | BE | 131 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BE | 136 | GLN |
| 26 | BE | 146 | VAL |
| 26 | BE | 149 | ILE |
| 26 | BE | 170 | ARG |
| 26 | BE | 171 | ASP |
| 26 | BE | 176 | ASP |
| 26 | BE | 178 | VAL |
| 26 | BE | 197 | GLU |
| 26 | BE | 198 | GLU |
| 26 | BE | 200 | LEU |
| 27 | BF | 14 | LYS |
| 27 | BF | 17 | MET |
| 27 | BF | 18 | THR |
| 27 | BF | 21 | ASN |
| 27 | BF | 25 | VAL |
| 27 | BF | 34 | ILE |
| 27 | BF | 35 | THR |
| 27 | BF | 36 | LEU |
| 27 | BF | 37 | ASN |
| 27 | BF | 40 | VAL |
| 27 | BF | 42 | GLU |
| 27 | BF | 44 | ILE |
| 27 | BF | 48 | LYS |
| 27 | BF | 49 | LEU |
| 27 | BF | 51 | ASP |
| 27 | BF | 78 | LYS |
| 27 | BF | 81 | GLN |
| 27 | BF | 83 | TYR |
| 27 | BF | 85 | ILE |
| 27 | BF | 104 | ILE |
| 27 | BF | 108 | VAL |
| 27 | BF | 120 | LYS |
| 27 | BF | 125 | ARG |
| 27 | BF | 132 | VAL |
| 27 | BF | 133 | ARG |
| 27 | BF | 134 | GLU |
| 27 | BF | 147 | ASP |
| 27 | BF | 152 | LEU |
| 27 | BF | 155 | THR |
| 27 | BF | 158 | THR |
| 27 | BF | 174 | ASP |
| 27 | BF | 178 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BG | 2 | SER |
| 28 | BG | 11 | VAL |
| 28 | BG | 33 | LEU |
| 28 | BG | 39 | ASP |
| 28 | BG | 55 | ARG |
| 28 | BG | 56 | ASP |
| 28 | BG | 67 | THR |
| 28 | BG | 69 | ARG |
| 28 | BG | 77 | ILE |
| 28 | BG | 84 | THR |
| 28 | BG | 87 | LEU |
| 28 | BG | 88 | GLN |
| 28 | BG | 99 | LYS |
| 28 | BG | 124 | GLU |
| 28 | BG | 133 | LEU |
| 28 | BG | 139 | GLN |
| 28 | BG | 152 | ARG |
| 28 | BG | 155 | GLU |
| 28 | BG | 172 | LYS |
| 29 | BH | 1 | MET |
| 29 | BH | 3 | VAL |
| 29 | BH | 6 | LEU |
| 29 | BH | 12 | LEU |
| 29 | BH | 15 | LEU |
| 29 | BH | 27 | ARG |
| 29 | BH | 50 | ARG |
| 29 | BH | 60 | GLU |
| 29 | BH | 62 | LEU |
| 29 | BH | 66 | ASN |
| 29 | BH | 75 | LEU |
| 29 | BH | 77 | THR |
| 29 | BH | 79 | THR |
| 29 | BH | 86 | ASP |
| 29 | BH | 91 | PHE |
| 29 | BH | 112 | LYS |
| 29 | BH | 119 | ASN |
| 29 | BH | 122 | LEU |
| 29 | BH | 123 | ARG |
| 29 | BH | 125 | THR |
| 29 | BH | 129 | GLU |
| 29 | BH | 131 | SER |
| 29 | BH | 137 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | BH | 142 | VAL |
| 29 | BH | 145 | ASN |
| 29 | BH | 146 | VAL |
| 30 | BI | 3 | LYS |
| 30 | BI | 9 | VAL |
| 30 | BI | 13 | VAL |
| 30 | BI | 17 | MET |
| 30 | BI | 19 | ASN |
| 30 | BI | 31 | GLN |
| 30 | BI | 34 | ASN |
| 30 | BI | 38 | PHE |
| 30 | BI | 45 | LYS |
| 30 | BI | 47 | ASP |
| 30 | BI | 50 | GLU |
| 30 | BI | 51 | LYS |
| 30 | BI | 62 | TYR |
| 30 | BI | 69 | PHE |
| 30 | BI | 72 | LYS |
| 30 | BI | 82 | LYS |
| 30 | BI | 86 | ILE |
| 30 | BI | 87 | LYS |
| 30 | BI | 90 | SER |
| 30 | BI | 94 | ASN |
| 30 | BI | 96 | ASP |
| 30 | BI | 103 | ARG |
| 30 | BI | 107 | GLN |
| 30 | BI | 125 | MET |
| 30 | BI | 128 | SER |
| 30 | BI | 134 | ARG |
| 30 | BI | 136 | MET |
| 31 | BJ | 30 | THR |
| 31 | BJ | 37 | ARG |
| 31 | BJ | 40 | HIS |
| 31 | BJ | 43 | GLU |
| 31 | BJ | 47 | HIS |
| 31 | BJ | 61 | LYS |
| 31 | BJ | 64 | VAL |
| 31 | BJ | 86 | GLN |
| 31 | BJ | 114 | LEU |
| 31 | BJ | 124 | VAL |
| 31 | BJ | 142 | ILE |
| 32 | BK | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BK | 40 | LYS |
| 32 | BK | 49 | ARG |
| 32 | BK | 51 | LYS |
| 32 | BK | 58 | LEU |
| 32 | BK | 66 | LYS |
| 32 | BK | 91 | SER |
| 32 | BK | 92 | GLU |
| 32 | BK | 105 | ARG |
| 32 | BK | 106 | GLU |
| 32 | BK | 110 | GLU |
| 32 | BK | 116 | ILE |
| 32 | BK | 117 | SER |
| 32 | BK | 121 | GLU |
| 33 | BL | 19 | LEU |
| 33 | BL | 40 | SER |
| 33 | BL | 60 | ARG |
| 33 | BL | 69 | ARG |
| 33 | BL | 82 | LEU |
| 33 | BL | 86 | GLU |
| 33 | BL | 94 | THR |
| 33 | BL | 100 | ILE |
| 33 | BL | 111 | ILE |
| 33 | BL | 115 | GLU |
| 33 | BL | 125 | LEU |
| 34 | BM | 20 | LEU |
| 34 | BM | 24 | THR |
| 34 | BM | 45 | GLN |
| 34 | BM | 55 | ARG |
| 34 | BM | 70 | ASP |
| 34 | BM | 80 | VAL |
| 34 | BM | 100 | LYS |
| 34 | BM | 112 | LEU |
| 34 | BM | 115 | GLU |
| 34 | BM | 126 | ILE |
| 35 | BN | 2 | ARG |
| 35 | BN | 33 | ILE |
| 35 | BN | 69 | ARG |
| 35 | BN | 90 | ARG |
| 35 | BN | 95 | THR |
| 35 | BN | 116 | VAL |
| 36 | BO | 3 | LYS |
| 36 | BO | 4 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BO | 5 | SER |
| 36 | BO | 9 | ARG |
| 36 | BO | 17 | LYS |
| 36 | BO | 18 | LEU |
| 36 | BO | 24 | THR |
| 36 | BO | 27 | VAL |
| 36 | BO | 28 | VAL |
| 36 | BO | 31 | THR |
| 36 | BO | 36 | TYR |
| 36 | BO | 45 | SER |
| 36 | BO | 47 | VAL |
| 36 | BO | 49 | VAL |
| 36 | BO | 54 | VAL |
| 36 | BO | 55 | GLU |
| 36 | BO | 60 | GLU |
| 36 | BO | 61 | GLN |
| 36 | BO | 65 | THR |
| 36 | BO | 87 | ILE |
| 36 | BO | 89 | ASP |
| 37 | BP | 6 | LYS |
| 37 | BP | 7 | GLN |
| 37 | BP | 12 | GLN |
| 37 | BP | 19 | SER |
| 37 | BP | 26 | VAL |
| 37 | BP | 27 | GLU |
| 37 | BP | 38 | LYS |
| 37 | BP | 53 | ARG |
| 37 | BP | 57 | SER |
| 37 | BP | 63 | LYS |
| 37 | BP | 64 | ILE |
| 37 | BP | 68 | GLU |
| 37 | BP | 88 | ARG |
| 37 | BP | 93 | ARG |
| 37 | BP | 96 | LYS |
| 37 | BP | 103 | ARG |
| 37 | BP | 109 | ARG |
| 37 | BP | 110 | ILE |
| 38 | BQ | 5 | LYS |
| 38 | BQ | 18 | LEU |
| 38 | BQ | 30 | ARG |
| 38 | BQ | 51 | ARG |
| 38 | BQ | 58 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | BQ | 78 | LYS |
| 38 | BQ | 85 | LYS |
| 38 | BQ | 87 | SER |
| 38 | BQ | 92 | ARG |
| 38 | BQ | 103 | LYS |
| 38 | BQ | 117 | LEU |
| 39 | BR | 10 | LYS |
| 39 | BR | 16 | GLU |
| 39 | BR | 20 | VAL |
| 39 | BR | 38 | VAL |
| 39 | BR | 46 | GLU |
| 39 | BR | 47 | VAL |
| 39 | BR | 48 | LYS |
| 39 | BR | 74 | ILE |
| 39 | BR | 85 | LYS |
| 39 | BR | 86 | GLN |
| 40 | BS | 6 | LYS |
| 40 | BS | 7 | HIS |
| 40 | BS | 8 | ARG |
| 40 | BS | 19 | LEU |
| 40 | BS | 25 | ARG |
| 40 | BS | 28 | LYS |
| 40 | BS | 30 | SER |
| 40 | BS | 47 | VAL |
| 40 | BS | 59 | GLU |
| 40 | BS | 69 | LEU |
| 40 | BS | 70 | LYS |
| 40 | BS | 81 | SER |
| 40 | BS | 82 | MET |
| 40 | BS | 90 | LYS |
| 40 | BS | 97 | LEU |
| 40 | BS | 101 | SER |
| 40 | BS | 109 | ASP |
| 41 | BT | 5 | GLU |
| 41 | BT | 12 | ARG |
| 41 | BT | 18 | GLU |
| 41 | BT | 27 | SER |
| 41 | BT | 30 | ILE |
| 41 | BT | 49 | LYS |
| 41 | BT | 68 | LYS |
| 41 | BT | 70 | HIS |
| 41 | BT | 73 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | BT | 79 | ASP |
| 41 | BT | 86 | THR |
| 41 | BT | 93 | LEU |
| 42 | BU | 5 | ILE |
| 42 | BU | 9 | ASP |
| 42 | BU | 26 | LYS |
| 42 | BU | 28 | VAL |
| 42 | BU | 29 | LEU |
| 42 | BU | 52 | LEU |
| 42 | BU | 68 | SER |
| 42 | BU | 72 | ILE |
| 42 | BU | 77 | THR |
| 42 | BU | 86 | ARG |
| 42 | BU | 99 | ASN |
| 43 | BV | 1 | MET |
| 43 | BV | 10 | LYS |
| 43 | BV | 14 | LYS |
| 43 | BV | 17 | SER |
| 43 | BV | 18 | ARG |
| 43 | BV | 29 | ILE |
| 43 | BV | 34 | LYS |
| 43 | BV | 41 | GLU |
| 43 | BV | 43 | ASP |
| 43 | BV | 61 | LEU |
| 43 | BV | 65 | VAL |
| 43 | BV | 66 | ASP |
| 43 | BV | 85 | LYS |
| 43 | BV | 92 | VAL |
| 43 | BV | 93 | ARG |
| 44 | BW | 20 | ARG |
| 44 | BW | 29 | GLU |
| 44 | BW | 38 | VAL |
| 44 | BW | 39 | ARG |
| 44 | BW | 41 | ARG |
| 44 | BW | 56 | ASP |
| 44 | BW | 64 | ASP |
| 44 | BW | 72 | LYS |
| 44 | BW | 81 | SER |
| 44 | BW | 85 | GLU |
| 45 | BX | 14 | THR |
| 45 | BX | 25 | THR |
| 45 | BX | 26 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | BX | 48 | THR |
| 45 | BX | 66 | THR |
| 45 | BX | 76 | GLU |
| 46 | BY | 5 | GLU |
| 46 | BY | 6 | LEU |
| 46 | BY | 16 | THR |
| 46 | BY | 22 | LEU |
| 46 | BY | 57 | LEU |
| 47 | BZ | 3 | LYS |
| 47 | BZ | 10 | THR |
| 47 | BZ | 19 | LYS |
| 47 | BZ | 31 | ARG |
| 47 | BZ | 36 | VAL |
| 47 | BZ | 57 | VAL |
| 47 | BZ | 58 | GLU |
| 48 | B0 | 18 | SER |
| 48 | B0 | 20 | ASP |
| 48 | B0 | 26 | THR |
| 48 | B0 | 36 | GLU |
| 48 | B0 | 40 | ARG |
| 49 | B1 | 46 | HIS |
| 49 | B1 | 47 | VAL |
| 49 | B1 | 51 | GLU |
| 50 | B2 | 4 | THR |
| 50 | B2 | 21 | ARG |
| 50 | B2 | 43 | THR |
| 50 | B2 | 45 | SER |
| 51 | B3 | 5 | LYS |
| 51 | B3 | 16 | LYS |
| 51 | B3 | 30 | ARG |
| 51 | B3 | 31 | HIS |
| 51 | B3 | 47 | LYS |
| 51 | B3 | 55 | LEU |
| 52 | B4 | 6 | SER |
| 52 | B4 | 18 | LYS |
| 53 | B5 | 21 | TYR |
| 53 | B5 | 23 | ILE |
| 53 | B5 | 38 | PHE |
| 53 | B5 | 47 | LYS |
| 53 | B5 | 48 | LEU |
| 53 | B5 | 64 | SER |
| 53 | B5 | 73 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | B5 | 76 | LEU |
| 53 | B5 | 78 | ILE |
| 53 | B5 | 86 | GLU |
| 53 | B5 | 93 | ASP |
| 53 | B5 | 94 | TYR |
| 53 | B5 | 100 | ILE |
| 2 | CB | 15 | HIS |
| 2 | CB | 16 | PHE |
| 2 | CB | 20 | THR |
| 2 | CB | 21 | ARG |
| 2 | CB | 22 | TYR |
| 2 | CB | 23 | TRP |
| 2 | CB | 26 | LYS |
| 2 | CB | 27 | MET |
| 2 | CB | 32 | PHE |
| 2 | CB | 35 | ARG |
| 2 | CB | 40 | ILE |
| 2 | CB | 43 | LEU |
| 2 | CB | 49 | MET |
| 2 | CB | 50 | PHE |
| 2 | CB | 56 | GLU |
| 2 | CB | 66 | LYS |
| 2 | CB | 67 | ILE |
| 2 | CB | 68 | LEU |
| 2 | CB | 73 | LYS |
| 2 | CB | 74 | ARG |
| 2 | CB | 77 | SER |
| 2 | CB | 80 | VAL |
| 2 | CB | 85 | LEU |
| 2 | CB | 87 | CYS |
| 2 | CB | 88 | ASP |
| 2 | CB | 94 | HIS |
| 2 | CB | 95 | ARG |
| 2 | CB | 96 | TRP |
| 2 | CB | 101 | LEU |
| 2 | CB | 106 | THR |
| 2 | CB | 111 | ILE |
| 2 | CB | 126 | PHE |
| 2 | CB | 127 | ASP |
| 2 | CB | 130 | THR |
| 2 | CB | 136 | MET |
| 2 | CB | 148 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CB | 163 | VAL |
| 2 | CB | 164 | ILE |
| 2 | CB | 168 | HIS |
| 2 | CB | 171 | ILE |
| 2 | CB | 174 | LYS |
| 2 | CB | 175 | GLU |
| 2 | CB | 179 | LEU |
| 2 | CB | 205 | ASP |
| 2 | CB | 207 | ILE |
| 2 | CB | 208 | ARG |
| 2 | CB | 210 | VAL |
| 2 | CB | 213 | TYR |
| 2 | CB | 222 | ARG |
| 2 | CB | 225 | ARG |
| 3 | CC | 3 | GLN |
| 3 | CC | 8 | ASN |
| 3 | CC | 16 | LYS |
| 3 | CC | 27 | LYS |
| 3 | CC | 37 | PHE |
| 3 | CC | 38 | LYS |
| 3 | CC | 43 | LEU |
| 3 | CC | 70 | THR |
| 3 | CC | 75 | ILE |
| 3 | CC | 80 | LYS |
| 3 | CC | 103 | ILE |
| 3 | CC | 107 | ARG |
| 3 | CC | 110 | GLU |
| 3 | CC | 121 | THR |
| 3 | CC | 131 | ARG |
| 3 | CC | 140 | ASN |
| 3 | CC | 153 | VAL |
| 3 | CC | 157 | LEU |
| 3 | CC | 167 | TRP |
| 3 | CC | 168 | TYR |
| 3 | CC | 175 | LEU |
| 3 | CC | 179 | ARG |
| 3 | CC | 185 | ASN |
| 3 | CC | 186 | THR |
| 3 | CC | 193 | TYR |
| 3 | CC | 200 | VAL |
| 4 | CD | 5 | LEU |
| 4 | CD | 8 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | CD | 9 | LEU |
| 4 | CD | 10 | LYS |
| 4 | CD | 23 | SER |
| 4 | CD | 30 | THR |
| 4 | CD | 32 | CYS |
| 4 | CD | 33 | LYS |
| 4 | CD | 44 | ARG |
| 4 | CD | 48 | LEU |
| 4 | CD | 50 | ASP |
| 4 | CD | 54 | GLN |
| 4 | CD | 55 | LEU |
| 4 | CD | 56 | ARG |
| 4 | CD | 58 | LYS |
| 4 | CD | 59 | GLN |
| 4 | CD | 81 | ARG |
| 4 | CD | 142 | VAL |
| 4 | CD | 148 | LYS |
| 4 | CD | 152 | GLN |
| 4 | CD | 155 | VAL |
| 4 | CD | 159 | LEU |
| 4 | CD | 161 | LEU |
| 4 | CD | 166 | GLU |
| 4 | CD | 169 | THR |
| 4 | CD | 191 | LEU |
| 4 | CD | 192 | SER |
| 4 | CD | 200 | ILE |
| 4 | CD | 206 | LYS |
| 5 | CE | 10 | GLU |
| 5 | CE | 15 | LEU |
| 5 | CE | 18 | VAL |
| 5 | CE | 24 | THR |
| 5 | CE | 25 | VAL |
| 5 | CE | 26 | LYS |
| 5 | CE | 32 | SER |
| 5 | CE | 45 | ARG |
| 5 | CE | 52 | LYS |
| 5 | CE | 70 | ASN |
| 5 | CE | 76 | LEU |
| 5 | CE | 81 | LEU |
| 5 | CE | 88 | VAL |
| 5 | CE | 93 | ARG |
| 5 | CE | 94 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CE | 100 | SER |
| 5 | CE | 105 | ILE |
| 5 | CE | 114 | VAL |
| 5 | CE | 115 | LEU |
| 5 | CE | 126 | LYS |
| 5 | CE | 136 | VAL |
| 5 | CE | 140 | THR |
| 5 | CE | 146 | ASN |
| 5 | CE | 149 | SER |
| 5 | CE | 151 | GLU |
| 5 | CE | 153 | VAL |
| 5 | CE | 156 | LYS |
| 6 | CF | 1 | MET |
| 6 | CF | 8 | PHE |
| 6 | CF | 16 | GLU |
| 6 | CF | 23 | GLU |
| 6 | CF | 24 | ARG |
| 6 | CF | 26 | THR |
| 6 | CF | 30 | THR |
| 6 | CF | 33 | GLU |
| 6 | CF | 35 | LYS |
| 6 | CF | 36 | ILE |
| 6 | CF | 38 | ARG |
| 6 | CF | 51 | ILE |
| 6 | CF | 53 | LYS |
| 6 | CF | 54 | LEU |
| 6 | CF | 55 | HIS |
| 6 | CF | 63 | ASN |
| 6 | CF | 64 | VAL |
| 6 | CF | 69 | GLU |
| 6 | CF | 71 | ILE |
| 6 | CF | 74 | LEU |
| 6 | CF | 75 | GLU |
| 6 | CF | 80 | PHE |
| 6 | CF | 85 | ILE |
| 6 | CF | 87 | SER |
| 6 | CF | 93 | LYS |
| 6 | CF | 97 | THR |
| 7 | CG | 4 | ARG |
| 7 | CG | 5 | ARG |
| 7 | CG | 6 | VAL |
| 7 | CG | 7 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CG | 12 | ILE |
| 7 | CG | 22 | LEU |
| 7 | CG | 43 | VAL |
| 7 | CG | 48 | GLU |
| 7 | CG | 59 | LEU |
| 7 | CG | 62 | PHE |
| 7 | CG | 64 | VAL |
| 7 | CG | 66 | LEU |
| 7 | CG | 67 | GLU |
| 7 | CG | 72 | THR |
| 7 | CG | 73 | VAL |
| 7 | CG | 78 | ARG |
| 7 | CG | 92 | ARG |
| 7 | CG | 94 | VAL |
| 7 | CG | 120 | LEU |
| 7 | CG | 123 | GLU |
| 7 | CG | 126 | ASP |
| 7 | CG | 129 | GLU |
| 7 | CG | 138 | ARG |
| 7 | CG | 140 | ASP |
| 7 | CG | 142 | HIS |
| 8 | CH | 13 | ARG |
| 8 | CH | 15 | ARG |
| 8 | CH | 26 | THR |
| 8 | CH | 32 | LEU |
| 8 | CH | 39 | VAL |
| 8 | CH | 42 | GLU |
| 8 | CH | 43 | GLU |
| 8 | CH | 45 | PHE |
| 8 | CH | 48 | ASP |
| 8 | CH | 52 | GLU |
| 8 | CH | 54 | ASP |
| 8 | CH | 67 | GLN |
| 8 | CH | 73 | GLU |
| 8 | CH | 74 | SER |
| 8 | CH | 75 | ILE |
| 8 | CH | 77 | ARG |
| 8 | CH | 83 | LEU |
| 8 | CH | 87 | LYS |
| 8 | CH | 99 | LEU |
| 8 | CH | 112 | THR |
| 8 | CH | 121 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CH | 125 | ILE |
| 9 | CI | 9 | THR |
| 9 | CI | 21 | ILE |
| 9 | CI | 28 | ILE |
| 9 | CI | 33 | ARG |
| 9 | CI | 36 | GLU |
| 9 | CI | 38 | TYR |
| 9 | CI | 49 | ARG |
| 9 | CI | 50 | GLN |
| 9 | CI | 55 | VAL |
| 9 | CI | 61 | LEU |
| 9 | CI | 62 | ASP |
| 9 | CI | 88 | MET |
| 9 | CI | 89 | GLU |
| 9 | CI | 94 | LEU |
| 9 | CI | 111 | VAL |
| 9 | CI | 127 | PHE |
| 9 | CI | 129 | LYS |
| 10 | CJ | 9 | ARG |
| 10 | CJ | 16 | ARG |
| 10 | CJ | 17 | LEU |
| 10 | CJ | 22 | THR |
| 10 | CJ | 25 | ILE |
| 10 | CJ | 30 | LYS |
| 10 | CJ | 51 | VAL |
| 10 | CJ | 53 | ILE |
| 10 | CJ | 59 | LYS |
| 10 | CJ | 71 | LEU |
| 10 | CJ | 80 | THR |
| 10 | CJ | 83 | THR |
| 10 | CJ | 87 | LEU |
| 10 | CJ | 88 | MET |
| 10 | CJ | 90 | LEU |
| 10 | CJ | 91 | ASP |
| 10 | CJ | 100 | ILE |
| 10 | CJ | 102 | LEU |
| 11 | CK | 14 | LYS |
| 11 | CK | 15 | GLN |
| 11 | CK | 26 | SER |
| 11 | CK | 33 | THR |
| 11 | CK | 64 | GLN |
| 11 | CK | 81 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | CK | 82 | LEU |
| 11 | CK | 83 | GLU |
| 11 | CK | 86 | VAL |
| 11 | CK | 93 | ARG |
| 11 | CK | 96 | THR |
| 11 | CK | 98 | ARG |
| 11 | CK | 106 | ARG |
| 11 | CK | 107 | ILE |
| 11 | CK | 108 | THR |
| 11 | CK | 109 | ASN |
| 11 | CK | 126 | LYS |
| 11 | CK | 127 | ARG |
| 11 | CK | 128 | ARG |
| 12 | CL | 3 | THR |
| 12 | CL | 4 | VAL |
| 12 | CL | 10 | LYS |
| 12 | CL | 18 | LYS |
| 12 | CL | 19 | SER |
| 12 | CL | 20 | ASN |
| 12 | CL | 29 | GLN |
| 12 | CL | 38 | TYR |
| 12 | CL | 44 | LYS |
| 12 | CL | 59 | ASN |
| 12 | CL | 63 | VAL |
| 12 | CL | 82 | ILE |
| 12 | CL | 86 | ARG |
| 12 | CL | 89 | ASP |
| 12 | CL | 93 | VAL |
| 12 | CL | 94 | ARG |
| 12 | CL | 97 | THR |
| 12 | CL | 107 | VAL |
| 12 | CL | 110 | ARG |
| 12 | CL | 111 | LYS |
| 12 | CL | 121 | ARG |
| 13 | CM | 8 | ASN |
| 13 | CM | 13 | LYS |
| 13 | CM | 14 | HIS |
| 13 | CM | 19 | LEU |
| 13 | CM | 29 | ARG |
| 13 | CM | 31 | LYS |
| 13 | CM | 41 | GLU |
| 13 | CM | 48 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | CM | 58 | ASP |
| 13 | CM | 59 | GLU |
| 13 | CM | 60 | VAL |
| 13 | CM | 63 | PHE |
| 13 | CM | 66 | GLU |
| 13 | CM | 90 | ARG |
| 13 | CM | 91 | HIS |
| 13 | CM | 101 | ARG |
| 13 | CM | 113 | ARG |
| 14 | CN | 10 | GLU |
| 14 | CN | 18 | ASP |
| 14 | CN | 23 | LYS |
| 14 | CN | 26 | GLU |
| 14 | CN | 28 | LYS |
| 14 | CN | 75 | ARG |
| 14 | CN | 77 | PHE |
| 14 | CN | 83 | LYS |
| 14 | CN | 100 | SER |
| 15 | CO | 17 | ARG |
| 15 | CO | 18 | ASP |
| 15 | CO | 26 | GLU |
| 15 | CO | 27 | VAL |
| 15 | CO | 38 | HIS |
| 15 | CO | 64 | ARG |
| 15 | CO | 70 | LEU |
| 15 | CO | 84 | ARG |
| 15 | CO | 87 | LEU |
| 15 | CO | 88 | ARG |
| 16 | CP | 1 | MET |
| 16 | CP | 5 | ARG |
| 16 | CP | 18 | GLN |
| 16 | CP | 20 | VAL |
| 16 | CP | 31 | ARG |
| 16 | CP | 46 | LYS |
| 16 | CP | 51 | ARG |
| 16 | CP | 55 | ASP |
| 16 | CP | 63 | GLN |
| 16 | CP | 74 | LEU |
| 16 | CP | 80 | LYS |
| 17 | CQ | 5 | ILE |
| 17 | CQ | 9 | GLN |
| 17 | CQ | 14 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | CQ | 17 | MET |
| 17 | CQ | 18 | GLU |
| 17 | CQ | 25 | ILE |
| 17 | CQ | 28 | PHE |
| 17 | CQ | 40 | ARG |
| 17 | CQ | 41 | THR |
| 17 | CQ | 48 | ASP |
| 17 | CQ | 50 | ASN |
| 17 | CQ | 52 | GLU |
| 17 | CQ | 55 | ILE |
| 17 | CQ | 61 | ILE |
| 17 | CQ | 62 | ARG |
| 17 | CQ | 63 | GLU |
| 17 | CQ | 65 | ARG |
| 17 | CQ | 70 | THR |
| 17 | CQ | 75 | LEU |
| 17 | CQ | 76 | VAL |
| 17 | CQ | 79 | VAL |
| 17 | CQ | 80 | GLU |
| 17 | CQ | 81 | LYS |
| 18 | CR | 21 | ILE |
| 18 | CR | 25 | ASP |
| 18 | CR | 33 | ILE |
| 18 | CR | 43 | ARG |
| 18 | CR | 45 | THR |
| 18 | CR | 47 | THR |
| 18 | CR | 54 | GLN |
| 18 | CR | 57 | ARG |
| 18 | CR | 59 | ILE |
| 18 | CR | 66 | SER |
| 19 | CS | 5 | LEU |
| 19 | CS | 6 | LYS |
| 19 | CS | 11 | ILE |
| 19 | CS | 13 | LEU |
| 19 | CS | 21 | LYS |
| 19 | CS | 23 | VAL |
| 19 | CS | 27 | ASP |
| 19 | CS | 31 | LEU |
| 19 | CS | 36 | ARG |
| 19 | CS | 43 | ASN |
| 19 | CS | 49 | ILE |
| 19 | CS | 58 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CT | 3 | ASN |
| 20 | CT | 6 | SER |
| 20 | CT | 8 | LYS |
| 20 | CT | 30 | THR |
| 20 | CT | 36 | TYR |
| 20 | CT | 59 | ASP |
| 20 | CT | 64 | LYS |
| 20 | CT | 69 | LYS |
| 21 | CU | 5 | LYS |
| 21 | CU | 12 | PHE |
| 21 | CU | 16 | LEU |
| 21 | CU | 18 | ARG |
| 21 | CU | 19 | PHE |
| 21 | CU | 24 | GLU |
| 21 | CU | 25 | LYS |
| 21 | CU | 28 | VAL |
| 21 | CU | 34 | ARG |
| 21 | CU | 37 | PHE |
| 21 | CU | 38 | TYR |
| 21 | CU | 42 | THR |
| 21 | CU | 47 | ARG |
| 21 | CU | 53 | VAL |
| 21 | CU | 54 | LYS |
| 24 | DC | 30 | PHE |
| 24 | DC | 63 | ARG |
| 24 | DC | 80 | ARG |
| 24 | DC | 103 | TYR |
| 24 | DC | 111 | LYS |
| 24 | DC | 116 | ILE |
| 24 | DC | 130 | LEU |
| 24 | DC | 153 | GLN |
| 24 | DC | 156 | ARG |
| 24 | DC | 157 | SER |
| 24 | DC | 167 | ARG |
| 24 | DC | 175 | ARG |
| 24 | DC | 195 | VAL |
| 24 | DC | 202 | LEU |
| 24 | DC | 203 | ARG |
| 24 | DC | 250 | VAL |
| 24 | DC | 259 | SER |
| 24 | DC | 262 | ARG |
| 24 | DC | 267 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DD | 4 | LEU |
| 25 | DD | 12 | THR |
| 25 | DD | 21 | SER |
| 25 | DD | 25 | THR |
| 25 | DD | 33 | ARG |
| 25 | DD | 55 | LYS |
| 25 | DD | 73 | VAL |
| 25 | DD | 77 | ARG |
| 25 | DD | 86 | GLU |
| 25 | DD | 95 | SER |
| 25 | DD | 103 | ASP |
| 25 | DD | 118 | PHE |
| 25 | DD | 129 | THR |
| 25 | DD | 138 | LEU |
| 25 | DD | 140 | HIS |
| 25 | DD | 146 | ILE |
| 25 | DD | 168 | GLU |
| 25 | DD | 170 | VAL |
| 25 | DD | 189 | VAL |
| 26 | DE | 9 | GLN |
| 26 | DE | 22 | ASP |
| 26 | DE | 40 | ARG |
| 26 | DE | 41 | GLN |
| 26 | DE | 57 | LYS |
| 26 | DE | 58 | LYS |
| 26 | DE | 69 | ARG |
| 26 | DE | 77 | ILE |
| 26 | DE | 78 | TRP |
| 26 | DE | 84 | THR |
| 26 | DE | 90 | GLN |
| 26 | DE | 91 | ASP |
| 26 | DE | 105 | LEU |
| 26 | DE | 107 | SER |
| 26 | DE | 108 | ILE |
| 26 | DE | 118 | LEU |
| 26 | DE | 126 | VAL |
| 26 | DE | 127 | GLU |
| 26 | DE | 131 | THR |
| 26 | DE | 137 | LYS |
| 26 | DE | 149 | ILE |
| 26 | DE | 150 | THR |
| 26 | DE | 163 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | DE | 164 | LEU |
| 26 | DE | 170 | ARG |
| 26 | DE | 173 | THR |
| 26 | DE | 187 | VAL |
| 26 | DE | 188 | MET |
| 27 | DF | 6 | ASP |
| 27 | DF | 7 | TYR |
| 27 | DF | 8 | TYR |
| 27 | DF | 14 | LYS |
| 27 | DF | 18 | THR |
| 27 | DF | 26 | MET |
| 27 | DF | 35 | THR |
| 27 | DF | 36 | LEU |
| 27 | DF | 38 | MET |
| 27 | DF | 44 | ILE |
| 27 | DF | 48 | LYS |
| 27 | DF | 52 | ASN |
| 27 | DF | 56 | ASP |
| 27 | DF | 64 | LYS |
| 27 | DF | 67 | ILE |
| 27 | DF | 74 | VAL |
| 27 | DF | 78 | LYS |
| 27 | DF | 110 | ARG |
| 27 | DF | 117 | LEU |
| 27 | DF | 121 | SER |
| 27 | DF | 125 | ARG |
| 27 | DF | 132 | VAL |
| 27 | DF | 140 | GLU |
| 27 | DF | 141 | ILE |
| 27 | DF | 143 | TYR |
| 27 | DF | 147 | ASP |
| 27 | DF | 150 | ARG |
| 27 | DF | 174 | ASP |
| 27 | DF | 177 | PHE |
| 28 | DG | 11 | VAL |
| 28 | DG | 24 | ILE |
| 28 | DG | 29 | LYS |
| 28 | DG | 30 | ASN |
| 28 | DG | 42 | GLU |
| 28 | DG | 45 | HIS |
| 28 | DG | 49 | THR |
| 28 | DG | 56 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | DG | 62 | TRP |
| 28 | DG | 69 | ARG |
| 28 | DG | 89 | LEU |
| 28 | DG | 90 | VAL |
| 28 | DG | 92 | VAL |
| 28 | DG | 98 | VAL |
| 28 | DG | 117 | LEU |
| 28 | DG | 124 | GLU |
| 28 | DG | 127 | THR |
| 28 | DG | 139 | GLN |
| 28 | DG | 149 | ARG |
| 28 | DG | 151 | TYR |
| 28 | DG | 155 | GLU |
| 28 | DG | 158 | LYS |
| 28 | DG | 166 | ASP |
| 29 | DH | 7 | ASP |
| 29 | DH | 12 | LEU |
| 29 | DH | 41 | LYS |
| 29 | DH | 42 | LYS |
| 29 | DH | 48 | GLU |
| 29 | DH | 50 | ARG |
| 29 | DH | 53 | GLU |
| 29 | DH | 54 | LEU |
| 29 | DH | 57 | LYS |
| 29 | DH | 62 | LEU |
| 29 | DH | 77 | THR |
| 29 | DH | 78 | VAL |
| 29 | DH | 87 | GLU |
| 29 | DH | 89 | LYS |
| 29 | DH | 94 | ILE |
| 29 | DH | 109 | GLU |
| 29 | DH | 114 | GLU |
| 29 | DH | 116 | ARG |
| 29 | DH | 117 | LEU |
| 29 | DH | 119 | ASN |
| 29 | DH | 121 | VAL |
| 29 | DH | 124 | THR |
| 29 | DH | 125 | THR |
| 29 | DH | 129 | GLU |
| 29 | DH | 142 | VAL |
| 29 | DH | 149 | GLU |
| 30 | DI | 3 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DI | 4 | LYS |
| 30 | DI | 8 | TYR |
| 30 | DI | 10 | LYS |
| 30 | DI | 11 | LEU |
| 30 | DI | 12 | GLN |
| 30 | DI | 24 | VAL |
| 30 | DI | 38 | PHE |
| 30 | DI | 40 | LYS |
| 30 | DI | 62 | TYR |
| 30 | DI | 68 | THR |
| 30 | DI | 69 | PHE |
| 30 | DI | 72 | LYS |
| 30 | DI | 79 | LEU |
| 30 | DI | 82 | LYS |
| 30 | DI | 86 | ILE |
| 30 | DI | 87 | LYS |
| 30 | DI | 88 | SER |
| 30 | DI | 92 | LYS |
| 30 | DI | 97 | LYS |
| 30 | DI | 98 | VAL |
| 30 | DI | 103 | ARG |
| 30 | DI | 105 | GLN |
| 30 | DI | 106 | LEU |
| 30 | DI | 112 | THR |
| 30 | DI | 117 | MET |
| 30 | DI | 122 | ILE |
| 30 | DI | 125 | MET |
| 30 | DI | 127 | ARG |
| 31 | DJ | 9 | GLU |
| 31 | DJ | 28 | LEU |
| 31 | DJ | 34 | ARG |
| 31 | DJ | 39 | LYS |
| 31 | DJ | 40 | HIS |
| 31 | DJ | 43 | GLU |
| 31 | DJ | 44 | TYR |
| 31 | DJ | 50 | THR |
| 31 | DJ | 62 | VAL |
| 31 | DJ | 65 | THR |
| 31 | DJ | 72 | LYS |
| 31 | DJ | 76 | HIS |
| 31 | DJ | 81 | ILE |
| 31 | DJ | 84 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | DJ | 85 | LYS |
| 31 | DJ | 96 | ARG |
| 31 | DJ | 101 | ILE |
| 31 | DJ | 103 | ILE |
| 31 | DJ | 109 | LEU |
| 31 | DJ | 118 | MET |
| 31 | DJ | 129 | GLU |
| 31 | DJ | 138 | GLN |
| 32 | DK | 25 | LEU |
| 32 | DK | 47 | ILE |
| 32 | DK | 49 | ARG |
| 32 | DK | 53 | LYS |
| 32 | DK | 56 | ASP |
| 32 | DK | 66 | LYS |
| 32 | DK | 70 | ARG |
| 32 | DK | 87 | LEU |
| 32 | DK | 92 | GLU |
| 32 | DK | 95 | ILE |
| 32 | DK | 104 | THR |
| 32 | DK | 110 | GLU |
| 32 | DK | 114 | LYS |
| 33 | DL | 2 | ARG |
| 33 | DL | 21 | ARG |
| 33 | DL | 25 | SER |
| 33 | DL | 29 | LYS |
| 33 | DL | 48 | ARG |
| 33 | DL | 59 | ARG |
| 33 | DL | 69 | ARG |
| 33 | DL | 78 | ARG |
| 33 | DL | 82 | LEU |
| 33 | DL | 86 | GLU |
| 33 | DL | 94 | THR |
| 33 | DL | 100 | ILE |
| 33 | DL | 104 | GLN |
| 33 | DL | 118 | THR |
| 33 | DL | 126 | ARG |
| 33 | DL | 136 | GLU |
| 34 | DM | 6 | ARG |
| 34 | DM | 14 | LYS |
| 34 | DM | 31 | PHE |
| 34 | DM | 47 | GLU |
| 34 | DM | 54 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DM | 59 | ARG |
| 34 | DM | 60 | GLN |
| 34 | DM | 70 | ASP |
| 34 | DM | 100 | LYS |
| 34 | DM | 108 | VAL |
| 34 | DM | 115 | GLU |
| 34 | DM | 119 | LEU |
| 34 | DM | 124 | LEU |
| 34 | DM | 128 | THR |
| 35 | DN | 1 | MET |
| 35 | DN | 2 | ARG |
| 35 | DN | 8 | ARG |
| 35 | DN | 10 | LEU |
| 35 | DN | 12 | ARG |
| 35 | DN | 14 | SER |
| 35 | DN | 20 | MET |
| 35 | DN | 33 | ILE |
| 35 | DN | 35 | LYS |
| 35 | DN | 51 | LEU |
| 35 | DN | 53 | THR |
| 35 | DN | 59 | SER |
| 35 | DN | 69 | ARG |
| 35 | DN | 70 | THR |
| 35 | DN | 71 | ARG |
| 35 | DN | 82 | GLU |
| 35 | DN | 83 | LEU |
| 35 | DN | 90 | ARG |
| 35 | DN | 95 | THR |
| 35 | DN | 100 | CYS |
| 35 | DN | 114 | GLU |
| 35 | DN | 115 | LEU |
| 35 | DN | 116 | VAL |
| 35 | DN | 118 | ARG |
| 36 | DO | 5 | SER |
| 36 | DO | 9 | ARG |
| 36 | DO | 18 | LEU |
| 36 | DO | 26 | LEU |
| 36 | DO | 31 | THR |
| 36 | DO | 35 | ILE |
| 36 | DO | 36 | TYR |
| 36 | DO | 46 | GLU |
| 36 | DO | 47 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | DO | 48 | LEU |
| 36 | DO | 56 | LYS |
| 36 | DO | 61 | GLN |
| 36 | DO | 78 | VAL |
| 36 | DO | 88 | LYS |
| 36 | DO | 93 | ASP |
| 36 | DO | 103 | VAL |
| 37 | DP | 4 | ILE |
| 37 | DP | 26 | VAL |
| 37 | DP | 34 | GLU |
| 37 | DP | 68 | GLU |
| 37 | DP | 73 | VAL |
| 37 | DP | 93 | ARG |
| 37 | DP | 109 | ARG |
| 37 | DP | 110 | ILE |
| 37 | DP | 112 | GLU |
| 38 | DQ | 6 | ARG |
| 38 | DQ | 9 | ILE |
| 38 | DQ | 11 | ARG |
| 38 | DQ | 25 | TYR |
| 38 | DQ | 41 | LYS |
| 38 | DQ | 51 | ARG |
| 38 | DQ | 52 | GLN |
| 38 | DQ | 60 | LEU |
| 38 | DQ | 97 | ASP |
| 38 | DQ | 104 | VAL |
| 38 | DQ | 117 | LEU |
| 39 | DR | 25 | LEU |
| 39 | DR | 33 | VAL |
| 39 | DR | 41 | ILE |
| 39 | DR | 46 | GLU |
| 39 | DR | 48 | LYS |
| 39 | DR | 58 | VAL |
| 39 | DR | 82 | HIS |
| 39 | DR | 90 | ARG |
| 40 | DS | 1 | MET |
| 40 | DS | 19 | LEU |
| 40 | DS | 20 | VAL |
| 40 | DS | 22 | ASP |
| 40 | DS | 23 | LEU |
| 40 | DS | 47 | VAL |
| 40 | DS | 67 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | DS | 70 | LYS |
| 40 | DS | 72 | THR |
| 40 | DS | 96 | ILE |
| 41 | DT | 3 | ARG |
| 41 | DT | 18 | GLU |
| 41 | DT | 22 | THR |
| 41 | DT | 30 | ILE |
| 41 | DT | 32 | LEU |
| 41 | DT | 44 | LYS |
| 41 | DT | 49 | LYS |
| 41 | DT | 50 | LEU |
| 41 | DT | 68 | LYS |
| 41 | DT | 69 | ARG |
| 41 | DT | 72 | GLN |
| 41 | DT | 74 | ILE |
| 41 | DT | 77 | ARG |
| 41 | DT | 79 | ASP |
| 42 | DU | 11 | VAL |
| 42 | DU | 18 | ASP |
| 42 | DU | 24 | LYS |
| 42 | DU | 34 | VAL |
| 42 | DU | 35 | ILE |
| 42 | DU | 45 | HIS |
| 42 | DU | 46 | GLN |
| 42 | DU | 49 | VAL |
| 42 | DU | 54 | GLN |
| 42 | DU | 67 | VAL |
| 42 | DU | 70 | VAL |
| 42 | DU | 81 | ASP |
| 42 | DU | 85 | PHE |
| 42 | DU | 91 | LYS |
| 42 | DU | 99 | ASN |
| 43 | DV | 2 | PHE |
| 43 | DV | 3 | THR |
| 43 | DV | 26 | PHE |
| 43 | DV | 29 | ILE |
| 43 | DV | 30 | ILE |
| 43 | DV | 42 | LEU |
| 43 | DV | 43 | ASP |
| 43 | DV | 45 | ASP |
| 43 | DV | 50 | MET |
| 43 | DV | 51 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | DV | 53 | LYS |
| 43 | DV | 65 | VAL |
| 43 | DV | 68 | LYS |
| 44 | DW | 20 | ARG |
| 44 | DW | 39 | ARG |
| 44 | DW | 41 | ARG |
| 44 | DW | 50 | ASN |
| 44 | DW | 56 | ASP |
| 44 | DW | 72 | LYS |
| 45 | DX | 4 | VAL |
| 45 | DX | 13 | VAL |
| 45 | DX | 46 | PHE |
| 45 | DX | 47 | VAL |
| 45 | DX | 50 | ARG |
| 45 | DX | 58 | VAL |
| 45 | DX | 64 | ILE |
| 45 | DX | 71 | LEU |
| 45 | DX | 74 | ARG |
| 46 | DY | 11 | VAL |
| 46 | DY | 13 | GLU |
| 46 | DY | 16 | THR |
| 46 | DY | 38 | GLN |
| 46 | DY | 39 | GLN |
| 46 | DY | 41 | HIS |
| 46 | DY | 45 | GLN |
| 46 | DY | 47 | ARG |
| 46 | DY | 49 | ASP |
| 46 | DY | 55 | THR |
| 46 | DY | 57 | LEU |
| 46 | DY | 58 | ASN |
| 47 | DZ | 3 | LYS |
| 47 | DZ | 6 | LYS |
| 47 | DZ | 10 | THR |
| 47 | DZ | 12 | SER |
| 47 | DZ | 17 | LEU |
| 47 | DZ | 25 | LEU |
| 47 | DZ | 31 | ARG |
| 47 | DZ | 36 | VAL |
| 47 | DZ | 52 | SER |
| 47 | DZ | 57 | VAL |
| 48 | D0 | 3 | VAL |
| 48 | D0 | 20 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | D0 | 22 | LEU |
| 48 | D0 | 28 | LEU |
| 49 | D1 | 5 | ILE |
| 49 | D1 | 12 | VAL |
| 49 | D1 | 26 | ASN |
| 49 | D1 | 42 | VAL |
| 49 | D1 | 46 | HIS |
| 49 | D1 | 47 | VAL |
| 50 | D2 | 4 | THR |
| 50 | D2 | 10 | LEU |
| 50 | D2 | 24 | THR |
| 50 | D2 | 41 | ARG |
| 50 | D2 | 42 | LEU |
| 50 | D2 | 43 | THR |
| 50 | D2 | 44 | VAL |
| 51 | D3 | 6 | THR |
| 51 | D3 | 30 | ARG |
| 51 | D3 | 31 | HIS |
| 51 | D3 | 47 | LYS |
| 51 | D3 | 49 | MET |
| 52 | D4 | 2 | LYS |
| 52 | D4 | 3 | VAL |
| 52 | D4 | 12 | ARG |
| 52 | D4 | 13 | ASN |
| 52 | D4 | 20 | ASP |
| 52 | D4 | 26 | ILE |
| 52 | D4 | 32 | LYS |
| 52 | D4 | 37 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 82 | GLN |
| 8 | AH | 18 | GLN |
| 9 | AI | 126 | GLN |
| 11 | AK | 22 | HIS |
| 11 | AK | 40 | ASN |
| 11 | AK | 109 | ASN |
| 15 | AO | 40 | GLN |
| 15 | AO | 50 | HIS |
| 17 | AQ | 45 | HIS |
| 19 | AS | 14 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AS | 52 | HIS |
| 24 | BC | 239 | ASN |
| 29 | BH | 119 | ASN |
| 29 | BH | 135 | HIS |
| 31 | BJ | 47 | HIS |
| 31 | BJ | 77 | HIS |
| 43 | BV | 87 | GLN |
| 44 | BW | 46 | HIS |
| 53 | B5 | 45 | HIS |
| 53 | B5 | 67 | HIS |
| 3 | CC | 176 | HIS |
| 5 | CE | 122 | ASN |
| 7 | CG | 97 | ASN |
| 9 | CI | 25 | ASN |
| 15 | CO | 42 | HIS |
| 15 | CO | 46 | HIS |
| 17 | CQ | 31 | HIS |
| 20 | CT | 61 | GLN |
| 24 | DC | 251 | GLN |
| 25 | DD | 140 | HIS |
| 28 | DG | 115 | HIS |
| 29 | DH | 28 | ASN |
| 29 | DH | 128 | HIS |
| 38 | DQ | 37 | GLN |
| 39 | DR | 66 | HIS |
| 39 | DR | 89 | HIS |
| 41 | DT | 15 | HIS |
| 42 | DU | 74 | ASN |
| 44 | DW | 46 | HIS |
| 45 | DX | 34 | HIS |
| 46 | DY | 41 | HIS |
| 46 | DY | 45 | GLN |
| 48 | D0 | 19 | HIS |
| 49 | D1 | 19 | HIS |
| 49 | D1 | 26 | ASN |
| 51 | D3 | 26 | HIS |
| 51 | D3 | 31 | HIS |
| 52 | D4 | 37 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1537/1539 (99%) | 324 (21%) | 11 (0%) |
| 1 | CA | 1538/1539 (99%) | 342 (22%) | 10 (0%) |
| 22 | BA | 2895/2903 (99%) | 579 (20%) | 24 (0%) |
| 22 | DA | 2895/2903 (99%) | 704 (24%) | 32 (1%) |
| 23 | BB | 118/119 (99%) | 16 (13%) | 0 |
| 23 | DB | 117/119 (98%) | 20 (17%) | 0 |
| All | All | 9100/9122 (99%) | 1985 (21%) | 77 (0%) |

All (1985) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 3 | A |
| 1 | AA | 4 | U |
| 1 | AA | 5 | U |
| 1 | AA | 6 | G |
| 1 | AA | 9 | G |
| 1 | AA | 13 | U |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 50 | A |
| 1 | AA | 51 | A |
| 1 | AA | 70 | U |
| 1 | AA | 71 | A |
| 1 | AA | 72 | A |
| 1 | AA | 73 | C |
| 1 | AA | 74 | A |
| 1 | AA | 75 | G |
| 1 | AA | 76 | G |
| 1 | AA | 80 | A |
| 1 | AA | 81 | A |
| 1 | AA | 82 | G |
| 1 | AA | 83 | C |
| 1 | AA | 85 | U |
| 1 | AA | 86 | G |
| 1 | AA | 89 | U |
| 1 | AA | 90 | C |
| 1 | AA | 91 | U |
| 1 | AA | 95 | C |
| 1 | AA | 97 | G |
| 1 | AA | 108 | G |
| 1 | AA | 111 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 116 | A |
| 1 | AA | 120 | A |
| 1 | AA | 121 | U |
| 1 | AA | 122 | G |
| 1 | AA | 127 | G |
| 1 | AA | 130 | A |
| 1 | AA | 131 | A |
| 1 | AA | 136 | C |
| 1 | AA | 137 | U |
| 1 | AA | 138 | G |
| 1 | AA | 140 | U |
| 1 | AA | 143 | A |
| 1 | AA | 144 | G |
| 1 | AA | 163 | C |
| 1 | AA | 168 | G |
| 1 | AA | 174 | A |
| 1 | AA | 177 | G |
| 1 | AA | 180 | U |
| 1 | AA | 181 | A |
| 1 | AA | 182 | A |
| 1 | AA | 183 | C |
| 1 | AA | 188 | C |
| 1 | AA | 195 | A |
| 1 | AA | 197 | A |
| 1 | AA | 205 | A |
| 1 | AA | 206 | C |
| 1 | AA | 210 | C |
| 1 | AA | 211 | G |
| 1 | AA | 217 | C |
| 1 | AA | 226 | G |
| 1 | AA | 240 | G |
| 1 | AA | 245 | U |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 262 | A |
| 1 | AA | 263 | A |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 281 | G |
| 1 | AA | 285 | C |
| 1 | AA | 289 | G |
| 1 | AA | 320 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 321 | A |
| 1 | AA | 327 | A |
| 1 | AA | 328 | C |
| 1 | AA | 329 | A |
| 1 | AA | 330 | C |
| 1 | AA | 331 | G |
| 1 | AA | 332 | G |
| 1 | AA | 346 | G |
| 1 | AA | 347 | G |
| 1 | AA | 352 | C |
| 1 | AA | 354 | G |
| 1 | AA | 367 | U |
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 376 | G |
| 1 | AA | 384 | G |
| 1 | AA | 392 | C |
| 1 | AA | 406 | G |
| 1 | AA | 411 | A |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 414 | A |
| 1 | AA | 421 | U |
| 1 | AA | 422 | C |
| 1 | AA | 429 | U |
| 1 | AA | 430 | A |
| 1 | AA | 435 | A |
| 1 | AA | 436 | C |
| 1 | AA | 445 | G |
| 1 | AA | 454 | G |
| 1 | AA | 457 | G |
| 1 | AA | 458 | U |
| 1 | AA | 462 | G |
| 1 | AA | 466 | A |
| 1 | AA | 467 | U |
| 1 | AA | 468 | A |
| 1 | AA | 476 | U |
| 1 | AA | 479 | U |
| 1 | AA | 481 | G |
| 1 | AA | 482 | A |
| 1 | AA | 484 | G |
| 1 | AA | 485 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 486 | U |
| 1 | AA | 495 | A |
| 1 | AA | 498 | A |
| 1 | AA | 501 | C |
| 1 | AA | 505 | G |
| 1 | AA | 511 | C |
| 1 | AA | 518 | C |
| 1 | AA | 521 | G |
| 1 | AA | 524 | G |
| 1 | AA | 527 | G |
| 1 | AA | 530 | G |
| 1 | AA | 532 | A |
| 1 | AA | 533 | A |
| 1 | AA | 541 | G |
| 1 | AA | 547 | A |
| 1 | AA | 559 | A |
| 1 | AA | 562 | U |
| 1 | AA | 564 | C |
| 1 | AA | 565 | U |
| 1 | AA | 566 | G |
| 1 | AA | 570 | G |
| 1 | AA | 573 | A |
| 1 | AA | 576 | C |
| 1 | AA | 588 | G |
| 1 | AA | 591 | U |
| 1 | AA | 615 | G |
| 1 | AA | 631 | C |
| 1 | AA | 632 | U |
| 1 | AA | 651 | C |
| 1 | AA | 652 | U |
| 1 | AA | 653 | U |
| 1 | AA | 661 | G |
| 1 | AA | 665 | A |
| 1 | AA | 671 | G |
| 1 | AA | 702 | A |
| 1 | AA | 703 | G |
| 1 | AA | 721 | G |
| 1 | AA | 723 | U |
| 1 | AA | 724 | G |
| 1 | AA | 731 | G |
| 1 | AA | 734 | G |
| 1 | AA | 748 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 750 | C |
| 1 | AA | 753 | A |
| 1 | AA | 755 | G |
| 1 | AA | 773 | G |
| 1 | AA | 777 | A |
| 1 | AA | 792 | A |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 814 | A |
| 1 | AA | 815 | A |
| 1 | AA | 817 | C |
| 1 | AA | 828 | U |
| 1 | AA | 832 | G |
| 1 | AA | 836 | G |
| 1 | AA | 841 | C |
| 1 | AA | 842 | U |
| 1 | AA | 843 | U |
| 1 | AA | 845 | A |
| 1 | AA | 846 | G |
| 1 | AA | 849 | G |
| 1 | AA | 851 | G |
| 1 | AA | 854 | U |
| 1 | AA | 859 | G |
| 1 | AA | 888 | G |
| 1 | AA | 892 | A |
| 1 | AA | 902 | G |
| 1 | AA | 910 | C |
| 1 | AA | 914 | A |
| 1 | AA | 921 | U |
| 1 | AA | 926 | G |
| 1 | AA | 927 | G |
| 1 | AA | 934 | C |
| 1 | AA | 935 | A |
| 1 | AA | 958 | A |
| 1 | AA | 960 | U |
| 1 | AA | 966 | G |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 973 | G |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 986 | U |
| 1 | AA | 987 | G |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1009 | U |
| 1 | AA | 1019 | A |
| 1 | AA | 1021 | A |
| 1 | AA | 1025 | U |
| 1 | AA | 1026 | G |
| 1 | AA | 1028 | C |
| 1 | AA | 1029 | U |
| 1 | AA | 1030 | U |
| 1 | AA | 1031 | C |
| 1 | AA | 1032 | G |
| 1 | AA | 1033 | G |
| 1 | AA | 1034 | G |
| 1 | AA | 1036 | A |
| 1 | AA | 1037 | C |
| 1 | AA | 1043 | G |
| 1 | AA | 1044 | A |
| 1 | AA | 1046 | A |
| 1 | AA | 1050 | G |
| 1 | AA | 1065 | U |
| 1 | AA | 1066 | C |
| 1 | AA | 1070 | U |
| 1 | AA | 1084 | G |
| 1 | AA | 1086 | U |
| 1 | AA | 1090 | U |
| 1 | AA | 1091 | U |
| 1 | AA | 1092 | A |
| 1 | AA | 1093 | A |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1098 | C |
| 1 | AA | 1101 | A |
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1133 | G |
| 1 | AA | 1135 | U |
| 1 | AA | 1136 | C |
| 1 | AA | 1137 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1140 | C |
| 1 | AA | 1141 | C |
| 1 | AA | 1142 | G |
| 1 | AA | 1143 | G |
| 1 | AA | 1145 | A |
| 1 | AA | 1146 | A |
| 1 | AA | 1152 | A |
| 1 | AA | 1154 | G |
| 1 | AA | 1159 | U |
| 1 | AA | 1160 | G |
| 1 | AA | 1161 | C |
| 1 | AA | 1167 | A |
| 1 | AA | 1168 | U |
| 1 | AA | 1171 | A |
| 1 | AA | 1181 | G |
| 1 | AA | 1183 | U |
| 1 | AA | 1184 | G |
| 1 | AA | 1196 | A |
| 1 | AA | 1197 | A |
| 1 | AA | 1202 | U |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1227 | A |
| 1 | AA | 1228 | C |
| 1 | AA | 1233 | G |
| 1 | AA | 1238 | A |
| 1 | AA | 1239 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1250 | A |
| 1 | AA | 1256 | A |
| 1 | AA | 1258 | G |
| 1 | AA | 1280 | A |
| 1 | AA | 1286 | U |
| 1 | AA | 1287 | A |
| 1 | AA | 1293 | C |
| 1 | AA | 1299 | A |
| 1 | AA | 1300 | G |
| 1 | AA | 1302 | C |
| 1 | AA | 1304 | G |
| 1 | AA | 1305 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1312 | G |
| 1 | AA | 1317 | C |
| 1 | AA | 1320 | C |
| 1 | AA | 1321 | U |
| 1 | AA | 1323 | G |
| 1 | AA | 1325 | C |
| 1 | AA | 1328 | C |
| 1 | AA | 1329 | A |
| 1 | AA | 1335 | U |
| 1 | AA | 1336 | C |
| 1 | AA | 1337 | G |
| 1 | AA | 1338 | G |
| 1 | AA | 1353 | G |
| 1 | AA | 1363 | A |
| 1 | AA | 1364 | U |
| 1 | AA | 1378 | C |
| 1 | AA | 1379 | G |
| 1 | AA | 1396 | A |
| 1 | AA | 1398 | A |
| 1 | AA | 1400 | C |
| 1 | AA | 1419 | G |
| 1 | AA | 1429 | A |
| 1 | AA | 1441 | A |
| 1 | AA | 1442 | G |
| 1 | AA | 1443 | C |
| 1 | AA | 1446 | A |
| 1 | AA | 1452 | C |
| 1 | AA | 1453 | G |
| 1 | AA | 1455 | G |
| 1 | AA | 1486 | G |
| 1 | AA | 1493 | A |
| 1 | AA | 1497 | G |
| 1 | AA | 1503 | A |
| 1 | AA | 1505 | G |
| 1 | AA | 1506 | U |
| 1 | AA | 1517 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 1 | AA | 1535 | C |
| 1 | AA | 1538 | C |
| 22 | BA | 10 | A |
| 22 | BA | 13 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 15 | G |
| 22 | BA | 27 | G |
| 22 | BA | 34 | U |
| 22 | BA | 35 | G |
| 22 | BA | 46 | G |
| 22 | BA | 61 | C |
| 22 | BA | 63 | A |
| 22 | BA | 71 | A |
| 22 | BA | 74 | A |
| 22 | BA | 75 | G |
| 22 | BA | 80 | G |
| 22 | BA | 103 | A |
| 22 | BA | 106 | C |
| 22 | BA | 118 | A |
| 22 | BA | 119 | A |
| 22 | BA | 120 | U |
| 22 | BA | 131 | A |
| 22 | BA | 138 | U |
| 22 | BA | 139 | U |
| 22 | BA | 140 | C |
| 22 | BA | 141 | G |
| 22 | BA | 142 | A |
| 22 | BA | 143 | C |
| 22 | BA | 180 | G |
| 22 | BA | 181 | A |
| 22 | BA | 196 | A |
| 22 | BA | 215 | G |
| 22 | BA | 216 | A |
| 22 | BA | 221 | A |
| 22 | BA | 222 | A |
| 22 | BA | 248 | G |
| 22 | BA | 255 | A |
| 22 | BA | 257 | C |
| 22 | BA | 265 | A |
| 22 | BA | 266 | G |
| 22 | BA | 271 | G |
| 22 | BA | 272 | A |
| 22 | BA | 276 | U |
| 22 | BA | 277 | G |
| 22 | BA | 279 | A |
| 22 | BA | 299 | A |
| 22 | BA | 302 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 311 | A |
| 22 | BA | 325 | G |
| 22 | BA | 329 | G |
| 22 | BA | 330 | A |
| 22 | BA | 340 | A |
| 22 | BA | 343 | C |
| 22 | BA | 353 | C |
| 22 | BA | 361 | G |
| 22 | BA | 362 | A |
| 22 | BA | 371 | A |
| 22 | BA | 372 | G |
| 22 | BA | 386 | G |
| 22 | BA | 389 | G |
| 22 | BA | 396 | G |
| 22 | BA | 404 | A |
| 22 | BA | 405 | U |
| 22 | BA | 411 | G |
| 22 | BA | 420 | C |
| 22 | BA | 424 | G |
| 22 | BA | 441 | U |
| 22 | BA | 450 | G |
| 22 | BA | 451 | U |
| 22 | BA | 456 | C |
| 22 | BA | 457 | A |
| 22 | BA | 468 | G |
| 22 | BA | 481 | G |
| 22 | BA | 482 | A |
| 22 | BA | 483 | A |
| 22 | BA | 491 | G |
| 22 | BA | 501 | A |
| 22 | BA | 504 | A |
| 22 | BA | 505 | A |
| 22 | BA | 508 | A |
| 22 | BA | 528 | A |
| 22 | BA | 531 | C |
| 22 | BA | 532 | A |
| 22 | BA | 544 | C |
| 22 | BA | 546 | U |
| 22 | BA | 547 | A |
| 22 | BA | 548 | G |
| 22 | BA | 549 | G |
| 22 | BA | 550 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 563 | A |
| 22 | BA | 573 | U |
| 22 | BA | 575 | A |
| 22 | BA | 585 | G |
| 22 | BA | 586 | A |
| 22 | BA | 603 | A |
| 22 | BA | 613 | A |
| 22 | BA | 615 | U |
| 22 | BA | 622 | G |
| 22 | BA | 627 | A |
| 22 | BA | 631 | A |
| 22 | BA | 637 | A |
| 22 | BA | 644 | A |
| 22 | BA | 645 | C |
| 22 | BA | 646 | U |
| 22 | BA | 647 | G |
| 22 | BA | 653 | U |
| 22 | BA | 654 | A |
| 22 | BA | 655 | A |
| 22 | BA | 664 | G |
| 22 | BA | 669 | G |
| 22 | BA | 670 | A |
| 22 | BA | 686 | U |
| 22 | BA | 702 | U |
| 22 | BA | 729 | G |
| 22 | BA | 730 | A |
| 22 | BA | 738 | G |
| 22 | BA | 740 | C |
| 22 | BA | 747 | U |
| 22 | BA | 759 | G |
| 22 | BA | 764 | A |
| 22 | BA | 765 | C |
| 22 | BA | 775 | G |
| 22 | BA | 776 | G |
| 22 | BA | 782 | A |
| 22 | BA | 783 | A |
| 22 | BA | 784 | G |
| 22 | BA | 785 | G |
| 22 | BA | 790 | U |
| 22 | BA | 791 | C |
| 22 | BA | 792 | A |
| 22 | BA | 801 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 805 | G |
| 22 | BA | 812 | C |
| 22 | BA | 814 | C |
| 22 | BA | 816 | C |
| 22 | BA | 819 | A |
| 22 | BA | 827 | U |
| 22 | BA | 828 | U |
| 22 | BA | 845 | A |
| 22 | BA | 846 | U |
| 22 | BA | 847 | U |
| 22 | BA | 858 | G |
| 22 | BA | 859 | G |
| 22 | BA | 866 | A |
| 22 | BA | 878 | A |
| 22 | BA | 879 | G |
| 22 | BA | 882 | G |
| 22 | BA | 885 | C |
| 22 | BA | 893 | C |
| 22 | BA | 896 | A |
| 22 | BA | 897 | C |
| 22 | BA | 910 | A |
| 22 | BA | 914 | G |
| 22 | BA | 915 | C |
| 22 | BA | 931 | U |
| 22 | BA | 932 | U |
| 22 | BA | 934 | U |
| 22 | BA | 941 | A |
| 22 | BA | 942 | G |
| 22 | BA | 946 | C |
| 22 | BA | 961 | C |
| 22 | BA | 974 | G |
| 22 | BA | 978 | G |
| 22 | BA | 982 | C |
| 22 | BA | 983 | A |
| 22 | BA | 984 | A |
| 22 | BA | 985 | C |
| 22 | BA | 990 | A |
| 22 | BA | 991 | C |
| 22 | BA | 995 | C |
| 22 | BA | 996 | A |
| 22 | BA | 999 | U |
| 22 | BA | 1005 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1012 | U |
| 22 | BA | 1013 | C |
| 22 | BA | 1022 | G |
| 22 | BA | 1026 | G |
| 22 | BA | 1033 | U |
| 22 | BA | 1040 | A |
| 22 | BA | 1046 | A |
| 22 | BA | 1047 | G |
| 22 | BA | 1058 | U |
| 22 | BA | 1061 | U |
| 22 | BA | 1062 | G |
| 22 | BA | 1063 | G |
| 22 | BA | 1065 | U |
| 22 | BA | 1066 | U |
| 22 | BA | 1067 | A |
| 22 | BA | 1068 | G |
| 22 | BA | 1069 | A |
| 22 | BA | 1070 | A |
| 22 | BA | 1071 | G |
| 22 | BA | 1072 | C |
| 22 | BA | 1073 | A |
| 22 | BA | 1074 | G |
| 22 | BA | 1075 | C |
| 22 | BA | 1077 | A |
| 22 | BA | 1079 | C |
| 22 | BA | 1080 | A |
| 22 | BA | 1081 | U |
| 22 | BA | 1082 | U |
| 22 | BA | 1087 | G |
| 22 | BA | 1088 | A |
| 22 | BA | 1089 | A |
| 22 | BA | 1092 | C |
| 22 | BA | 1093 | G |
| 22 | BA | 1095 | A |
| 22 | BA | 1097 | U |
| 22 | BA | 1098 | A |
| 22 | BA | 1099 | G |
| 22 | BA | 1100 | C |
| 22 | BA | 1101 | U |
| 22 | BA | 1103 | A |
| 22 | BA | 1104 | C |
| 22 | BA | 1112 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1132 | U |
| 22 | BA | 1133 | A |
| 22 | BA | 1135 | C |
| 22 | BA | 1136 | G |
| 22 | BA | 1138 | G |
| 22 | BA | 1139 | G |
| 22 | BA | 1142 | A |
| 22 | BA | 1144 | A |
| 22 | BA | 1168 | G |
| 22 | BA | 1170 | C |
| 22 | BA | 1171 | G |
| 22 | BA | 1172 | C |
| 22 | BA | 1174 | U |
| 22 | BA | 1175 | A |
| 22 | BA | 1176 | U |
| 22 | BA | 1178 | C |
| 22 | BA | 1179 | G |
| 22 | BA | 1180 | U |
| 22 | BA | 1186 | G |
| 22 | BA | 1189 | A |
| 22 | BA | 1218 | G |
| 22 | BA | 1230 | A |
| 22 | BA | 1238 | G |
| 22 | BA | 1252 | G |
| 22 | BA | 1253 | A |
| 22 | BA | 1256 | G |
| 22 | BA | 1266 | G |
| 22 | BA | 1271 | G |
| 22 | BA | 1272 | A |
| 22 | BA | 1275 | A |
| 22 | BA | 1294 | U |
| 22 | BA | 1300 | G |
| 22 | BA | 1301 | A |
| 22 | BA | 1303 | G |
| 22 | BA | 1305 | C |
| 22 | BA | 1320 | C |
| 22 | BA | 1325 | U |
| 22 | BA | 1332 | G |
| 22 | BA | 1345 | C |
| 22 | BA | 1348 | C |
| 22 | BA | 1352 | U |
| 22 | BA | 1355 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1357 | C |
| 22 | BA | 1359 | A |
| 22 | BA | 1365 | A |
| 22 | BA | 1374 | G |
| 22 | BA | 1377 | G |
| 22 | BA | 1378 | A |
| 22 | BA | 1379 | U |
| 22 | BA | 1383 | A |
| 22 | BA | 1384 | A |
| 22 | BA | 1386 | C |
| 22 | BA | 1406 | U |
| 22 | BA | 1407 | G |
| 22 | BA | 1411 | U |
| 22 | BA | 1416 | G |
| 22 | BA | 1419 | A |
| 22 | BA | 1420 | A |
| 22 | BA | 1428 | C |
| 22 | BA | 1435 | G |
| 22 | BA | 1437 | C |
| 22 | BA | 1452 | G |
| 22 | BA | 1453 | A |
| 22 | BA | 1458 | U |
| 22 | BA | 1461 | C |
| 22 | BA | 1467 | U |
| 22 | BA | 1482 | G |
| 22 | BA | 1483 | G |
| 22 | BA | 1493 | C |
| 22 | BA | 1494 | A |
| 22 | BA | 1495 | A |
| 22 | BA | 1504 | A |
| 22 | BA | 1508 | A |
| 22 | BA | 1510 | G |
| 22 | BA | 1515 | A |
| 22 | BA | 1530 | G |
| 22 | BA | 1532 | A |
| 22 | BA | 1533 | C |
| 22 | BA | 1534 | U |
| 22 | BA | 1535 | A |
| 22 | BA | 1536 | C |
| 22 | BA | 1547 | C |
| 22 | BA | 1548 | A |
| 22 | BA | 1554 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1555 | G |
| 22 | BA | 1560 | G |
| 22 | BA | 1569 | A |
| 22 | BA | 1578 | U |
| 22 | BA | 1579 | A |
| 22 | BA | 1583 | A |
| 22 | BA | 1584 | U |
| 22 | BA | 1585 | C |
| 22 | BA | 1593 | A |
| 22 | BA | 1597 | A |
| 22 | BA | 1606 | C |
| 22 | BA | 1607 | C |
| 22 | BA | 1608 | A |
| 22 | BA | 1632 | A |
| 22 | BA | 1647 | U |
| 22 | BA | 1648 | U |
| 22 | BA | 1649 | G |
| 22 | BA | 1653 | G |
| 22 | BA | 1674 | G |
| 22 | BA | 1685 | C |
| 22 | BA | 1688 | U |
| 22 | BA | 1689 | A |
| 22 | BA | 1714 | U |
| 22 | BA | 1715 | G |
| 22 | BA | 1718 | G |
| 22 | BA | 1729 | U |
| 22 | BA | 1730 | C |
| 22 | BA | 1736 | U |
| 22 | BA | 1738 | G |
| 22 | BA | 1744 | A |
| 22 | BA | 1758 | U |
| 22 | BA | 1764 | C |
| 22 | BA | 1773 | A |
| 22 | BA | 1776 | G |
| 22 | BA | 1782 | U |
| 22 | BA | 1786 | A |
| 22 | BA | 1795 | C |
| 22 | BA | 1800 | C |
| 22 | BA | 1801 | A |
| 22 | BA | 1808 | A |
| 22 | BA | 1813 | G |
| 22 | BA | 1816 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1828 | G |
| 22 | BA | 1829 | A |
| 22 | BA | 1835 | G |
| 22 | BA | 1840 | G |
| 22 | BA | 1841 | U |
| 22 | BA | 1842 | G |
| 22 | BA | 1847 | A |
| 22 | BA | 1849 | G |
| 22 | BA | 1853 | A |
| 22 | BA | 1870 | C |
| 22 | BA | 1871 | A |
| 22 | BA | 1872 | A |
| 22 | BA | 1873 | G |
| 22 | BA | 1876 | A |
| 22 | BA | 1880 | U |
| 22 | BA | 1885 | A |
| 22 | BA | 1888 | G |
| 22 | BA | 1890 | A |
| 22 | BA | 1900 | A |
| 22 | BA | 1906 | G |
| 22 | BA | 1909 | C |
| 22 | BA | 1912 | A |
| 22 | BA | 1913 | A |
| 22 | BA | 1914 | C |
| 22 | BA | 1915 | U |
| 22 | BA | 1916 | A |
| 22 | BA | 1917 | U |
| 22 | BA | 1919 | A |
| 22 | BA | 1920 | C |
| 22 | BA | 1923 | U |
| 22 | BA | 1924 | C |
| 22 | BA | 1925 | C |
| 22 | BA | 1926 | U |
| 22 | BA | 1929 | G |
| 22 | BA | 1930 | G |
| 22 | BA | 1931 | U |
| 22 | BA | 1932 | A |
| 22 | BA | 1938 | A |
| 22 | BA | 1955 | U |
| 22 | BA | 1959 | G |
| 22 | BA | 1964 | G |
| 22 | BA | 1965 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1967 | C |
| 22 | BA | 1970 | A |
| 22 | BA | 1972 | G |
| 22 | BA | 1975 | G |
| 22 | BA | 1986 | C |
| 22 | BA | 1991 | U |
| 22 | BA | 1992 | G |
| 22 | BA | 1993 | U |
| 22 | BA | 1995 | U |
| 22 | BA | 1997 | C |
| 22 | BA | 2009 | A |
| 22 | BA | 2022 | U |
| 22 | BA | 2023 | C |
| 22 | BA | 2031 | A |
| 22 | BA | 2033 | A |
| 22 | BA | 2043 | C |
| 22 | BA | 2055 | C |
| 22 | BA | 2056 | G |
| 22 | BA | 2060 | A |
| 22 | BA | 2061 | G |
| 22 | BA | 2062 | A |
| 22 | BA | 2064 | C |
| 22 | BA | 2069 | G |
| 22 | BA | 2072 | C |
| 22 | BA | 2092 | U |
| 22 | BA | 2093 | G |
| 22 | BA | 2097 | A |
| 22 | BA | 2098 | U |
| 22 | BA | 2099 | U |
| 22 | BA | 2100 | G |
| 22 | BA | 2102 | G |
| 22 | BA | 2103 | C |
| 22 | BA | 2106 | U |
| 22 | BA | 2110 | G |
| 22 | BA | 2111 | U |
| 22 | BA | 2112 | G |
| 22 | BA | 2113 | U |
| 22 | BA | 2115 | G |
| 22 | BA | 2116 | G |
| 22 | BA | 2117 | A |
| 22 | BA | 2118 | U |
| 22 | BA | 2119 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2122 | U |
| 22 | BA | 2126 | A |
| 22 | BA | 2127 | G |
| 22 | BA | 2128 | G |
| 22 | BA | 2129 | C |
| 22 | BA | 2132 | U |
| 22 | BA | 2133 | G |
| 22 | BA | 2134 | A |
| 22 | BA | 2136 | G |
| 22 | BA | 2138 | G |
| 22 | BA | 2139 | U |
| 22 | BA | 2145 | C |
| 22 | BA | 2147 | A |
| 22 | BA | 2148 | G |
| 22 | BA | 2162 | G |
| 22 | BA | 2163 | A |
| 22 | BA | 2164 | C |
| 22 | BA | 2165 | C |
| 22 | BA | 2166 | U |
| 22 | BA | 2167 | U |
| 22 | BA | 2169 | A |
| 22 | BA | 2170 | A |
| 22 | BA | 2171 | A |
| 22 | BA | 2172 | U |
| 22 | BA | 2173 | A |
| 22 | BA | 2174 | C |
| 22 | BA | 2178 | C |
| 22 | BA | 2179 | C |
| 22 | BA | 2181 | U |
| 22 | BA | 2182 | U |
| 22 | BA | 2187 | U |
| 22 | BA | 2190 | G |
| 22 | BA | 2197 | U |
| 22 | BA | 2198 | A |
| 22 | BA | 2203 | U |
| 22 | BA | 2204 | G |
| 22 | BA | 2210 | U |
| 22 | BA | 2211 | A |
| 22 | BA | 2212 | A |
| 22 | BA | 2214 | C |
| 22 | BA | 2220 | U |
| 22 | BA | 2225 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2238 | G |
| 22 | BA | 2239 | G |
| 22 | BA | 2248 | C |
| 22 | BA | 2250 | G |
| 22 | BA | 2268 | A |
| 22 | BA | 2272 | U |
| 22 | BA | 2278 | A |
| 22 | BA | 2283 | C |
| 22 | BA | 2286 | G |
| 22 | BA | 2287 | A |
| 22 | BA | 2296 | U |
| 22 | BA | 2297 | A |
| 22 | BA | 2305 | U |
| 22 | BA | 2308 | G |
| 22 | BA | 2309 | A |
| 22 | BA | 2311 | A |
| 22 | BA | 2322 | A |
| 22 | BA | 2325 | G |
| 22 | BA | 2327 | A |
| 22 | BA | 2331 | G |
| 22 | BA | 2335 | A |
| 22 | BA | 2345 | G |
| 22 | BA | 2346 | A |
| 22 | BA | 2347 | C |
| 22 | BA | 2361 | G |
| 22 | BA | 2383 | G |
| 22 | BA | 2385 | C |
| 22 | BA | 2389 | G |
| 22 | BA | 2394 | C |
| 22 | BA | 2402 | U |
| 22 | BA | 2403 | C |
| 22 | BA | 2406 | A |
| 22 | BA | 2412 | A |
| 22 | BA | 2420 | C |
| 22 | BA | 2422 | C |
| 22 | BA | 2424 | C |
| 22 | BA | 2425 | A |
| 22 | BA | 2428 | G |
| 22 | BA | 2429 | G |
| 22 | BA | 2430 | A |
| 22 | BA | 2431 | U |
| 22 | BA | 2435 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2441 | U |
| 22 | BA | 2448 | A |
| 22 | BA | 2465 | C |
| 22 | BA | 2474 | U |
| 22 | BA | 2476 | A |
| 22 | BA | 2478 | A |
| 22 | BA | 2484 | G |
| 22 | BA | 2487 | G |
| 22 | BA | 2490 | G |
| 22 | BA | 2491 | U |
| 22 | BA | 2497 | A |
| 22 | BA | 2502 | G |
| 22 | BA | 2503 | A |
| 22 | BA | 2504 | U |
| 22 | BA | 2505 | G |
| 22 | BA | 2506 | U |
| 22 | BA | 2508 | G |
| 22 | BA | 2515 | C |
| 22 | BA | 2518 | A |
| 22 | BA | 2529 | G |
| 22 | BA | 2535 | G |
| 22 | BA | 2554 | U |
| 22 | BA | 2555 | U |
| 22 | BA | 2566 | A |
| 22 | BA | 2567 | G |
| 22 | BA | 2573 | C |
| 22 | BA | 2576 | G |
| 22 | BA | 2578 | G |
| 22 | BA | 2594 | C |
| 22 | BA | 2602 | A |
| 22 | BA | 2603 | G |
| 22 | BA | 2609 | U |
| 22 | BA | 2613 | U |
| 22 | BA | 2615 | U |
| 22 | BA | 2629 | U |
| 22 | BA | 2652 | C |
| 22 | BA | 2662 | A |
| 22 | BA | 2688 | G |
| 22 | BA | 2689 | U |
| 22 | BA | 2690 | U |
| 22 | BA | 2714 | G |
| 22 | BA | 2726 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2729 | G |
| 22 | BA | 2732 | G |
| 22 | BA | 2733 | A |
| 22 | BA | 2744 | G |
| 22 | BA | 2748 | A |
| 22 | BA | 2757 | A |
| 22 | BA | 2765 | A |
| 22 | BA | 2778 | A |
| 22 | BA | 2791 | G |
| 22 | BA | 2792 | A |
| 22 | BA | 2798 | U |
| 22 | BA | 2799 | A |
| 22 | BA | 2800 | A |
| 22 | BA | 2803 | G |
| 22 | BA | 2811 | G |
| 22 | BA | 2820 | A |
| 22 | BA | 2821 | A |
| 22 | BA | 2825 | G |
| 22 | BA | 2827 | C |
| 22 | BA | 2835 | A |
| 22 | BA | 2862 | G |
| 22 | BA | 2867 | G |
| 22 | BA | 2873 | A |
| 22 | BA | 2874 | C |
| 22 | BA | 2879 | A |
| 22 | BA | 2880 | C |
| 22 | BA | 2883 | A |
| 22 | BA | 2884 | U |
| 22 | BA | 2885 | G |
| 22 | BA | 2887 | A |
| 22 | BA | 2903 | U |
| 23 | BB | 2 | G |
| 23 | BB | 9 | G |
| 23 | BB | 15 | A |
| 23 | BB | 16 | G |
| 23 | BB | 25 | U |
| 23 | BB | 35 | C |
| 23 | BB | 42 | C |
| 23 | BB | 44 | G |
| 23 | BB | 45 | A |
| 23 | BB | 56 | G |
| 23 | BB | 66 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | BB | 89 | U |
| 23 | BB | 90 | C |
| 23 | BB | 91 | C |
| 23 | BB | 109 | A |
| 23 | BB | 119 | A |
| 1 | CA | 3 | A |
| 1 | CA | 5 | U |
| 1 | CA | 6 | G |
| 1 | CA | 9 | G |
| 1 | CA | 21 | G |
| 1 | CA | 32 | A |
| 1 | CA | 39 | G |
| 1 | CA | 47 | C |
| 1 | CA | 48 | C |
| 1 | CA | 51 | A |
| 1 | CA | 52 | C |
| 1 | CA | 55 | A |
| 1 | CA | 65 | A |
| 1 | CA | 67 | C |
| 1 | CA | 68 | G |
| 1 | CA | 70 | U |
| 1 | CA | 71 | A |
| 1 | CA | 73 | C |
| 1 | CA | 74 | A |
| 1 | CA | 75 | G |
| 1 | CA | 79 | G |
| 1 | CA | 80 | A |
| 1 | CA | 84 | U |
| 1 | CA | 85 | U |
| 1 | CA | 86 | G |
| 1 | CA | 87 | C |
| 1 | CA | 88 | U |
| 1 | CA | 91 | U |
| 1 | CA | 93 | U |
| 1 | CA | 94 | G |
| 1 | CA | 116 | A |
| 1 | CA | 117 | G |
| 1 | CA | 120 | A |
| 1 | CA | 121 | U |
| 1 | CA | 122 | G |
| 1 | CA | 129 | A |
| 1 | CA | 130 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 131 | A |
| 1 | CA | 135 | C |
| 1 | CA | 137 | U |
| 1 | CA | 142 | G |
| 1 | CA | 143 | A |
| 1 | CA | 144 | G |
| 1 | CA | 154 | U |
| 1 | CA | 155 | A |
| 1 | CA | 156 | C |
| 1 | CA | 159 | G |
| 1 | CA | 173 | U |
| 1 | CA | 174 | A |
| 1 | CA | 176 | C |
| 1 | CA | 181 | A |
| 1 | CA | 182 | A |
| 1 | CA | 183 | C |
| 1 | CA | 184 | G |
| 1 | CA | 185 | U |
| 1 | CA | 186 | C |
| 1 | CA | 191 | G |
| 1 | CA | 197 | A |
| 1 | CA | 200 | G |
| 1 | CA | 201 | G |
| 1 | CA | 204 | G |
| 1 | CA | 207 | C |
| 1 | CA | 208 | U |
| 1 | CA | 209 | U |
| 1 | CA | 210 | C |
| 1 | CA | 211 | G |
| 1 | CA | 212 | G |
| 1 | CA | 214 | C |
| 1 | CA | 240 | G |
| 1 | CA | 241 | G |
| 1 | CA | 244 | U |
| 1 | CA | 245 | U |
| 1 | CA | 247 | G |
| 1 | CA | 250 | A |
| 1 | CA | 251 | G |
| 1 | CA | 253 | A |
| 1 | CA | 254 | G |
| 1 | CA | 259 | G |
| 1 | CA | 266 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 267 | C |
| 1 | CA | 268 | U |
| 1 | CA | 269 | C |
| 1 | CA | 280 | C |
| 1 | CA | 289 | G |
| 1 | CA | 294 | U |
| 1 | CA | 316 | C |
| 1 | CA | 321 | A |
| 1 | CA | 328 | C |
| 1 | CA | 329 | A |
| 1 | CA | 330 | C |
| 1 | CA | 332 | G |
| 1 | CA | 345 | C |
| 1 | CA | 347 | G |
| 1 | CA | 352 | C |
| 1 | CA | 354 | G |
| 1 | CA | 367 | U |
| 1 | CA | 372 | C |
| 1 | CA | 376 | G |
| 1 | CA | 378 | G |
| 1 | CA | 384 | G |
| 1 | CA | 389 | A |
| 1 | CA | 390 | U |
| 1 | CA | 398 | U |
| 1 | CA | 404 | G |
| 1 | CA | 406 | G |
| 1 | CA | 409 | U |
| 1 | CA | 411 | A |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 421 | U |
| 1 | CA | 422 | C |
| 1 | CA | 424 | G |
| 1 | CA | 427 | U |
| 1 | CA | 429 | U |
| 1 | CA | 430 | A |
| 1 | CA | 439 | U |
| 1 | CA | 440 | C |
| 1 | CA | 446 | G |
| 1 | CA | 459 | A |
| 1 | CA | 463 | U |
| 1 | CA | 467 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 468 | A |
| 1 | CA | 473 | U |
| 1 | CA | 474 | G |
| 1 | CA | 478 | A |
| 1 | CA | 479 | U |
| 1 | CA | 481 | G |
| 1 | CA | 484 | G |
| 1 | CA | 485 | U |
| 1 | CA | 486 | U |
| 1 | CA | 498 | A |
| 1 | CA | 505 | G |
| 1 | CA | 509 | A |
| 1 | CA | 511 | C |
| 1 | CA | 518 | C |
| 1 | CA | 519 | C |
| 1 | CA | 524 | G |
| 1 | CA | 527 | G |
| 1 | CA | 530 | G |
| 1 | CA | 531 | U |
| 1 | CA | 532 | A |
| 1 | CA | 533 | A |
| 1 | CA | 545 | C |
| 1 | CA | 547 | A |
| 1 | CA | 550 | G |
| 1 | CA | 559 | A |
| 1 | CA | 564 | C |
| 1 | CA | 568 | G |
| 1 | CA | 570 | G |
| 1 | CA | 572 | A |
| 1 | CA | 573 | A |
| 1 | CA | 576 | C |
| 1 | CA | 582 | C |
| 1 | CA | 615 | G |
| 1 | CA | 619 | U |
| 1 | CA | 622 | A |
| 1 | CA | 628 | G |
| 1 | CA | 636 | U |
| 1 | CA | 650 | G |
| 1 | CA | 653 | U |
| 1 | CA | 654 | G |
| 1 | CA | 665 | A |
| 1 | CA | 687 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 695 | A |
| 1 | CA | 702 | A |
| 1 | CA | 721 | G |
| 1 | CA | 723 | U |
| 1 | CA | 724 | G |
| 1 | CA | 731 | G |
| 1 | CA | 747 | A |
| 1 | CA | 755 | G |
| 1 | CA | 765 | G |
| 1 | CA | 777 | A |
| 1 | CA | 785 | G |
| 1 | CA | 787 | A |
| 1 | CA | 793 | U |
| 1 | CA | 794 | A |
| 1 | CA | 802 | A |
| 1 | CA | 812 | G |
| 1 | CA | 815 | A |
| 1 | CA | 817 | C |
| 1 | CA | 828 | U |
| 1 | CA | 832 | G |
| 1 | CA | 841 | C |
| 1 | CA | 842 | U |
| 1 | CA | 843 | U |
| 1 | CA | 844 | G |
| 1 | CA | 845 | A |
| 1 | CA | 846 | G |
| 1 | CA | 849 | G |
| 1 | CA | 874 | G |
| 1 | CA | 876 | C |
| 1 | CA | 880 | C |
| 1 | CA | 906 | A |
| 1 | CA | 914 | A |
| 1 | CA | 922 | G |
| 1 | CA | 926 | G |
| 1 | CA | 934 | C |
| 1 | CA | 935 | A |
| 1 | CA | 960 | U |
| 1 | CA | 964 | A |
| 1 | CA | 969 | A |
| 1 | CA | 971 | G |
| 1 | CA | 975 | A |
| 1 | CA | 976 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 977 | A |
| 1 | CA | 983 | A |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |
| 1 | CA | 993 | G |
| 1 | CA | 994 | A |
| 1 | CA | 995 | C |
| 1 | CA | 996 | A |
| 1 | CA | 1004 | A |
| 1 | CA | 1008 | U |
| 1 | CA | 1018 | G |
| 1 | CA | 1020 | G |
| 1 | CA | 1022 | A |
| 1 | CA | 1025 | U |
| 1 | CA | 1026 | G |
| 1 | CA | 1027 | C |
| 1 | CA | 1028 | C |
| 1 | CA | 1030 | U |
| 1 | CA | 1031 | C |
| 1 | CA | 1032 | G |
| 1 | CA | 1033 | G |
| 1 | CA | 1034 | G |
| 1 | CA | 1037 | C |
| 1 | CA | 1039 | G |
| 1 | CA | 1042 | A |
| 1 | CA | 1043 | G |
| 1 | CA | 1044 | A |
| 1 | CA | 1047 | G |
| 1 | CA | 1050 | G |
| 1 | CA | 1052 | U |
| 1 | CA | 1054 | C |
| 1 | CA | 1055 | A |
| 1 | CA | 1065 | U |
| 1 | CA | 1070 | U |
| 1 | CA | 1072 | G |
| 1 | CA | 1073 | U |
| 1 | CA | 1086 | U |
| 1 | CA | 1089 | G |
| 1 | CA | 1094 | G |
| 1 | CA | 1095 | U |
| 1 | CA | 1096 | C |
| 1 | CA | 1101 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1104 | G |
| 1 | CA | 1124 | G |
| 1 | CA | 1125 | U |
| 1 | CA | 1129 | C |
| 1 | CA | 1133 | G |
| 1 | CA | 1134 | G |
| 1 | CA | 1136 | C |
| 1 | CA | 1137 | C |
| 1 | CA | 1139 | G |
| 1 | CA | 1140 | C |
| 1 | CA | 1141 | C |
| 1 | CA | 1142 | G |
| 1 | CA | 1145 | A |
| 1 | CA | 1154 | G |
| 1 | CA | 1157 | A |
| 1 | CA | 1159 | U |
| 1 | CA | 1160 | G |
| 1 | CA | 1161 | C |
| 1 | CA | 1168 | U |
| 1 | CA | 1181 | G |
| 1 | CA | 1184 | G |
| 1 | CA | 1187 | G |
| 1 | CA | 1196 | A |
| 1 | CA | 1197 | A |
| 1 | CA | 1198 | G |
| 1 | CA | 1202 | U |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1222 | G |
| 1 | CA | 1227 | A |
| 1 | CA | 1228 | C |
| 1 | CA | 1230 | C |
| 1 | CA | 1236 | A |
| 1 | CA | 1238 | A |
| 1 | CA | 1239 | A |
| 1 | CA | 1240 | U |
| 1 | CA | 1253 | G |
| 1 | CA | 1256 | A |
| 1 | CA | 1257 | A |
| 1 | CA | 1259 | C |
| 1 | CA | 1260 | G |
| 1 | CA | 1275 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1280 | A |
| 1 | CA | 1285 | A |
| 1 | CA | 1286 | U |
| 1 | CA | 1287 | A |
| 1 | CA | 1297 | G |
| 1 | CA | 1299 | A |
| 1 | CA | 1301 | U |
| 1 | CA | 1305 | G |
| 1 | CA | 1312 | G |
| 1 | CA | 1317 | C |
| 1 | CA | 1318 | A |
| 1 | CA | 1320 | C |
| 1 | CA | 1322 | C |
| 1 | CA | 1323 | G |
| 1 | CA | 1324 | A |
| 1 | CA | 1332 | A |
| 1 | CA | 1336 | C |
| 1 | CA | 1337 | G |
| 1 | CA | 1338 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1353 | G |
| 1 | CA | 1362 | A |
| 1 | CA | 1363 | A |
| 1 | CA | 1368 | A |
| 1 | CA | 1379 | G |
| 1 | CA | 1381 | U |
| 1 | CA | 1382 | C |
| 1 | CA | 1418 | A |
| 1 | CA | 1441 | A |
| 1 | CA | 1442 | G |
| 1 | CA | 1446 | A |
| 1 | CA | 1451 | U |
| 1 | CA | 1452 | C |
| 1 | CA | 1454 | G |
| 1 | CA | 1475 | G |
| 1 | CA | 1477 | U |
| 1 | CA | 1491 | G |
| 1 | CA | 1492 | A |
| 1 | CA | 1497 | G |
| 1 | CA | 1499 | A |
| 1 | CA | 1503 | A |
| 1 | CA | 1505 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1506 | U |
| 1 | CA | 1507 | A |
| 1 | CA | 1509 | C |
| 1 | CA | 1517 | G |
| 1 | CA | 1519 | A |
| 1 | CA | 1529 | G |
| 1 | CA | 1530 | G |
| 1 | CA | 1533 | C |
| 1 | CA | 1534 | A |
| 1 | CA | 1535 | C |
| 1 | CA | 1536 | C |
| 22 | DA | 10 | A |
| 22 | DA | 15 | G |
| 22 | DA | 32 | C |
| 22 | DA | 34 | U |
| 22 | DA | 39 | G |
| 22 | DA | 42 | A |
| 22 | DA | 43 | G |
| 22 | DA | 46 | G |
| 22 | DA | 57 | C |
| 22 | DA | 61 | C |
| 22 | DA | 64 | A |
| 22 | DA | 66 | C |
| 22 | DA | 70 | G |
| 22 | DA | 71 | A |
| 22 | DA | 73 | A |
| 22 | DA | 74 | A |
| 22 | DA | 75 | G |
| 22 | DA | 80 | G |
| 22 | DA | 81 | G |
| 22 | DA | 82 | U |
| 22 | DA | 83 | A |
| 22 | DA | 84 | A |
| 22 | DA | 85 | G |
| 22 | DA | 87 | U |
| 22 | DA | 91 | A |
| 22 | DA | 96 | C |
| 22 | DA | 97 | C |
| 22 | DA | 98 | G |
| 22 | DA | 101 | A |
| 22 | DA | 103 | A |
| 22 | DA | 104 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 111 | A |
| 22 | DA | 118 | A |
| 22 | DA | 119 | A |
| 22 | DA | 120 | U |
| 22 | DA | 121 | G |
| 22 | DA | 128 | C |
| 22 | DA | 137 | U |
| 22 | DA | 138 | U |
| 22 | DA | 139 | U |
| 22 | DA | 140 | C |
| 22 | DA | 141 | G |
| 22 | DA | 142 | A |
| 22 | DA | 143 | C |
| 22 | DA | 145 | C |
| 22 | DA | 150 | U |
| 22 | DA | 155 | A |
| 22 | DA | 158 | U |
| 22 | DA | 159 | G |
| 22 | DA | 162 | U |
| 22 | DA | 166 | U |
| 22 | DA | 178 | G |
| 22 | DA | 180 | G |
| 22 | DA | 184 | C |
| 22 | DA | 185 | G |
| 22 | DA | 196 | A |
| 22 | DA | 198 | C |
| 22 | DA | 202 | U |
| 22 | DA | 206 | U |
| 22 | DA | 216 | A |
| 22 | DA | 221 | A |
| 22 | DA | 222 | A |
| 22 | DA | 223 | A |
| 22 | DA | 224 | U |
| 22 | DA | 225 | C |
| 22 | DA | 228 | C |
| 22 | DA | 233 | A |
| 22 | DA | 245 | G |
| 22 | DA | 248 | G |
| 22 | DA | 249 | C |
| 22 | DA | 251 | A |
| 22 | DA | 258 | G |
| 22 | DA | 262 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 265 | A |
| 22 | DA | 266 | G |
| 22 | DA | 271 | G |
| 22 | DA | 272 | A |
| 22 | DA | 276 | U |
| 22 | DA | 279 | A |
| 22 | DA | 281 | C |
| 22 | DA | 285 | G |
| 22 | DA | 291 | G |
| 22 | DA | 294 | A |
| 22 | DA | 311 | A |
| 22 | DA | 321 | U |
| 22 | DA | 329 | G |
| 22 | DA | 330 | A |
| 22 | DA | 335 | C |
| 22 | DA | 346 | A |
| 22 | DA | 348 | A |
| 22 | DA | 350 | G |
| 22 | DA | 359 | G |
| 22 | DA | 361 | G |
| 22 | DA | 362 | A |
| 22 | DA | 367 | G |
| 22 | DA | 370 | G |
| 22 | DA | 371 | A |
| 22 | DA | 372 | G |
| 22 | DA | 380 | G |
| 22 | DA | 385 | C |
| 22 | DA | 386 | G |
| 22 | DA | 387 | U |
| 22 | DA | 392 | U |
| 22 | DA | 396 | G |
| 22 | DA | 401 | A |
| 22 | DA | 405 | U |
| 22 | DA | 411 | G |
| 22 | DA | 412 | A |
| 22 | DA | 417 | C |
| 22 | DA | 420 | C |
| 22 | DA | 421 | C |
| 22 | DA | 424 | G |
| 22 | DA | 426 | C |
| 22 | DA | 430 | A |
| 22 | DA | 435 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 444 | C |
| 22 | DA | 446 | G |
| 22 | DA | 448 | U |
| 22 | DA | 451 | U |
| 22 | DA | 455 | C |
| 22 | DA | 461 | C |
| 22 | DA | 462 | C |
| 22 | DA | 478 | A |
| 22 | DA | 480 | A |
| 22 | DA | 481 | G |
| 22 | DA | 490 | C |
| 22 | DA | 491 | G |
| 22 | DA | 496 | G |
| 22 | DA | 504 | A |
| 22 | DA | 505 | A |
| 22 | DA | 508 | A |
| 22 | DA | 509 | C |
| 22 | DA | 510 | C |
| 22 | DA | 511 | U |
| 22 | DA | 528 | A |
| 22 | DA | 531 | C |
| 22 | DA | 532 | A |
| 22 | DA | 533 | G |
| 22 | DA | 542 | C |
| 22 | DA | 543 | G |
| 22 | DA | 544 | C |
| 22 | DA | 546 | U |
| 22 | DA | 547 | A |
| 22 | DA | 548 | G |
| 22 | DA | 549 | G |
| 22 | DA | 550 | C |
| 22 | DA | 563 | A |
| 22 | DA | 564 | C |
| 22 | DA | 568 | U |
| 22 | DA | 569 | U |
| 22 | DA | 572 | A |
| 22 | DA | 573 | U |
| 22 | DA | 575 | A |
| 22 | DA | 586 | A |
| 22 | DA | 588 | U |
| 22 | DA | 603 | A |
| 22 | DA | 613 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 614 | A |
| 22 | DA | 615 | U |
| 22 | DA | 622 | G |
| 22 | DA | 627 | A |
| 22 | DA | 628 | G |
| 22 | DA | 631 | A |
| 22 | DA | 637 | A |
| 22 | DA | 642 | U |
| 22 | DA | 645 | C |
| 22 | DA | 646 | U |
| 22 | DA | 647 | G |
| 22 | DA | 648 | G |
| 22 | DA | 654 | A |
| 22 | DA | 655 | A |
| 22 | DA | 656 | G |
| 22 | DA | 657 | U |
| 22 | DA | 662 | G |
| 22 | DA | 664 | G |
| 22 | DA | 672 | C |
| 22 | DA | 682 | G |
| 22 | DA | 684 | G |
| 22 | DA | 685 | A |
| 22 | DA | 686 | U |
| 22 | DA | 694 | U |
| 22 | DA | 695 | G |
| 22 | DA | 701 | G |
| 22 | DA | 702 | U |
| 22 | DA | 717 | C |
| 22 | DA | 726 | G |
| 22 | DA | 727 | A |
| 22 | DA | 728 | G |
| 22 | DA | 729 | G |
| 22 | DA | 730 | A |
| 22 | DA | 740 | C |
| 22 | DA | 747 | U |
| 22 | DA | 748 | G |
| 22 | DA | 752 | A |
| 22 | DA | 757 | G |
| 22 | DA | 758 | C |
| 22 | DA | 771 | G |
| 22 | DA | 773 | U |
| 22 | DA | 775 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 776 | G |
| 22 | DA | 782 | A |
| 22 | DA | 784 | G |
| 22 | DA | 785 | G |
| 22 | DA | 790 | U |
| 22 | DA | 792 | A |
| 22 | DA | 793 | A |
| 22 | DA | 798 | G |
| 22 | DA | 800 | A |
| 22 | DA | 801 | G |
| 22 | DA | 802 | A |
| 22 | DA | 805 | G |
| 22 | DA | 812 | C |
| 22 | DA | 814 | C |
| 22 | DA | 815 | C |
| 22 | DA | 819 | A |
| 22 | DA | 826 | U |
| 22 | DA | 827 | U |
| 22 | DA | 828 | U |
| 22 | DA | 829 | A |
| 22 | DA | 830 | G |
| 22 | DA | 844 | A |
| 22 | DA | 845 | A |
| 22 | DA | 846 | U |
| 22 | DA | 847 | U |
| 22 | DA | 858 | G |
| 22 | DA | 859 | G |
| 22 | DA | 878 | A |
| 22 | DA | 881 | G |
| 22 | DA | 882 | G |
| 22 | DA | 885 | C |
| 22 | DA | 896 | A |
| 22 | DA | 897 | C |
| 22 | DA | 907 | G |
| 22 | DA | 910 | A |
| 22 | DA | 914 | G |
| 22 | DA | 915 | C |
| 22 | DA | 931 | U |
| 22 | DA | 932 | U |
| 22 | DA | 933 | A |
| 22 | DA | 941 | A |
| 22 | DA | 946 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 951 | C |
| 22 | DA | 953 | G |
| 22 | DA | 958 | U |
| 22 | DA | 959 | A |
| 22 | DA | 961 | C |
| 22 | DA | 974 | G |
| 22 | DA | 983 | A |
| 22 | DA | 995 | C |
| 22 | DA | 996 | A |
| 22 | DA | 1012 | U |
| 22 | DA | 1013 | C |
| 22 | DA | 1022 | G |
| 22 | DA | 1023 | U |
| 22 | DA | 1025 | G |
| 22 | DA | 1026 | G |
| 22 | DA | 1033 | U |
| 22 | DA | 1046 | A |
| 22 | DA | 1047 | G |
| 22 | DA | 1051 | G |
| 22 | DA | 1057 | A |
| 22 | DA | 1058 | U |
| 22 | DA | 1061 | U |
| 22 | DA | 1062 | G |
| 22 | DA | 1065 | U |
| 22 | DA | 1066 | U |
| 22 | DA | 1068 | G |
| 22 | DA | 1069 | A |
| 22 | DA | 1070 | A |
| 22 | DA | 1071 | G |
| 22 | DA | 1072 | C |
| 22 | DA | 1074 | G |
| 22 | DA | 1075 | C |
| 22 | DA | 1077 | A |
| 22 | DA | 1088 | A |
| 22 | DA | 1089 | A |
| 22 | DA | 1092 | C |
| 22 | DA | 1094 | U |
| 22 | DA | 1096 | A |
| 22 | DA | 1097 | U |
| 22 | DA | 1100 | C |
| 22 | DA | 1101 | U |
| 22 | DA | 1104 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1110 | G |
| 22 | DA | 1112 | G |
| 22 | DA | 1115 | G |
| 22 | DA | 1116 | G |
| 22 | DA | 1119 | U |
| 22 | DA | 1122 | G |
| 22 | DA | 1128 | G |
| 22 | DA | 1132 | U |
| 22 | DA | 1135 | C |
| 22 | DA | 1136 | G |
| 22 | DA | 1139 | G |
| 22 | DA | 1142 | A |
| 22 | DA | 1153 | C |
| 22 | DA | 1155 | A |
| 22 | DA | 1171 | G |
| 22 | DA | 1172 | C |
| 22 | DA | 1175 | A |
| 22 | DA | 1176 | U |
| 22 | DA | 1178 | C |
| 22 | DA | 1179 | G |
| 22 | DA | 1180 | U |
| 22 | DA | 1183 | U |
| 22 | DA | 1186 | G |
| 22 | DA | 1199 | U |
| 22 | DA | 1204 | A |
| 22 | DA | 1205 | A |
| 22 | DA | 1212 | G |
| 22 | DA | 1227 | G |
| 22 | DA | 1230 | A |
| 22 | DA | 1231 | U |
| 22 | DA | 1235 | G |
| 22 | DA | 1236 | G |
| 22 | DA | 1237 | A |
| 22 | DA | 1238 | G |
| 22 | DA | 1242 | U |
| 22 | DA | 1243 | C |
| 22 | DA | 1244 | A |
| 22 | DA | 1247 | A |
| 22 | DA | 1248 | G |
| 22 | DA | 1250 | G |
| 22 | DA | 1253 | A |
| 22 | DA | 1256 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1266 | G |
| 22 | DA | 1268 | A |
| 22 | DA | 1272 | A |
| 22 | DA | 1276 | A |
| 22 | DA | 1282 | U |
| 22 | DA | 1288 | G |
| 22 | DA | 1289 | C |
| 22 | DA | 1293 | C |
| 22 | DA | 1294 | U |
| 22 | DA | 1300 | G |
| 22 | DA | 1301 | A |
| 22 | DA | 1321 | A |
| 22 | DA | 1330 | C |
| 22 | DA | 1339 | G |
| 22 | DA | 1344 | U |
| 22 | DA | 1345 | C |
| 22 | DA | 1352 | U |
| 22 | DA | 1355 | G |
| 22 | DA | 1359 | A |
| 22 | DA | 1365 | A |
| 22 | DA | 1374 | G |
| 22 | DA | 1376 | C |
| 22 | DA | 1378 | A |
| 22 | DA | 1379 | U |
| 22 | DA | 1380 | G |
| 22 | DA | 1383 | A |
| 22 | DA | 1384 | A |
| 22 | DA | 1391 | U |
| 22 | DA | 1393 | A |
| 22 | DA | 1395 | A |
| 22 | DA | 1411 | U |
| 22 | DA | 1416 | G |
| 22 | DA | 1418 | G |
| 22 | DA | 1419 | A |
| 22 | DA | 1420 | A |
| 22 | DA | 1428 | C |
| 22 | DA | 1434 | A |
| 22 | DA | 1446 | C |
| 22 | DA | 1452 | G |
| 22 | DA | 1453 | A |
| 22 | DA | 1454 | C |
| 22 | DA | 1456 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1458 | U |
| 22 | DA | 1462 | C |
| 22 | DA | 1465 | G |
| 22 | DA | 1468 | U |
| 22 | DA | 1471 | G |
| 22 | DA | 1476 | U |
| 22 | DA | 1482 | G |
| 22 | DA | 1493 | C |
| 22 | DA | 1503 | A |
| 22 | DA | 1504 | A |
| 22 | DA | 1509 | A |
| 22 | DA | 1510 | G |
| 22 | DA | 1515 | A |
| 22 | DA | 1523 | U |
| 22 | DA | 1524 | G |
| 22 | DA | 1527 | G |
| 22 | DA | 1530 | G |
| 22 | DA | 1531 | C |
| 22 | DA | 1533 | C |
| 22 | DA | 1534 | U |
| 22 | DA | 1535 | A |
| 22 | DA | 1536 | C |
| 22 | DA | 1537 | G |
| 22 | DA | 1540 | G |
| 22 | DA | 1555 | G |
| 22 | DA | 1560 | G |
| 22 | DA | 1566 | A |
| 22 | DA | 1569 | A |
| 22 | DA | 1576 | U |
| 22 | DA | 1578 | U |
| 22 | DA | 1581 | G |
| 22 | DA | 1582 | C |
| 22 | DA | 1583 | A |
| 22 | DA | 1584 | U |
| 22 | DA | 1585 | C |
| 22 | DA | 1587 | G |
| 22 | DA | 1592 | C |
| 22 | DA | 1602 | U |
| 22 | DA | 1603 | A |
| 22 | DA | 1606 | C |
| 22 | DA | 1607 | C |
| 22 | DA | 1608 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1610 | A |
| 22 | DA | 1613 | G |
| 22 | DA | 1616 | A |
| 22 | DA | 1626 | A |
| 22 | DA | 1634 | A |
| 22 | DA | 1645 | G |
| 22 | DA | 1646 | C |
| 22 | DA | 1647 | U |
| 22 | DA | 1648 | U |
| 22 | DA | 1649 | G |
| 22 | DA | 1651 | G |
| 22 | DA | 1652 | A |
| 22 | DA | 1660 | G |
| 22 | DA | 1663 | G |
| 22 | DA | 1664 | A |
| 22 | DA | 1674 | G |
| 22 | DA | 1715 | G |
| 22 | DA | 1729 | U |
| 22 | DA | 1730 | C |
| 22 | DA | 1732 | C |
| 22 | DA | 1738 | G |
| 22 | DA | 1740 | G |
| 22 | DA | 1744 | A |
| 22 | DA | 1750 | G |
| 22 | DA | 1758 | U |
| 22 | DA | 1759 | A |
| 22 | DA | 1764 | C |
| 22 | DA | 1767 | G |
| 22 | DA | 1773 | A |
| 22 | DA | 1781 | U |
| 22 | DA | 1782 | U |
| 22 | DA | 1791 | A |
| 22 | DA | 1793 | C |
| 22 | DA | 1800 | C |
| 22 | DA | 1801 | A |
| 22 | DA | 1802 | A |
| 22 | DA | 1808 | A |
| 22 | DA | 1810 | A |
| 22 | DA | 1812 | U |
| 22 | DA | 1816 | C |
| 22 | DA | 1817 | G |
| 22 | DA | 1828 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1829 | A |
| 22 | DA | 1833 | C |
| 22 | DA | 1848 | A |
| 22 | DA | 1858 | A |
| 22 | DA | 1870 | C |
| 22 | DA | 1871 | A |
| 22 | DA | 1872 | A |
| 22 | DA | 1873 | G |
| 22 | DA | 1876 | A |
| 22 | DA | 1878 | G |
| 22 | DA | 1880 | U |
| 22 | DA | 1882 | U |
| 22 | DA | 1889 | A |
| 22 | DA | 1903 | G |
| 22 | DA | 1906 | G |
| 22 | DA | 1914 | C |
| 22 | DA | 1920 | C |
| 22 | DA | 1926 | U |
| 22 | DA | 1927 | A |
| 22 | DA | 1929 | G |
| 22 | DA | 1930 | G |
| 22 | DA | 1937 | A |
| 22 | DA | 1938 | A |
| 22 | DA | 1945 | G |
| 22 | DA | 1955 | U |
| 22 | DA | 1965 | C |
| 22 | DA | 1966 | A |
| 22 | DA | 1967 | C |
| 22 | DA | 1970 | A |
| 22 | DA | 1971 | U |
| 22 | DA | 1972 | G |
| 22 | DA | 1975 | G |
| 22 | DA | 1981 | A |
| 22 | DA | 1987 | A |
| 22 | DA | 1991 | U |
| 22 | DA | 1992 | G |
| 22 | DA | 1993 | U |
| 22 | DA | 1997 | C |
| 22 | DA | 2004 | G |
| 22 | DA | 2007 | U |
| 22 | DA | 2018 | G |
| 22 | DA | 2020 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2021 | C |
| 22 | DA | 2022 | U |
| 22 | DA | 2023 | C |
| 22 | DA | 2030 | A |
| 22 | DA | 2031 | A |
| 22 | DA | 2033 | A |
| 22 | DA | 2043 | C |
| 22 | DA | 2049 | G |
| 22 | DA | 2055 | C |
| 22 | DA | 2056 | G |
| 22 | DA | 2060 | A |
| 22 | DA | 2061 | G |
| 22 | DA | 2062 | A |
| 22 | DA | 2064 | C |
| 22 | DA | 2069 | G |
| 22 | DA | 2072 | C |
| 22 | DA | 2075 | U |
| 22 | DA | 2080 | A |
| 22 | DA | 2087 | G |
| 22 | DA | 2092 | U |
| 22 | DA | 2093 | G |
| 22 | DA | 2108 | A |
| 22 | DA | 2109 | U |
| 22 | DA | 2110 | G |
| 22 | DA | 2111 | U |
| 22 | DA | 2112 | G |
| 22 | DA | 2113 | U |
| 22 | DA | 2115 | G |
| 22 | DA | 2116 | G |
| 22 | DA | 2117 | A |
| 22 | DA | 2118 | U |
| 22 | DA | 2119 | A |
| 22 | DA | 2120 | G |
| 22 | DA | 2125 | G |
| 22 | DA | 2126 | A |
| 22 | DA | 2127 | G |
| 22 | DA | 2128 | G |
| 22 | DA | 2131 | U |
| 22 | DA | 2132 | U |
| 22 | DA | 2133 | G |
| 22 | DA | 2135 | A |
| 22 | DA | 2137 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2143 | C |
| 22 | DA | 2146 | C |
| 22 | DA | 2147 | A |
| 22 | DA | 2149 | U |
| 22 | DA | 2158 | A |
| 22 | DA | 2162 | G |
| 22 | DA | 2163 | A |
| 22 | DA | 2164 | C |
| 22 | DA | 2165 | C |
| 22 | DA | 2166 | U |
| 22 | DA | 2169 | A |
| 22 | DA | 2170 | A |
| 22 | DA | 2171 | A |
| 22 | DA | 2172 | U |
| 22 | DA | 2189 | U |
| 22 | DA | 2190 | G |
| 22 | DA | 2194 | U |
| 22 | DA | 2198 | A |
| 22 | DA | 2203 | U |
| 22 | DA | 2204 | G |
| 22 | DA | 2207 | C |
| 22 | DA | 2211 | A |
| 22 | DA | 2212 | A |
| 22 | DA | 2215 | C |
| 22 | DA | 2225 | A |
| 22 | DA | 2226 | C |
| 22 | DA | 2230 | G |
| 22 | DA | 2238 | G |
| 22 | DA | 2239 | G |
| 22 | DA | 2242 | G |
| 22 | DA | 2243 | U |
| 22 | DA | 2245 | U |
| 22 | DA | 2246 | G |
| 22 | DA | 2250 | G |
| 22 | DA | 2268 | A |
| 22 | DA | 2273 | A |
| 22 | DA | 2279 | G |
| 22 | DA | 2280 | G |
| 22 | DA | 2283 | C |
| 22 | DA | 2285 | C |
| 22 | DA | 2287 | A |
| 22 | DA | 2289 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2305 | U |
| 22 | DA | 2307 | G |
| 22 | DA | 2308 | G |
| 22 | DA | 2309 | A |
| 22 | DA | 2310 | C |
| 22 | DA | 2311 | A |
| 22 | DA | 2313 | C |
| 22 | DA | 2321 | U |
| 22 | DA | 2322 | A |
| 22 | DA | 2325 | G |
| 22 | DA | 2327 | A |
| 22 | DA | 2333 | A |
| 22 | DA | 2345 | G |
| 22 | DA | 2347 | C |
| 22 | DA | 2350 | C |
| 22 | DA | 2354 | C |
| 22 | DA | 2356 | U |
| 22 | DA | 2357 | G |
| 22 | DA | 2361 | G |
| 22 | DA | 2383 | G |
| 22 | DA | 2385 | C |
| 22 | DA | 2397 | G |
| 22 | DA | 2402 | U |
| 22 | DA | 2406 | A |
| 22 | DA | 2407 | A |
| 22 | DA | 2409 | G |
| 22 | DA | 2410 | G |
| 22 | DA | 2412 | A |
| 22 | DA | 2417 | C |
| 22 | DA | 2423 | U |
| 22 | DA | 2424 | C |
| 22 | DA | 2425 | A |
| 22 | DA | 2426 | A |
| 22 | DA | 2429 | G |
| 22 | DA | 2430 | A |
| 22 | DA | 2431 | U |
| 22 | DA | 2435 | A |
| 22 | DA | 2440 | C |
| 22 | DA | 2441 | U |
| 22 | DA | 2446 | G |
| 22 | DA | 2447 | G |
| 22 | DA | 2448 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2449 | U |
| 22 | DA | 2465 | C |
| 22 | DA | 2470 | G |
| 22 | DA | 2476 | A |
| 22 | DA | 2491 | U |
| 22 | DA | 2502 | G |
| 22 | DA | 2503 | A |
| 22 | DA | 2505 | G |
| 22 | DA | 2517 | C |
| 22 | DA | 2518 | A |
| 22 | DA | 2525 | G |
| 22 | DA | 2529 | G |
| 22 | DA | 2535 | G |
| 22 | DA | 2547 | A |
| 22 | DA | 2550 | G |
| 22 | DA | 2554 | U |
| 22 | DA | 2556 | C |
| 22 | DA | 2559 | C |
| 22 | DA | 2563 | U |
| 22 | DA | 2566 | A |
| 22 | DA | 2567 | G |
| 22 | DA | 2578 | G |
| 22 | DA | 2585 | U |
| 22 | DA | 2586 | U |
| 22 | DA | 2600 | A |
| 22 | DA | 2602 | A |
| 22 | DA | 2603 | G |
| 22 | DA | 2609 | U |
| 22 | DA | 2613 | U |
| 22 | DA | 2615 | U |
| 22 | DA | 2619 | C |
| 22 | DA | 2624 | G |
| 22 | DA | 2629 | U |
| 22 | DA | 2630 | G |
| 22 | DA | 2644 | G |
| 22 | DA | 2646 | C |
| 22 | DA | 2648 | G |
| 22 | DA | 2656 | U |
| 22 | DA | 2661 | G |
| 22 | DA | 2663 | G |
| 22 | DA | 2665 | A |
| 22 | DA | 2689 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2690 | U |
| 22 | DA | 2691 | C |
| 22 | DA | 2714 | G |
| 22 | DA | 2716 | C |
| 22 | DA | 2718 | G |
| 22 | DA | 2719 | G |
| 22 | DA | 2726 | A |
| 22 | DA | 2727 | A |
| 22 | DA | 2729 | G |
| 22 | DA | 2739 | U |
| 22 | DA | 2741 | A |
| 22 | DA | 2748 | A |
| 22 | DA | 2751 | G |
| 22 | DA | 2757 | A |
| 22 | DA | 2778 | A |
| 22 | DA | 2791 | G |
| 22 | DA | 2794 | C |
| 22 | DA | 2799 | A |
| 22 | DA | 2803 | G |
| 22 | DA | 2807 | U |
| 22 | DA | 2809 | A |
| 22 | DA | 2812 | G |
| 22 | DA | 2818 | U |
| 22 | DA | 2820 | A |
| 22 | DA | 2821 | A |
| 22 | DA | 2823 | A |
| 22 | DA | 2826 | A |
| 22 | DA | 2833 | U |
| 22 | DA | 2834 | G |
| 22 | DA | 2835 | A |
| 22 | DA | 2843 | G |
| 22 | DA | 2850 | A |
| 22 | DA | 2852 | G |
| 22 | DA | 2855 | C |
| 22 | DA | 2861 | U |
| 22 | DA | 2867 | G |
| 22 | DA | 2871 | U |
| 22 | DA | 2872 | A |
| 22 | DA | 2879 | A |
| 22 | DA | 2880 | C |
| 22 | DA | 2883 | A |
| 22 | DA | 2891 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2897 | U |
| 23 | DB | 13 | G |
| 23 | DB | 15 | A |
| 23 | DB | 16 | G |
| 23 | DB | 24 | G |
| 23 | DB | 35 | C |
| 23 | DB | 36 | C |
| 23 | DB | 44 | G |
| 23 | DB | 51 | G |
| 23 | DB | 54 | G |
| 23 | DB | 56 | G |
| 23 | DB | 61 | G |
| 23 | DB | 66 | A |
| 23 | DB | 87 | U |
| 23 | DB | 88 | C |
| 23 | DB | 89 | U |
| 23 | DB | 90 | C |
| 23 | DB | 99 | A |
| 23 | DB | 109 | A |
| 23 | DB | 110 | C |
| 23 | DB | 111 | U |

All (77) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 209 | U |
| 1 | AA | 351 | G |
| 1 | AA | 429 | U |
| 1 | AA | 484 | G |
| 1 | AA | 722 | G |
| 1 | AA | 1031 | C |
| 1 | AA | 1049 | U |
| 1 | AA | 1145 | A |
| 1 | AA | 1201 | A |
| 1 | AA | 1211 | U |
| 1 | AA | 1505 | G |
| 22 | BA | 70 | G |
| 22 | BA | 199 | A |
| 22 | BA | 271 | G |
| 22 | BA | 404 | A |
| 22 | BA | 455 | C |
| 22 | BA | 764 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 784 | G |
| 22 | BA | 800 | A |
| 22 | BA | 960 | A |
| 22 | BA | 984 | A |
| 22 | BA | 995 | C |
| 22 | BA | 1344 | U |
| 22 | BA | 1378 | A |
| 22 | BA | 1494 | A |
| 22 | BA | 1554 | U |
| 22 | BA | 1583 | A |
| 22 | BA | 1606 | C |
| 22 | BA | 1757 | A |
| 22 | BA | 1875 | G |
| 22 | BA | 2127 | G |
| 22 | BA | 2211 | A |
| 22 | BA | 2286 | G |
| 22 | BA | 2326 | C |
| 22 | BA | 2873 | A |
| 1 | CA | 85 | U |
| 1 | CA | 115 | G |
| 1 | CA | 209 | U |
| 1 | CA | 429 | U |
| 1 | CA | 484 | G |
| 1 | CA | 1049 | U |
| 1 | CA | 1201 | A |
| 1 | CA | 1211 | U |
| 1 | CA | 1279 | G |
| 1 | CA | 1317 | C |
| 22 | DA | 271 | G |
| 22 | DA | 404 | A |
| 22 | DA | 479 | A |
| 22 | DA | 613 | A |
| 22 | DA | 800 | A |
| 22 | DA | 846 | U |
| 22 | DA | 877 | A |
| 22 | DA | 1237 | A |
| 22 | DA | 1275 | A |
| 22 | DA | 1344 | U |
| 22 | DA | 1378 | A |
| 22 | DA | 1475 | G |
| 22 | DA | 1514 | G |
| 22 | DA | 1606 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1847 | A |
| 22 | DA | 1875 | G |
| 22 | DA | 2109 | U |
| 22 | DA | 2127 | G |
| 22 | DA | 2145 | C |
| 22 | DA | 2146 | C |
| 22 | DA | 2157 | G |
| 22 | DA | 2162 | G |
| 22 | DA | 2211 | A |
| 22 | DA | 2225 | A |
| 22 | DA | 2286 | G |
| 22 | DA | 2308 | G |
| 22 | DA | 2326 | C |
| 22 | DA | 2425 | A |
| 22 | DA | 2602 | A |
| 22 | DA | 2655 | G |
| 22 | DA | 2756 | U |
| 22 | DA | 2820 | A |

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

10 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 | $\# Z > 2$ |
| 54 | MHW | D6 | 1 | 54 | 9,9,10 | 1.95 | 1 (11%) | 10,11,13 | 3.07 | 4 (40%) |
| 54 | MHV | D6 | 6 | 54 | 7,9,10 | 1.19 | 0 | 7,11,13 | 3.21 | 4 (57%) |
| 54 | MHW | B6 | 1 | 54 | 9,9,10 | 1.64 | 1 (11%) | 10,11,13 | 2.86 | 4 (40%) |
| 54 | 004 | B6 | 7 | 54 | 9,10,11 | 1.52 | 1 (11%) | 9,12,14 | 2.03 | 3 (33%) |
| 54 | DBB | B6 | 3 | 54 | 4,5,6 | 1.31 | 0 | 1,5,7 | 2.61 | 1 (100%) |
| 54 | MHU | B6 | 5 | 54 | 14,15,16 | 1.80 | 3 (21%) | 18,19,21 | 1.27 | 3 (16%) |
| 54 | MHV | B6 | 6 | 54 | 7,9,10 | 1.59 | 1 (14%) | 7,11,13 | 3.44 | 4 (57%) |
| 54 | MHU | D6 | 5 | 54 | 14,15,16 | 1.63 | 3 (21%) | 18,19,21 | 1.15 | 2 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 54 | DBB | D6 | 3 | 54 | 4,5,6 | 1.18 | 0 | 1,5,7 | 1.37 | 0 |
| 54 | 004 | D6 | 7 | 54 | 9,10,11 | 0.78 | 0 | 9,12,14 | 0.60 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 54 | MHW | D6 | 1 | 54 | - | 0/2/2/4 | 0/1/1/1 |
| 54 | MHV | D6 | 6 | 54 | - | 0/1/12/14 | 0/1/1/1 |
| 54 | MHW | B6 | 1 | 54 | - | 0/2/2/4 | 0/1/1/1 |
| 54 | 004 | B6 | 7 | 54 | - | 1/4/6/8 | 0/1/1/1 |
| 54 | DBB | B6 | 3 | 54 | - | 1/3/4/6 | - |
| 54 | MHU | B6 | 5 | 54 | - | 0/9/12/14 | 0/1/1/1 |
| 54 | MHV | B6 | 6 | 54 | - | 0/1/12/14 | 0/1/1/1 |
| 54 | MHU | D6 | 5 | 54 | - | 0/9/12/14 | 0/1/1/1 |
| 54 | DBB | D6 | 3 | 54 | - | 0/3/4/6 | - |
| 54 | 004 | D6 | 7 | 54 | - | 2/4/6/8 | 0/1/1/1 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 54 | D6 | 1 | MHW | CA-C | 5.22 | 1.54 | 1.48 |
| 54 | B6 | 5 | MHU | CZ-NZ | 5.22 | 1.49 | 1.37 |
| 54 | D6 | 5 | MHU | CZ-NZ | 4.69 | 1.48 | 1.37 |
| 54 | B6 | 7 | 004 | CB-CA | -4.30 | 1.48 | 1.52 |
| 54 | B6 | 1 | MHW | CA-C | 3.99 | 1.52 | 1.48 |
| 54 | B6 | 6 | MHV | CB-CG | -2.97 | 1.45 | 1.50 |
| 54 | B6 | 5 | MHU | CD2-CE2 | 2.18 | 1.42 | 1.38 |
| 54 | B6 | 5 | MHU | CB-CG | 2.15 | 1.56 | 1.51 |
| 54 | D6 | 5 | MHU | CB-CG | 2.10 | 1.56 | 1.51 |
| 54 | D6 | 5 | MHU | CD2-CE2 | 2.00 | 1.42 | 1.38 |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 54 | D6 | 1 | MHW | CD-CE-N | 6.55 | 134.13 | 123.43 |
| 54 | B6 | 1 | MHW | CD-CE-N | 5.89 | 133.04 | 123.43 |
| 54 | B6 | 6 | MHV | CD2-CG-CB | 5.52 | 124.11 | 115.89 |
| 54 | D6 | 6 | MHV | CD2-CE-N | -5.22 | 98.62 | 110.03 |
| 54 | D6 | 6 | MHV | CD2-CG-CB | 5.13 | 123.53 | 115.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 54 | D6 | 1 | MHW | CG2-CD-CE | -4.90 | 111.66 | 118.91 |
| 54 | B6 | 6 | MHV | CD2-CE-N | -4.80 | 99.55 | 110.03 |
| 54 | B6 | 6 | MHV | OD1-CG-CB | -4.49 | 116.26 | 121.96 |
| 54 | D6 | 1 | MHW | O-C-CA | -4.12 | 120.32 | 124.22 |
| 54 | B6 | 7 | 004 | CB-CA-N | -4.10 | 102.59 | 112.40 |
| 54 | B6 | 1 | MHW | O-C-CA | -4.02 | 120.42 | 124.22 |
| 54 | B6 | 1 | MHW | CG2-CD-CE | -3.89 | 113.14 | 118.91 |
| 54 | B6 | 7 | 004 | CG2-CB-CG1 | 3.23 | 122.32 | 118.29 |
| 54 | B6 | 1 | MHW | C-CA-N | 2.96 | 120.20 | 115.41 |
| 54 | D6 | 6 | MHV | OD1-CG-CD2 | -2.84 | 117.19 | 122.05 |
| 54 | D6 | 1 | MHW | C-CA-N | 2.71 | 119.80 | 115.41 |
| 54 | B6 | 3 | DBB | CG-CB-CA | -2.61 | 107.44 | 113.42 |
| 54 | D6 | 5 | MHU | O-C-CA | -2.57 | 118.03 | 124.78 |
| 54 | D6 | 5 | MHU | CE2-CZ-NZ | -2.45 | 118.31 | 121.63 |
| 54 | B6 | 5 | MHU | CB-CA-C | -2.35 | 107.20 | 111.65 |
| 54 | B6 | 5 | MHU | CE2-CZ-NZ | -2.30 | 118.52 | 121.63 |
| 54 | B6 | 5 | MHU | CB-CA-N | 2.24 | 114.13 | 110.65 |
| 54 | D6 | 6 | MHV | OD1-CG-CB | -2.11 | 119.28 | 121.96 |
| 54 | B6 | 6 | MHV | CB-CA-N | -2.10 | 108.17 | 112.50 |
| 54 | B6 | 7 | 004 | CD1-CG1-CB | -2.09 | 118.06 | 120.65 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 54 | B6 | 3 | DBB | N-CA-CB-CG |
| 54 | D6 | 7 | 004 | C-CA-CB-CG1 |
| 54 | D6 | 7 | 004 | C-CA-CB-CG2 |
| 54 | B6 | 7 | 004 | C-CA-CB-CG1 |

There are no ring outliers.

6 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 54 | D6 | 1 | MHW | 2 | 0 |
| 54 | D6 | 6 | MHV | 1 | 0 |
| 54 | B6 | 7 | 004 | 1 | 0 |
| 54 | D6 | 5 | MHU | 3 | 0 |
| 54 | D6 | 3 | DBB | 1 | 0 |
| 54 | D6 | 7 | 004 | 4 | 0 |

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 500 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$ |
| 56 | DOL | BA | 3001 | - | 43,50,50 | 2.86 | 13 (30%) | 51,70,70 | 2.88 | 14 (27%) |
| 56 | DOL | DA | 3001 | - | 43,50,50 | 2.90 | 13 (30%) | 51,70,70 | 2.81 | 13 (25%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 56 | DOL | BA | 3001 | - | - | 18/58/77/77 | 0/2/3/3 |
| 56 | DOL | DA | 3001 | - | - | 10/58/77/77 | 0/2/3/3 |

All (26) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 56 | DA | 3001 | DOL | O15-C14 | 9.27 | 1.37 | 1.21 |
| 56 | BA | 3001 | DOL | O15-C14 | 8.90 | 1.36 | 1.21 |
| 56 | DA | 3001 | DOL | C22-C23 | 8.04 | 1.53 | 1.32 |
| 56 | BA | 3001 | DOL | C22-C23 | 7.76 | 1.52 | 1.32 |
| 56 | DA | 3001 | DOL | O38-C37 | 6.42 | 1.37 | 1.21 |
| 56 | BA | 3001 | DOL | O38-C37 | 6.18 | 1.36 | 1.21 |
| 56 | BA | 3001 | DOL | C26-N25 | 5.92 | 1.47 | 1.34 |
| 56 | DA | 3001 | DOL | C26-N25 | 5.90 | 1.47 | 1.34 |
| 56 | DA | 3001 | DOL | C19-C20 | 5.25 | 1.51 | 1.34 |
| 56 | DA | 3001 | DOL | C6-N5 | 5.09 | 1.46 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 56 | BA | 3001 | DOL | C19-C20 | 4.99 | 1.50 | 1.34 |
| 56 | BA | 3001 | DOL | C6-N5 | 4.46 | 1.44 | 1.34 |
| 56 | BA | 3001 | DOL | O36-C32 | -3.60 | 1.39 | 1.44 |
| 56 | DA | 3001 | DOL | C28-C29 | 3.54 | 1.40 | 1.32 |
| 56 | BA | 3001 | DOL | C28-C29 | 3.53 | 1.40 | 1.32 |
| 56 | BA | 3001 | DOL | C16-C17 | -3.46 | 1.49 | 1.54 |
| 56 | DA | 3001 | DOL | C16-C17 | -3.39 | 1.49 | 1.54 |
| 56 | DA | 3001 | DOL | O18-C17 | -3.09 | 1.38 | 1.43 |
| 56 | BA | 3001 | DOL | O36-C37 | -2.99 | 1.27 | 1.34 |
| 56 | DA | 3001 | DOL | C22-C20 | 2.86 | 1.52 | 1.45 |
| 56 | BA | 3001 | DOL | O18-C17 | -2.78 | 1.38 | 1.43 |
| 56 | BA | 3001 | DOL | C22-C20 | 2.76 | 1.51 | 1.45 |
| 56 | DA | 3001 | DOL | O36-C32 | -2.59 | 1.40 | 1.44 |
| 56 | DA | 3001 | DOL | O36-C37 | -2.28 | 1.29 | 1.34 |
| 56 | BA | 3001 | DOL | C3-C4 | 2.22 | 1.57 | 1.52 |
| 56 | DA | 3001 | DOL | C3-C4 | 2.06 | 1.56 | 1.52 |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 56 | DA | 3001 | DOL | O40-S39-O41 | -15.45 | 100.57 | 118.19 |
| 56 | BA | 3001 | DOL | O40-S39-O41 | -14.66 | 101.47 | 118.19 |
| 56 | BA | 3001 | DOL | C8-C6-N5 | 6.55 | 127.31 | 119.76 |
| 56 | BA | 3001 | DOL | C29-C28-C26 | -5.90 | 107.93 | 122.69 |
| 56 | DA | 3001 | DOL | C4-N5-C1 | -5.06 | 106.22 | 112.45 |
| 56 | BA | 3001 | DOL | C23-C22-C20 | -4.62 | 118.91 | 125.89 |
| 56 | DA | 3001 | DOL | C29-C28-C26 | -4.25 | 112.07 | 122.69 |
| 56 | DA | 3001 | DOL | O36-C37-C1 | 4.17 | 120.04 | 111.52 |
| 56 | BA | 3001 | DOL | O7-C6-N5 | -3.97 | 115.16 | 121.59 |
| 56 | DA | 3001 | DOL | C30-C29-C28 | -3.80 | 116.08 | 126.44 |
| 56 | DA | 3001 | DOL | C23-C22-C20 | -3.72 | 120.27 | 125.89 |
| 56 | DA | 3001 | DOL | C3-C2-C1 | 3.57 | 109.05 | 103.13 |
| 56 | BA | 3001 | DOL | C4-N5-C1 | -3.27 | 108.42 | 112.45 |
| 56 | BA | 3001 | DOL | C28-C26-N25 | 2.98 | 120.59 | 114.97 |
| 56 | BA | 3001 | DOL | C30-C29-C28 | -2.95 | 118.37 | 126.44 |
| 56 | DA | 3001 | DOL | O36-C32-C30 | 2.70 | 111.60 | 107.09 |
| 56 | DA | 3001 | DOL | C32-O36-C37 | 2.61 | 122.27 | 117.78 |
| 56 | DA | 3001 | DOL | O38-C37-C1 | -2.59 | 119.52 | 124.53 |
| 56 | BA | 3001 | DOL | O36-C37-C1 | 2.56 | 116.76 | 111.52 |
| 56 | DA | 3001 | DOL | C31-C30-C32 | 2.49 | 115.71 | 111.11 |
| 56 | BA | 3001 | DOL | C12-C8-C6 | -2.31 | 120.33 | 128.43 |
| 56 | BA | 3001 | DOL | C24-N25-C26 | -2.28 | 118.35 | 122.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56 | BA | 3001 | DOL | C16-C17-C19 | -2.22 | 106.93 | 111.10 |
| 56 | BA | 3001 | DOL | C31-C30-C32 | 2.13 | 115.04 | 111.11 |
| 56 | DA | 3001 | DOL | C28-C26-N25 | 2.08 | 118.89 | 114.97 |
| 56 | DA | 3001 | DOL | C1-N5-C6 | 2.04 | 128.31 | 120.88 |
| 56 | BA | 3001 | DOL | C32-O36-C37 | 2.02 | 121.25 | 117.78 |

There are no chirality outliers.

All (28) torsion outliers are listed below:

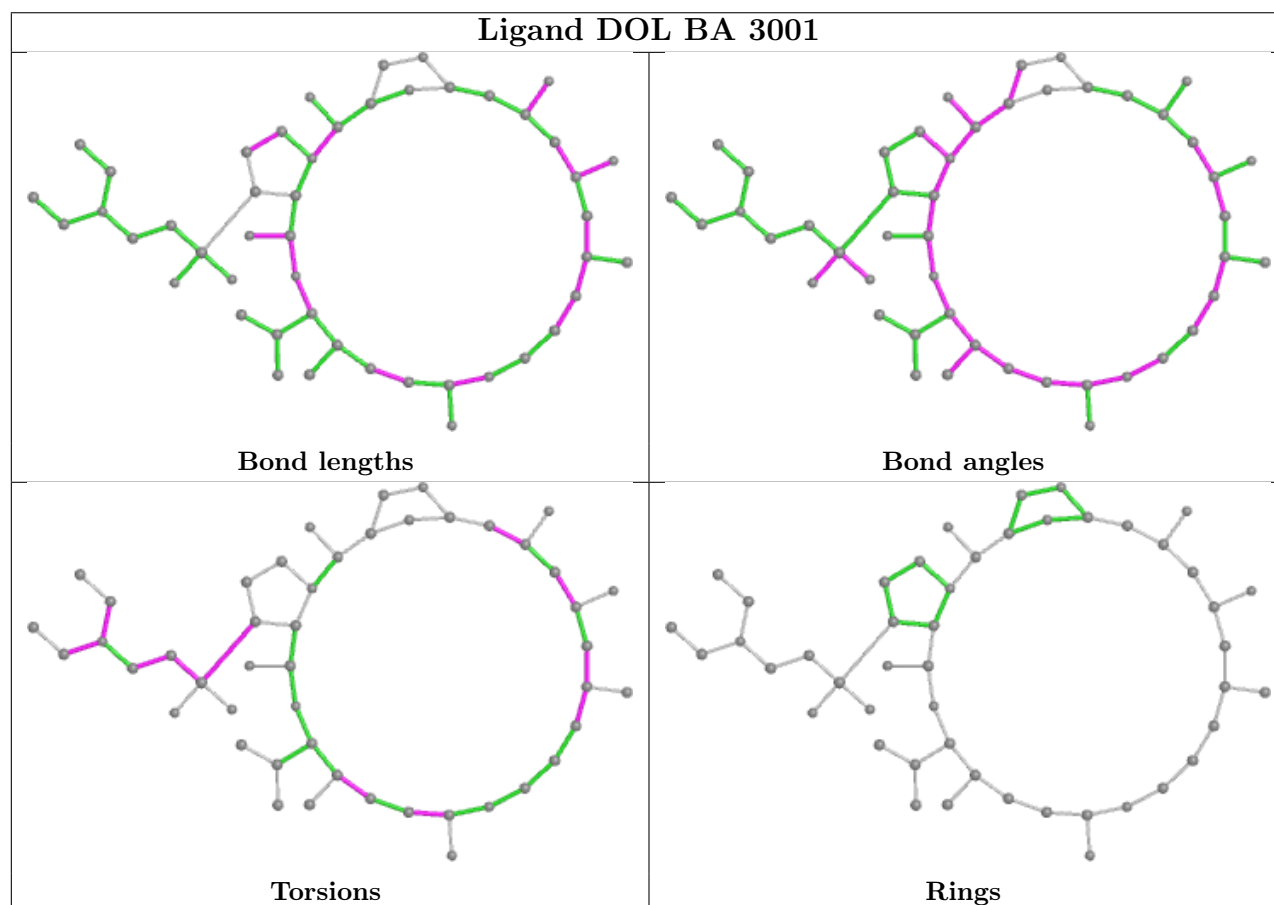
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 56 | BA | 3001 | DOL | C1-C2-S39-O40 |
| 56 | BA | 3001 | DOL | C1-C2-S39-C42 |
| 56 | BA | 3001 | DOL | S39-C42-C43-N44 |
| 56 | BA | 3001 | DOL | C14-C16-C17-O18 |
| 56 | BA | 3001 | DOL | C17-C19-C20-C22 |
| 56 | BA | 3001 | DOL | C21-C20-C22-C23 |
| 56 | DA | 3001 | DOL | C1-C2-S39-C42 |
| 56 | DA | 3001 | DOL | N25-C26-C28-C29 |
| 56 | BA | 3001 | DOL | C19-C20-C22-C23 |
| 56 | DA | 3001 | DOL | O27-C26-C28-C29 |
| 56 | DA | 3001 | DOL | C46-C45-N44-C47 |
| 56 | DA | 3001 | DOL | C28-C29-C30-C31 |
| 56 | DA | 3001 | DOL | C46-C45-N44-C43 |
| 56 | BA | 3001 | DOL | C46-C45-N44-C47 |
| 56 | BA | 3001 | DOL | C46-C45-N44-C43 |
| 56 | BA | 3001 | DOL | C48-C47-N44-C45 |
| 56 | DA | 3001 | DOL | C3-C2-S39-O40 |
| 56 | BA | 3001 | DOL | C14-C16-C17-C19 |
| 56 | BA | 3001 | DOL | C43-C42-S39-C2 |
| 56 | BA | 3001 | DOL | N25-C26-C28-C29 |
| 56 | BA | 3001 | DOL | C10-C13-C14-O15 |
| 56 | DA | 3001 | DOL | C10-C13-C14-O15 |
| 56 | BA | 3001 | DOL | C10-C13-C14-C16 |
| 56 | DA | 3001 | DOL | C10-C13-C14-C16 |
| 56 | BA | 3001 | DOL | C28-C29-C30-C31 |
| 56 | BA | 3001 | DOL | O27-C26-C28-C29 |
| 56 | BA | 3001 | DOL | C3-C2-S39-O40 |
| 56 | DA | 3001 | DOL | C42-C43-N44-C45 |

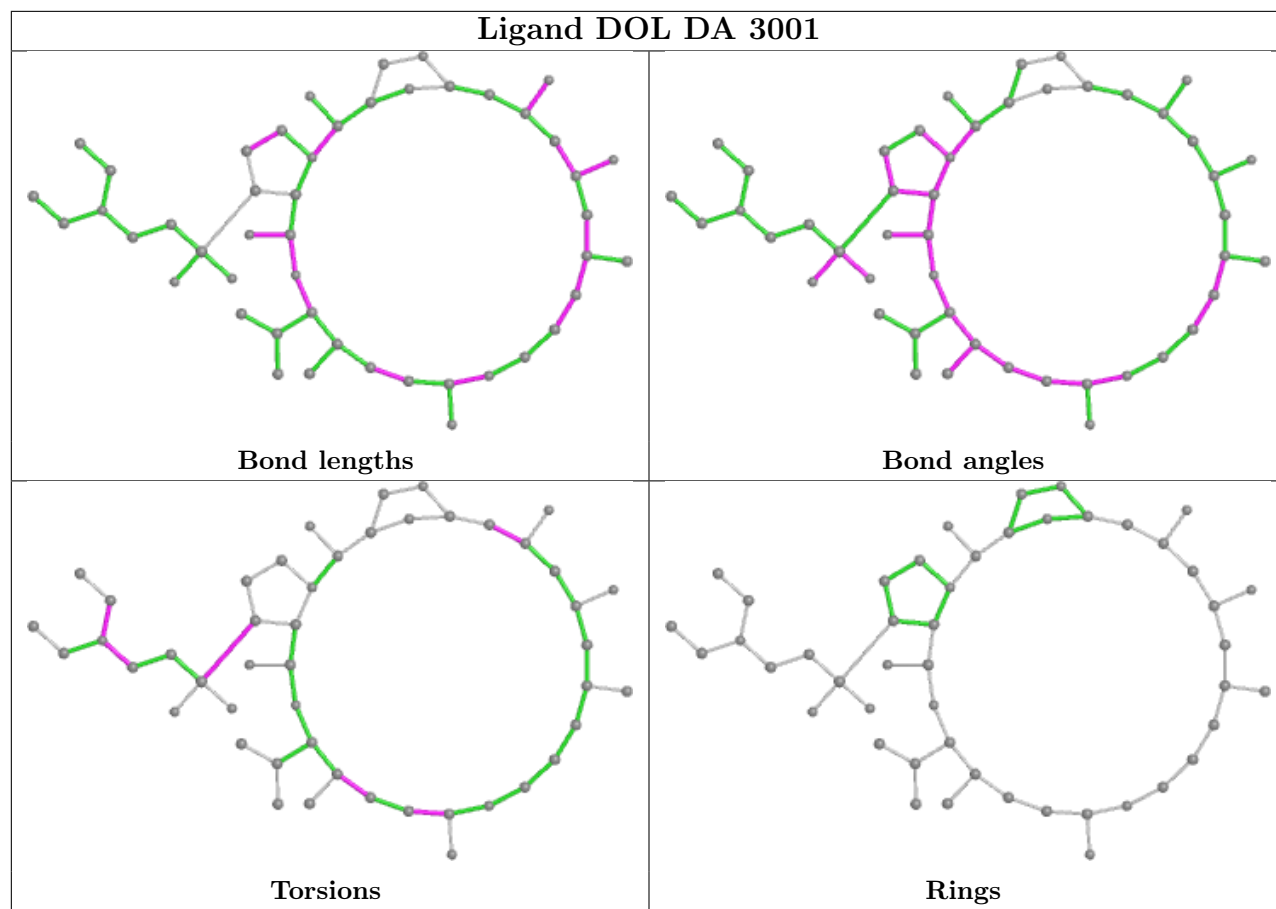
There are no ring outliers.

2 monomers are involved in 40 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56 | BA | 3001 | DOL | 15 | 0 |
| 56 | DA | 3001 | DOL | 25 | 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 | 1538/1539 (99%) | -0.16 | 22 (1%) 75 70 | 10, 49, 132, 182 | 0 |
| 1 | CA | 1539/1539 (100%) | 0.16 | 55 (3%) 42 32 | 22, 70, 146, 178 | 0 |
| 2 | AB | 218/218 (100%) | 0.80 | 29 (13%) 3 2 | 36, 73, 100, 117 | 0 |
| 2 | CB | 218/218 (100%) | 1.05 | 45 (20%) 1 0 | 57, 86, 108, 121 | 0 |
| 3 | AC | 206/206 (100%) | 0.15 | 10 (4%) 29 20 | 33, 57, 78, 95 | 0 |
| 3 | CC | 206/206 (100%) | 1.19 | 50 (24%) 0 0 | 55, 80, 96, 107 | 0 |
| 4 | AD | 205/205 (100%) | 0.36 | 8 (3%) 39 29 | 31, 56, 79, 99 | 0 |
| 4 | CD | 205/205 (100%) | -0.03 | 5 (2%) 59 49 | 13, 35, 60, 82 | 0 |
| 5 | AE | 150/150 (100%) | 0.10 | 2 (1%) 77 72 | 26, 47, 78, 93 | 0 |
| 5 | CE | 150/150 (100%) | 0.18 | 1 (0%) 87 84 | 25, 52, 84, 104 | 0 |
| 6 | AF | 100/100 (100%) | -0.18 | 1 (1%) 82 77 | 32, 54, 73, 77 | 0 |
| 6 | CF | 100/100 (100%) | 0.53 | 10 (10%) 7 4 | 41, 74, 92, 103 | 0 |
| 7 | AG | 151/151 (100%) | 0.26 | 3 (1%) 65 56 | 51, 75, 92, 100 | 0 |
| 7 | CG | 151/151 (100%) | 2.56 | 85 (56%) 0 0 | 82, 106, 114, 118 | 0 |
| 8 | AH | 129/129 (100%) | 0.18 | 2 (1%) 72 66 | 29, 46, 67, 79 | 0 |
| 8 | CH | 129/129 (100%) | 0.45 | 10 (7%) 13 7 | 46, 64, 80, 94 | 0 |
| 9 | AI | 127/127 (100%) | 0.93 | 22 (17%) 1 1 | 40, 74, 98, 107 | 0 |
| 9 | CI | 127/127 (100%) | 1.84 | 45 (35%) 0 0 | 79, 96, 112, 121 | 0 |
| 10 | AJ | 98/98 (100%) | 0.64 | 7 (7%) 16 9 | 38, 66, 86, 116 | 0 |
| 10 | CJ | 98/98 (100%) | 2.70 | 59 (60%) 0 0 | 72, 97, 115, 123 | 0 |
| 11 | AK | 117/117 (100%) | 0.49 | 10 (8%) 10 5 | 25, 60, 89, 119 | 0 |
| 11 | CK | 117/117 (100%) | 0.23 | 2 (1%) 70 63 | 35, 68, 79, 90 | 0 |
| 12 | AL | 123/123 (100%) | 0.15 | 6 (4%) 29 20 | 20, 34, 65, 97 | 0 |
| 12 | CL | 123/123 (100%) | 0.32 | 3 (2%) 59 49 | 30, 50, 74, 95 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | AM | 114/114 (100%) | 0.42 | 10 (8%) 10 5 | 47, 69, 91, 103 | 0 |
| 13 | CM | 114/114 (100%) | 3.11 | 76 (66%) 0 0 | 93, 113, 122, 125 | 0 |
| 14 | AN | 96/100 (96%) | 0.67 | 11 (11%) 4 2 | 36, 60, 96, 105 | 0 |
| 14 | CN | 96/100 (96%) | 2.16 | 44 (45%) 0 0 | 70, 96, 115, 122 | 0 |
| 15 | AO | 88/88 (100%) | 0.35 | 3 (3%) 45 35 | 29, 47, 64, 91 | 0 |
| 15 | CO | 88/88 (100%) | 0.32 | 3 (3%) 45 35 | 36, 64, 80, 102 | 0 |
| 16 | AP | 82/82 (100%) | 0.69 | 6 (7%) 15 8 | 34, 47, 83, 109 | 0 |
| 16 | CP | 82/82 (100%) | 0.98 | 11 (13%) 3 1 | 45, 62, 91, 112 | 0 |
| 17 | AQ | 80/80 (100%) | 0.26 | 3 (3%) 40 30 | 27, 48, 75, 111 | 0 |
| 17 | CQ | 80/80 (100%) | 1.14 | 19 (23%) 0 0 | 42, 77, 97, 99 | 0 |
| 18 | AR | 55/55 (100%) | 0.22 | 3 (5%) 25 16 | 40, 52, 77, 102 | 0 |
| 18 | CR | 55/55 (100%) | 0.28 | 4 (7%) 15 8 | 36, 54, 78, 108 | 0 |
| 19 | AS | 79/79 (100%) | 0.70 | 13 (16%) 1 1 | 54, 70, 88, 97 | 0 |
| 19 | CS | 79/79 (100%) | 3.96 | 58 (73%) 0 0 | 95, 114, 122, 128 | 0 |
| 20 | AT | 85/85 (100%) | 0.43 | 4 (4%) 31 22 | 35, 48, 68, 96 | 0 |
| 20 | CT | 85/85 (100%) | 1.81 | 33 (38%) 0 0 | 53, 78, 96, 101 | 0 |
| 21 | AU | 51/51 (100%) | 1.26 | 12 (23%) 0 0 | 41, 74, 95, 105 | 0 |
| 21 | CU | 51/51 (100%) | 0.68 | 6 (11%) 4 2 | 42, 69, 98, 102 | 0 |
| 22 | BA | 2897/2903 (99%) | 0.14 | 106 (3%) 41 31 | 0, 14, 129, 195 | 0 |
| 22 | DA | 2897/2903 (99%) | 0.40 | 129 (4%) 33 23 | 41, 85, 148, 181 | 0 |
| 23 | BB | 119/119 (100%) | -0.36 | 0 100 100 | 2, 23, 46, 81 | 0 |
| 23 | DB | 118/119 (99%) | 0.19 | 4 (3%) 45 35 | 69, 115, 134, 142 | 0 |
| 24 | BC | 271/271 (100%) | -0.18 | 1 (0%) 92 91 | 2, 18, 35, 55 | 0 |
| 24 | DC | 271/271 (100%) | 0.73 | 32 (11%) 4 2 | 46, 64, 77, 95 | 0 |
| 25 | BD | 209/209 (100%) | -0.25 | 0 100 100 | 0, 9, 34, 65 | 0 |
| 25 | DD | 209/209 (100%) | 1.16 | 44 (21%) 1 0 | 53, 72, 87, 97 | 0 |
| 26 | BE | 201/201 (100%) | -0.30 | 0 100 100 | 1, 23, 54, 88 | 0 |
| 26 | DE | 201/201 (100%) | 1.86 | 80 (39%) 0 0 | 52, 89, 105, 113 | 0 |
| 27 | BF | 177/177 (100%) | 0.19 | 4 (2%) 60 51 | 21, 40, 74, 88 | 0 |
| 27 | DF | 177/177 (100%) | 3.27 | 128 (72%) 0 0 | 94, 113, 124, 131 | 0 |
| 28 | BG | 176/176 (100%) | 0.04 | 3 (1%) 70 63 | 15, 35, 58, 72 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | DG | 176/176 (100%) | 2.22 | 89 (50%) 0 0 | 78, 96, 110, 121 | 0 |
| 29 | BH | 149/149 (100%) | 3.01 | 73 (48%) 0 0 | 25, 102, 121, 129 | 0 |
| 29 | DH | 149/149 (100%) | 1.18 | 30 (20%) 1 0 | 25, 92, 107, 115 | 0 |
| 30 | BI | 141/141 (100%) | 3.56 | 100 (70%) 0 0 | 89, 116, 126, 134 | 0 |
| 30 | DI | 141/141 (100%) | 4.83 | 120 (85%) 0 0 | 105, 124, 135, 142 | 0 |
| 31 | BJ | 142/142 (100%) | -0.27 | 0 100 100 | 1, 6, 26, 35 | 0 |
| 31 | DJ | 142/142 (100%) | 0.84 | 16 (11%) 5 3 | 49, 69, 83, 91 | 0 |
| 32 | BK | 122/122 (100%) | -0.34 | 0 100 100 | 3, 11, 28, 60 | 0 |
| 32 | DK | 122/122 (100%) | 1.12 | 29 (23%) 0 0 | 48, 66, 84, 95 | 0 |
| 33 | BL | 143/143 (100%) | -0.13 | 0 100 100 | 1, 18, 42, 65 | 0 |
| 33 | DL | 143/143 (100%) | 1.95 | 62 (43%) 0 0 | 43, 87, 98, 115 | 0 |
| 34 | BM | 136/136 (100%) | -0.38 | 0 100 100 | 1, 10, 24, 85 | 0 |
| 34 | DM | 136/136 (100%) | 1.01 | 26 (19%) 1 1 | 44, 70, 85, 99 | 0 |
| 35 | BN | 120/120 (100%) | -0.25 | 0 100 100 | 2, 7, 17, 65 | 0 |
| 35 | DN | 120/120 (100%) | 1.29 | 28 (23%) 0 0 | 58, 78, 92, 112 | 0 |
| 36 | BO | 116/116 (100%) | -0.21 | 0 100 100 | 14, 24, 42, 54 | 0 |
| 36 | DO | 116/116 (100%) | 2.77 | 75 (64%) 0 0 | 85, 99, 110, 117 | 0 |
| 37 | BP | 114/114 (100%) | -0.22 | 1 (0%) 84 80 | 6, 16, 41, 71 | 0 |
| 37 | DP | 114/114 (100%) | 1.07 | 27 (23%) 0 0 | 61, 74, 86, 94 | 0 |
| 38 | BQ | 117/117 (100%) | -0.31 | 0 100 100 | 0, 3, 12, 30 | 0 |
| 38 | DQ | 117/117 (100%) | 1.15 | 25 (21%) 0 0 | 55, 70, 81, 89 | 0 |
| 39 | BR | 103/103 (100%) | -0.29 | 0 100 100 | 0, 11, 31, 56 | 0 |
| 39 | DR | 103/103 (100%) | 1.66 | 35 (33%) 0 0 | 57, 80, 92, 103 | 0 |
| 40 | BS | 110/110 (100%) | -0.22 | 0 100 100 | 1, 4, 21, 68 | 0 |
| 40 | DS | 110/110 (100%) | 2.12 | 53 (48%) 0 0 | 60, 79, 94, 105 | 0 |
| 41 | BT | 93/93 (100%) | 0.19 | 3 (3%) 47 37 | 10, 24, 68, 98 | 0 |
| 41 | DT | 93/93 (100%) | 2.71 | 57 (61%) 0 0 | 73, 91, 106, 115 | 0 |
| 42 | BU | 102/102 (100%) | -0.22 | 2 (1%) 65 56 | 10, 25, 58, 77 | 0 |
| 42 | DU | 102/102 (100%) | 3.20 | 65 (63%) 0 0 | 77, 95, 109, 120 | 0 |
| 43 | BV | 94/94 (100%) | -0.27 | 0 100 100 | 4, 18, 39, 52 | 0 |
| 43 | DV | 94/94 (100%) | 1.14 | 21 (22%) 0 0 | 72, 86, 98, 105 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BW | 76/76 (100%) | -0.15 | 2 (2%) 56 46 | 4, 11, 27, 57 | 0 |
| 44 | DW | 75/76 (98%) | 2.04 | 39 (52%) 0 0 | 58, 83, 93, 104 | 0 |
| 45 | BX | 77/77 (100%) | -0.24 | 0 100 100 | 8, 22, 48, 68 | 0 |
| 45 | DX | 77/77 (100%) | 1.11 | 15 (19%) 1 0 | 47, 72, 87, 91 | 0 |
| 46 | BY | 63/63 (100%) | 0.23 | 3 (4%) 30 21 | 18, 38, 71, 94 | 0 |
| 46 | DY | 63/63 (100%) | 1.95 | 30 (47%) 0 0 | 81, 99, 106, 109 | 0 |
| 47 | BZ | 58/58 (100%) | -0.22 | 0 100 100 | 2, 6, 25, 34 | 0 |
| 47 | DZ | 58/58 (100%) | 0.83 | 7 (12%) 4 2 | 60, 73, 85, 103 | 0 |
| 48 | B0 | 56/56 (100%) | -0.30 | 0 100 100 | 0, 7, 33, 60 | 0 |
| 48 | D0 | 56/56 (100%) | 1.49 | 17 (30%) 0 0 | 51, 82, 95, 103 | 0 |
| 49 | B1 | 50/50 (100%) | -0.23 | 1 (2%) 65 56 | 13, 25, 49, 57 | 0 |
| 49 | D1 | 50/50 (100%) | 1.73 | 15 (30%) 0 0 | 73, 89, 94, 106 | 0 |
| 50 | B2 | 46/46 (100%) | -0.14 | 1 (2%) 62 52 | 4, 8, 15, 79 | 0 |
| 50 | D2 | 46/46 (100%) | 1.94 | 19 (41%) 0 0 | 58, 72, 86, 101 | 0 |
| 51 | B3 | 64/64 (100%) | -0.18 | 0 100 100 | 4, 9, 17, 29 | 0 |
| 51 | D3 | 64/64 (100%) | 1.69 | 26 (40%) 0 0 | 60, 75, 84, 94 | 0 |
| 52 | B4 | 38/38 (100%) | -0.13 | 0 100 100 | 5, 15, 29, 52 | 0 |
| 52 | D4 | 38/38 (100%) | 2.23 | 18 (47%) 0 0 | 62, 77, 88, 98 | 0 |
| 53 | B5 | 191/228 (83%) | 6.24 | 186 (97%) 0 0 | 100, 121, 133, 141 | 0 |
| 54 | B6 | 2/8 (25%) | 0.45 | 0 100 100 | 1, 1, 1, 1 | 0 |
| 54 | D6 | 2/8 (25%) | -0.02 | 0 100 100 | 46, 46, 46, 51 | 0 |
| All | All | 20738/20810 (99%) | 0.62 | 2658 (12%) 3 2 | 0, 63, 124, 195 | 0 |

All (2658) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | BI | 53 | LEU | 25.2 |
| 53 | B5 | 55 | SER | 19.9 |
| 22 | BA | 2101 | A | 17.4 |
| 22 | BA | 2184 | A | 17.4 |
| 53 | B5 | 207 | GLY | 16.3 |
| 22 | BA | 2185 | U | 16.2 |
| 10 | AJ | 102 | LEU | 16.0 |
| 29 | BH | 130 | VAL | 14.7 |
| 30 | DI | 6 | GLN | 14.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | B5 | 223 | VAL | 14.3 |
| 53 | B5 | 48 | LEU | 14.1 |
| 7 | CG | 62 | PHE | 14.1 |
| 29 | BH | 97 | ARG | 13.9 |
| 22 | BA | 2100 | G | 13.6 |
| 22 | BA | 2102 | G | 13.4 |
| 30 | DI | 68 | THR | 13.2 |
| 22 | BA | 2159 | G | 13.1 |
| 22 | BA | 2135 | A | 12.8 |
| 1 | CA | 1536 | C | 12.6 |
| 30 | DI | 67 | PHE | 12.6 |
| 22 | BA | 2183 | A | 12.6 |
| 29 | BH | 102 | ALA | 12.5 |
| 53 | B5 | 111 | PHE | 12.4 |
| 22 | BA | 2103 | C | 12.3 |
| 29 | BH | 96 | THR | 12.2 |
| 1 | AA | 1535 | C | 12.1 |
| 53 | B5 | 208 | THR | 12.1 |
| 20 | CT | 4 | ILE | 12.1 |
| 22 | BA | 2148 | G | 11.9 |
| 2 | AB | 157 | LEU | 11.9 |
| 53 | B5 | 218 | THR | 11.8 |
| 22 | BA | 2147 | A | 11.8 |
| 22 | BA | 2139 | U | 11.6 |
| 53 | B5 | 157 | ILE | 11.6 |
| 53 | B5 | 66 | PRO | 11.6 |
| 29 | BH | 113 | SER | 11.4 |
| 22 | BA | 2104 | C | 11.3 |
| 22 | BA | 2160 | C | 11.3 |
| 30 | DI | 66 | SER | 11.2 |
| 53 | B5 | 173 | HIS | 11.2 |
| 53 | B5 | 140 | ASN | 11.2 |
| 30 | DI | 58 | VAL | 11.1 |
| 53 | B5 | 122 | GLY | 11.1 |
| 42 | DU | 36 | VAL | 11.0 |
| 53 | B5 | 62 | THR | 11.0 |
| 53 | B5 | 183 | PRO | 10.9 |
| 22 | BA | 2138 | G | 10.8 |
| 30 | BI | 2 | ALA | 10.8 |
| 22 | BA | 2158 | A | 10.7 |
| 22 | BA | 2140 | G | 10.7 |
| 36 | DO | 40 | ILE | 10.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 53 | B5 | 224 | ARG | 10.7 |
| 53 | B5 | 108 | TRP | 10.7 |
| 30 | BI | 3 | LYS | 10.7 |
| 53 | B5 | 52 | PRO | 10.5 |
| 53 | B5 | 131 | ILE | 10.5 |
| 19 | CS | 66 | MET | 10.4 |
| 53 | B5 | 67 | HIS | 10.4 |
| 53 | B5 | 50 | ILE | 10.3 |
| 53 | B5 | 206 | LYS | 10.2 |
| 53 | B5 | 198 | GLU | 10.2 |
| 22 | BA | 2165 | C | 10.2 |
| 22 | BA | 2143 | C | 10.2 |
| 30 | DI | 59 | ILE | 10.1 |
| 42 | DU | 26 | LYS | 10.1 |
| 53 | B5 | 217 | THR | 10.1 |
| 22 | BA | 2174 | C | 10.1 |
| 22 | BA | 2136 | G | 10.0 |
| 53 | B5 | 59 | VAL | 10.0 |
| 27 | DF | 156 | ILE | 10.0 |
| 30 | DI | 4 | LYS | 10.0 |
| 30 | DI | 69 | PHE | 9.9 |
| 22 | DA | 1175 | A | 9.9 |
| 22 | BA | 2156 | G | 9.9 |
| 22 | BA | 2145 | C | 9.8 |
| 30 | DI | 3 | LYS | 9.8 |
| 29 | BH | 146 | VAL | 9.8 |
| 53 | B5 | 182 | PRO | 9.8 |
| 19 | CS | 37 | ARG | 9.8 |
| 29 | BH | 69 | ALA | 9.6 |
| 13 | CM | 84 | GLY | 9.6 |
| 19 | CS | 24 | GLU | 9.6 |
| 22 | BA | 2117 | A | 9.6 |
| 4 | CD | 25 | VAL | 9.5 |
| 27 | DF | 130 | MET | 9.5 |
| 30 | BI | 79 | LEU | 9.4 |
| 22 | BA | 2144 | G | 9.4 |
| 19 | CS | 74 | PHE | 9.4 |
| 53 | B5 | 106 | ASP | 9.3 |
| 27 | DF | 129 | SER | 9.2 |
| 53 | B5 | 181 | PHE | 9.1 |
| 30 | BI | 67 | PHE | 9.1 |
| 29 | BH | 136 | SER | 9.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | DL | 92 | LEU | 9.1 |
| 30 | BI | 13 | VAL | 9.1 |
| 22 | BA | 2142 | A | 9.1 |
| 27 | DF | 128 | TYR | 9.1 |
| 42 | DU | 60 | GLU | 9.0 |
| 22 | BA | 2182 | U | 9.0 |
| 9 | CI | 128 | SER | 9.0 |
| 22 | BA | 2177 | C | 9.0 |
| 29 | BH | 112 | LYS | 9.0 |
| 1 | CA | 1539 | C | 9.0 |
| 30 | BI | 68 | THR | 9.0 |
| 36 | DO | 24 | THR | 9.0 |
| 53 | B5 | 199 | ALA | 8.9 |
| 30 | BI | 12 | GLN | 8.9 |
| 22 | BA | 2099 | U | 8.9 |
| 1 | AA | 1536 | C | 8.9 |
| 53 | B5 | 134 | PRO | 8.8 |
| 22 | BA | 2178 | C | 8.8 |
| 22 | BA | 2155 | U | 8.7 |
| 22 | BA | 2157 | G | 8.7 |
| 19 | CS | 67 | VAL | 8.7 |
| 41 | DT | 34 | VAL | 8.7 |
| 53 | B5 | 107 | GLY | 8.7 |
| 30 | BI | 4 | LYS | 8.7 |
| 30 | DI | 2 | ALA | 8.7 |
| 22 | BA | 2161 | C | 8.7 |
| 53 | B5 | 53 | ARG | 8.7 |
| 22 | BA | 2141 | G | 8.7 |
| 1 | CA | 1535 | C | 8.6 |
| 53 | B5 | 156 | GLU | 8.6 |
| 53 | B5 | 20 | VAL | 8.6 |
| 27 | DF | 155 | THR | 8.6 |
| 53 | B5 | 147 | GLY | 8.6 |
| 30 | DI | 53 | LEU | 8.6 |
| 41 | DT | 15 | HIS | 8.6 |
| 29 | BH | 105 | ALA | 8.5 |
| 30 | DI | 42 | PHE | 8.5 |
| 30 | DI | 11 | LEU | 8.5 |
| 53 | B5 | 68 | GLY | 8.4 |
| 53 | B5 | 174 | ALA | 8.4 |
| 2 | AB | 156 | GLY | 8.4 |
| 42 | DU | 78 | GLY | 8.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 10 | CJ | 77 | VAL | 8.4 |
| 30 | BI | 5 | VAL | 8.4 |
| 29 | BH | 106 | ALA | 8.4 |
| 30 | DI | 60 | THR | 8.4 |
| 22 | BA | 2115 | G | 8.3 |
| 53 | B5 | 96 | GLY | 8.3 |
| 53 | B5 | 95 | VAL | 8.3 |
| 22 | BA | 2127 | G | 8.3 |
| 19 | CS | 30 | PRO | 8.2 |
| 53 | B5 | 45 | HIS | 8.2 |
| 22 | BA | 2162 | G | 8.2 |
| 7 | CG | 66 | LEU | 8.2 |
| 41 | DT | 43 | ILE | 8.2 |
| 29 | BH | 98 | ASP | 8.2 |
| 22 | BA | 2150 | C | 8.2 |
| 19 | CS | 60 | VAL | 8.2 |
| 42 | DU | 52 | LEU | 8.2 |
| 30 | BI | 41 | ALA | 8.1 |
| 30 | BI | 11 | LEU | 8.1 |
| 53 | B5 | 70 | GLY | 8.1 |
| 42 | DU | 25 | VAL | 8.1 |
| 30 | BI | 69 | PHE | 8.1 |
| 30 | DI | 85 | GLY | 8.0 |
| 10 | CJ | 74 | VAL | 8.0 |
| 19 | CS | 39 | THR | 8.0 |
| 22 | BA | 2123 | G | 8.0 |
| 22 | BA | 2175 | C | 8.0 |
| 53 | B5 | 143 | ALA | 8.0 |
| 14 | CN | 36 | ALA | 8.0 |
| 29 | BH | 115 | VAL | 8.0 |
| 53 | B5 | 219 | MET | 8.0 |
| 16 | AP | 81 | ALA | 7.9 |
| 53 | B5 | 194 | ILE | 7.9 |
| 53 | B5 | 76 | LEU | 7.9 |
| 29 | BH | 68 | ARG | 7.9 |
| 52 | D4 | 10 | LEU | 7.9 |
| 30 | DI | 46 | THR | 7.9 |
| 53 | B5 | 180 | SER | 7.9 |
| 30 | DI | 80 | LEU | 7.8 |
| 27 | DF | 35 | THR | 7.8 |
| 7 | CG | 18 | PHE | 7.8 |
| 29 | BH | 148 | ALA | 7.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 19 | CS | 44 | MET | 7.8 |
| 1 | CA | 1537 | U | 7.8 |
| 22 | BA | 2124 | G | 7.8 |
| 30 | DI | 13 | VAL | 7.8 |
| 29 | BH | 144 | VAL | 7.8 |
| 30 | BI | 54 | PRO | 7.8 |
| 53 | B5 | 109 | MET | 7.7 |
| 29 | BH | 120 | GLY | 7.7 |
| 40 | DS | 92 | ARG | 7.7 |
| 9 | CI | 43 | THR | 7.7 |
| 53 | B5 | 158 | LYS | 7.7 |
| 42 | DU | 51 | ALA | 7.7 |
| 16 | CP | 47 | GLU | 7.7 |
| 53 | B5 | 200 | HIS | 7.7 |
| 53 | B5 | 221 | PRO | 7.6 |
| 9 | CI | 130 | ARG | 7.6 |
| 22 | BA | 2179 | C | 7.6 |
| 53 | B5 | 61 | GLY | 7.6 |
| 7 | CG | 39 | ALA | 7.6 |
| 33 | DL | 144 | GLU | 7.6 |
| 22 | BA | 2116 | G | 7.6 |
| 30 | DI | 7 | ALA | 7.5 |
| 22 | BA | 2163 | A | 7.5 |
| 22 | BA | 2176 | A | 7.5 |
| 53 | B5 | 77 | ALA | 7.5 |
| 53 | B5 | 203 | GLU | 7.5 |
| 50 | D2 | 42 | LEU | 7.5 |
| 19 | CS | 43 | ASN | 7.5 |
| 53 | B5 | 214 | TYR | 7.5 |
| 27 | DF | 67 | ILE | 7.5 |
| 53 | B5 | 212 | SER | 7.5 |
| 28 | DG | 43 | VAL | 7.5 |
| 47 | DZ | 2 | ALA | 7.5 |
| 30 | DI | 52 | GLY | 7.4 |
| 53 | B5 | 73 | VAL | 7.4 |
| 30 | BI | 87 | LYS | 7.4 |
| 53 | B5 | 148 | PHE | 7.4 |
| 41 | DT | 2 | ILE | 7.4 |
| 53 | B5 | 132 | LEU | 7.4 |
| 30 | DI | 34 | ASN | 7.4 |
| 22 | BA | 2121 | G | 7.4 |
| 22 | BA | 2169 | A | 7.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 30 | DI | 48 | SER | 7.3 |
| 22 | BA | 2166 | U | 7.3 |
| 30 | DI | 70 | VAL | 7.3 |
| 30 | DI | 22 | PRO | 7.3 |
| 22 | DA | 1537 | G | 7.3 |
| 53 | B5 | 225 | ILE | 7.3 |
| 9 | AI | 130 | ARG | 7.3 |
| 22 | BA | 2113 | U | 7.3 |
| 42 | DU | 39 | ILE | 7.3 |
| 22 | BA | 2149 | U | 7.3 |
| 22 | BA | 2172 | U | 7.3 |
| 53 | B5 | 196 | ALA | 7.3 |
| 13 | CM | 63 | PHE | 7.2 |
| 19 | CS | 71 | LEU | 7.2 |
| 13 | CM | 96 | PRO | 7.2 |
| 22 | BA | 2173 | A | 7.2 |
| 30 | DI | 120 | ALA | 7.2 |
| 35 | DN | 28 | LEU | 7.2 |
| 42 | DU | 89 | ASP | 7.2 |
| 30 | DI | 63 | ALA | 7.1 |
| 53 | B5 | 84 | ILE | 7.1 |
| 29 | BH | 91 | PHE | 7.1 |
| 15 | AO | 89 | ARG | 7.1 |
| 33 | DL | 121 | THR | 7.1 |
| 53 | B5 | 205 | ALA | 7.1 |
| 53 | B5 | 141 | PRO | 7.1 |
| 13 | CM | 86 | TYR | 7.1 |
| 53 | B5 | 169 | THR | 7.1 |
| 53 | B5 | 165 | ARG | 7.0 |
| 46 | BY | 63 | ALA | 7.0 |
| 53 | B5 | 170 | GLY | 7.0 |
| 53 | B5 | 171 | ALA | 7.0 |
| 48 | D0 | 27 | SER | 7.0 |
| 33 | DL | 101 | ILE | 7.0 |
| 53 | B5 | 87 | ALA | 7.0 |
| 29 | BH | 110 | VAL | 7.0 |
| 22 | BA | 2120 | G | 7.0 |
| 22 | BA | 2152 | G | 6.9 |
| 53 | B5 | 27 | ALA | 6.9 |
| 16 | AP | 80 | LYS | 6.9 |
| 7 | CG | 15 | ASP | 6.9 |
| 7 | CG | 43 | VAL | 6.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | BH | 55 | GLU | 6.9 |
| 45 | DX | 49 | LEU | 6.9 |
| 41 | DT | 55 | VAL | 6.8 |
| 44 | DW | 38 | VAL | 6.8 |
| 7 | CG | 59 | LEU | 6.8 |
| 53 | B5 | 64 | SER | 6.8 |
| 53 | B5 | 97 | GLY | 6.8 |
| 30 | DI | 54 | PRO | 6.8 |
| 27 | DF | 39 | GLY | 6.8 |
| 42 | DU | 77 | THR | 6.8 |
| 30 | DI | 76 | ALA | 6.8 |
| 29 | BH | 101 | ASP | 6.8 |
| 30 | DI | 24 | VAL | 6.8 |
| 53 | B5 | 100 | ILE | 6.8 |
| 27 | DF | 91 | LEU | 6.7 |
| 22 | BA | 2153 | C | 6.7 |
| 22 | BA | 2112 | G | 6.7 |
| 53 | B5 | 72 | GLN | 6.7 |
| 30 | DI | 61 | VAL | 6.7 |
| 27 | DF | 66 | LEU | 6.7 |
| 29 | BH | 54 | LEU | 6.7 |
| 53 | B5 | 161 | ARG | 6.6 |
| 42 | DU | 35 | ILE | 6.6 |
| 9 | CI | 129 | LYS | 6.6 |
| 53 | B5 | 94 | TYR | 6.6 |
| 28 | DG | 103 | ILE | 6.6 |
| 36 | DO | 26 | LEU | 6.6 |
| 10 | CJ | 45 | ARG | 6.6 |
| 33 | DL | 73 | ILE | 6.6 |
| 19 | CS | 42 | PRO | 6.5 |
| 1 | CA | 209 | U | 6.5 |
| 53 | B5 | 86 | GLU | 6.5 |
| 27 | DF | 65 | PRO | 6.5 |
| 30 | DI | 47 | ASP | 6.5 |
| 42 | DU | 12 | ILE | 6.5 |
| 53 | B5 | 167 | ASP | 6.5 |
| 53 | B5 | 78 | ILE | 6.5 |
| 2 | CB | 161 | LEU | 6.5 |
| 53 | B5 | 142 | LYS | 6.5 |
| 19 | CS | 63 | THR | 6.5 |
| 1 | AA | 1538 | C | 6.4 |
| 42 | DU | 62 | GLU | 6.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | DU | 31 | SER | 6.4 |
| 19 | CS | 49 | ILE | 6.4 |
| 7 | CG | 75 | VAL | 6.4 |
| 22 | BA | 2111 | U | 6.4 |
| 53 | B5 | 69 | LEU | 6.4 |
| 53 | B5 | 179 | ALA | 6.4 |
| 13 | CM | 98 | ARG | 6.4 |
| 27 | DF | 170 | LEU | 6.4 |
| 41 | DT | 10 | VAL | 6.4 |
| 30 | DI | 78 | VAL | 6.4 |
| 30 | BI | 22 | PRO | 6.4 |
| 10 | CJ | 87 | LEU | 6.4 |
| 22 | BA | 2110 | G | 6.4 |
| 27 | DF | 86 | GLY | 6.4 |
| 4 | AD | 36 | GLN | 6.4 |
| 29 | BH | 87 | GLU | 6.4 |
| 9 | AI | 129 | LYS | 6.3 |
| 41 | DT | 8 | LEU | 6.3 |
| 30 | BI | 101 | ILE | 6.3 |
| 19 | CS | 15 | LEU | 6.3 |
| 22 | BA | 2105 | U | 6.3 |
| 27 | DF | 122 | PHE | 6.3 |
| 1 | CA | 1032 | G | 6.3 |
| 22 | BA | 2107 | G | 6.3 |
| 30 | DI | 32 | GLY | 6.3 |
| 30 | BI | 114 | ALA | 6.3 |
| 30 | BI | 55 | ILE | 6.3 |
| 27 | DF | 21 | ASN | 6.3 |
| 22 | BA | 2114 | A | 6.3 |
| 26 | DE | 119 | ILE | 6.3 |
| 53 | B5 | 166 | ASN | 6.3 |
| 36 | DO | 51 | ALA | 6.3 |
| 14 | CN | 47 | LYS | 6.3 |
| 30 | BI | 17 | MET | 6.2 |
| 30 | DI | 18 | ALA | 6.2 |
| 22 | BA | 2130 | U | 6.2 |
| 50 | B2 | 46 | LYS | 6.2 |
| 53 | B5 | 110 | ASP | 6.2 |
| 22 | DA | 1536 | C | 6.2 |
| 30 | DI | 82 | LYS | 6.2 |
| 53 | B5 | 197 | LEU | 6.2 |
| 53 | B5 | 204 | GLY | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | DE | 175 | ILE | 6.2 |
| 30 | DI | 55 | ILE | 6.2 |
| 22 | BA | 2125 | G | 6.1 |
| 30 | DI | 8 | TYR | 6.1 |
| 8 | AH | 2 | SER | 6.1 |
| 53 | B5 | 162 | ILE | 6.1 |
| 28 | DG | 9 | VAL | 6.1 |
| 30 | DI | 20 | PRO | 6.1 |
| 30 | BI | 66 | SER | 6.1 |
| 29 | BH | 67 | ALA | 6.1 |
| 36 | DO | 25 | ARG | 6.1 |
| 19 | CS | 40 | ILE | 6.1 |
| 27 | DF | 85 | ILE | 6.1 |
| 53 | B5 | 85 | LYS | 6.1 |
| 22 | BA | 2137 | U | 6.1 |
| 13 | CM | 95 | LEU | 6.1 |
| 26 | DE | 143 | LEU | 6.1 |
| 28 | DG | 32 | GLU | 6.1 |
| 53 | B5 | 149 | ASN | 6.1 |
| 21 | CU | 38 | TYR | 6.1 |
| 30 | DI | 41 | ALA | 6.1 |
| 30 | DI | 139 | VAL | 6.1 |
| 53 | B5 | 155 | ARG | 6.1 |
| 29 | DH | 136 | SER | 6.1 |
| 53 | B5 | 160 | GLY | 6.1 |
| 28 | DG | 45 | HIS | 6.1 |
| 14 | CN | 2 | ALA | 6.1 |
| 53 | B5 | 46 | ALA | 6.1 |
| 53 | B5 | 195 | ARG | 6.1 |
| 2 | CB | 67 | ILE | 6.1 |
| 1 | CA | 94 | G | 6.1 |
| 22 | BA | 2168 | G | 6.1 |
| 7 | AG | 5 | ARG | 6.0 |
| 13 | CM | 45 | ILE | 6.0 |
| 27 | DF | 117 | LEU | 6.0 |
| 49 | D1 | 36 | LEU | 6.0 |
| 40 | DS | 40 | ASN | 6.0 |
| 50 | D2 | 33 | ARG | 6.0 |
| 27 | DF | 23 | ASN | 6.0 |
| 27 | DF | 54 | ALA | 6.0 |
| 27 | DF | 154 | ILE | 6.0 |
| 29 | BH | 109 | GLU | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | B5 | 213 | VAL | 6.0 |
| 29 | BH | 85 | GLY | 6.0 |
| 29 | DH | 142 | VAL | 6.0 |
| 30 | DI | 15 | ALA | 6.0 |
| 22 | BA | 2118 | U | 6.0 |
| 29 | BH | 72 | ILE | 6.0 |
| 29 | BH | 121 | VAL | 6.0 |
| 28 | DG | 2 | SER | 6.0 |
| 7 | CG | 17 | LYS | 5.9 |
| 29 | BH | 86 | ASP | 5.9 |
| 10 | CJ | 10 | LEU | 5.9 |
| 13 | CM | 85 | CYS | 5.9 |
| 22 | BA | 2154 | A | 5.9 |
| 53 | B5 | 146 | VAL | 5.9 |
| 20 | CT | 81 | ALA | 5.9 |
| 19 | CS | 47 | LEU | 5.9 |
| 30 | BI | 71 | THR | 5.9 |
| 1 | AA | 1539 | C | 5.9 |
| 13 | CM | 47 | GLU | 5.9 |
| 16 | CP | 80 | LYS | 5.9 |
| 19 | CS | 29 | LYS | 5.9 |
| 7 | CG | 53 | ARG | 5.9 |
| 22 | BA | 2134 | A | 5.8 |
| 27 | DF | 93 | GLY | 5.9 |
| 13 | CM | 69 | LEU | 5.8 |
| 53 | B5 | 145 | THR | 5.8 |
| 27 | DF | 89 | VAL | 5.8 |
| 9 | AI | 43 | THR | 5.8 |
| 28 | DG | 33 | LEU | 5.8 |
| 53 | B5 | 65 | LEU | 5.8 |
| 42 | DU | 63 | ALA | 5.8 |
| 30 | DI | 130 | GLU | 5.8 |
| 16 | CP | 39 | PHE | 5.8 |
| 29 | BH | 123 | ARG | 5.8 |
| 42 | DU | 87 | PHE | 5.8 |
| 53 | B5 | 58 | ASN | 5.8 |
| 1 | CA | 1534 | A | 5.8 |
| 7 | CG | 151 | PHE | 5.8 |
| 30 | DI | 121 | ASP | 5.8 |
| 22 | BA | 2164 | C | 5.8 |
| 40 | DS | 3 | THR | 5.8 |
| 41 | DT | 76 | ARG | 5.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 49 | D1 | 53 | LYS | 5.8 |
| 53 | B5 | 54 | ARG | 5.8 |
| 30 | DI | 39 | CYS | 5.8 |
| 41 | DT | 42 | GLU | 5.8 |
| 46 | DY | 59 | GLU | 5.7 |
| 36 | DO | 107 | ALA | 5.7 |
| 10 | CJ | 73 | LEU | 5.7 |
| 30 | DI | 21 | SER | 5.7 |
| 53 | B5 | 81 | GLY | 5.7 |
| 53 | B5 | 42 | VAL | 5.7 |
| 13 | CM | 103 | LYS | 5.7 |
| 19 | CS | 31 | LEU | 5.7 |
| 27 | DF | 113 | ASP | 5.7 |
| 30 | DI | 35 | ILE | 5.7 |
| 1 | CA | 1538 | C | 5.7 |
| 28 | DG | 102 | VAL | 5.7 |
| 53 | B5 | 130 | ARG | 5.7 |
| 7 | CG | 16 | PRO | 5.7 |
| 1 | CA | 1030 | U | 5.7 |
| 29 | DH | 12 | LEU | 5.7 |
| 48 | D0 | 26 | THR | 5.7 |
| 30 | DI | 5 | VAL | 5.7 |
| 30 | DI | 75 | PRO | 5.7 |
| 44 | DW | 63 | ALA | 5.6 |
| 53 | B5 | 209 | PHE | 5.6 |
| 12 | AL | 124 | ALA | 5.6 |
| 22 | BA | 2126 | A | 5.6 |
| 40 | DS | 84 | ARG | 5.6 |
| 28 | DG | 105 | LEU | 5.6 |
| 21 | AU | 38 | TYR | 5.6 |
| 30 | BI | 8 | TYR | 5.6 |
| 29 | DH | 47 | PHE | 5.6 |
| 33 | DL | 89 | VAL | 5.6 |
| 30 | DI | 31 | GLN | 5.6 |
| 6 | CF | 91 | ARG | 5.6 |
| 53 | B5 | 123 | ALA | 5.6 |
| 13 | CM | 83 | LEU | 5.6 |
| 42 | DU | 32 | GLY | 5.6 |
| 42 | DU | 20 | GLY | 5.6 |
| 53 | B5 | 98 | GLU | 5.6 |
| 30 | BI | 52 | GLY | 5.6 |
| 53 | B5 | 104 | ILE | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | DT | 71 | GLY | 5.6 |
| 27 | DF | 32 | GLU | 5.6 |
| 30 | DI | 98 | VAL | 5.5 |
| 29 | DH | 6 | LEU | 5.5 |
| 19 | CS | 12 | ASP | 5.5 |
| 33 | DL | 70 | LYS | 5.5 |
| 19 | CS | 41 | PHE | 5.5 |
| 27 | DF | 152 | LEU | 5.5 |
| 9 | CI | 68 | LYS | 5.5 |
| 30 | BI | 135 | SER | 5.5 |
| 42 | DU | 50 | PRO | 5.5 |
| 32 | DK | 68 | GLY | 5.5 |
| 30 | DI | 62 | TYR | 5.5 |
| 21 | CU | 35 | ARG | 5.5 |
| 36 | DO | 117 | PHE | 5.5 |
| 30 | DI | 83 | ALA | 5.5 |
| 49 | D1 | 47 | VAL | 5.5 |
| 22 | BA | 138 | U | 5.5 |
| 1 | AA | 1030 | U | 5.5 |
| 29 | BH | 119 | ASN | 5.4 |
| 14 | AN | 30 | ILE | 5.4 |
| 14 | CN | 51 | LEU | 5.4 |
| 26 | DE | 13 | THR | 5.4 |
| 26 | DE | 128 | ALA | 5.4 |
| 13 | CM | 70 | ARG | 5.4 |
| 30 | BI | 38 | PHE | 5.4 |
| 53 | B5 | 121 | MET | 5.4 |
| 41 | DT | 81 | LYS | 5.4 |
| 14 | AN | 21 | PHE | 5.4 |
| 53 | B5 | 210 | LEU | 5.4 |
| 44 | DW | 25 | ARG | 5.4 |
| 30 | DI | 79 | LEU | 5.4 |
| 36 | DO | 41 | ALA | 5.4 |
| 53 | B5 | 39 | ASP | 5.4 |
| 29 | BH | 58 | LEU | 5.4 |
| 28 | DG | 92 | VAL | 5.4 |
| 30 | BI | 58 | VAL | 5.4 |
| 1 | AA | 78 | A | 5.4 |
| 13 | CM | 12 | HIS | 5.4 |
| 22 | BA | 2181 | U | 5.4 |
| 25 | DD | 60 | VAL | 5.4 |
| 40 | DS | 36 | LEU | 5.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 52 | D4 | 25 | VAL | 5.3 |
| 50 | D2 | 46 | LYS | 5.3 |
| 10 | CJ | 100 | ILE | 5.3 |
| 53 | B5 | 164 | PHE | 5.3 |
| 30 | DI | 64 | ASP | 5.3 |
| 28 | DG | 62 | TRP | 5.3 |
| 42 | DU | 21 | LYS | 5.3 |
| 42 | DU | 80 | ALA | 5.3 |
| 53 | B5 | 192 | ALA | 5.3 |
| 8 | CH | 2 | SER | 5.3 |
| 13 | CM | 39 | ILE | 5.3 |
| 10 | CJ | 76 | ILE | 5.3 |
| 13 | CM | 46 | SER | 5.3 |
| 30 | BI | 142 | ASP | 5.3 |
| 42 | DU | 90 | GLY | 5.3 |
| 40 | DS | 4 | ILE | 5.3 |
| 12 | CL | 124 | ALA | 5.3 |
| 35 | DN | 111 | ALA | 5.3 |
| 3 | CC | 193 | TYR | 5.3 |
| 13 | CM | 58 | ASP | 5.3 |
| 30 | DI | 77 | ALA | 5.3 |
| 14 | CN | 20 | TYR | 5.2 |
| 27 | DF | 114 | PHE | 5.2 |
| 22 | BA | 2131 | U | 5.2 |
| 9 | CI | 58 | VAL | 5.2 |
| 51 | D3 | 14 | PHE | 5.2 |
| 7 | CG | 57 | SER | 5.2 |
| 30 | DI | 140 | VAL | 5.2 |
| 19 | CS | 28 | LYS | 5.2 |
| 30 | DI | 44 | ALA | 5.2 |
| 36 | DO | 60 | GLU | 5.2 |
| 1 | CA | 1540 | U | 5.2 |
| 27 | DF | 87 | CYS | 5.2 |
| 30 | BI | 39 | CYS | 5.2 |
| 51 | D3 | 61 | CYS | 5.2 |
| 9 | CI | 38 | TYR | 5.2 |
| 26 | DE | 131 | THR | 5.2 |
| 53 | B5 | 47 | LYS | 5.2 |
| 39 | DR | 37 | GLU | 5.2 |
| 40 | DS | 68 | ASP | 5.2 |
| 31 | DJ | 47 | HIS | 5.2 |
| 53 | B5 | 202 | PRO | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 30 | DI | 118 | THR | 5.2 |
| 53 | B5 | 150 | ILE | 5.2 |
| 14 | CN | 24 | ARG | 5.2 |
| 10 | CJ | 8 | ILE | 5.1 |
| 22 | BA | 546 | U | 5.1 |
| 30 | BI | 14 | ALA | 5.1 |
| 53 | B5 | 63 | VAL | 5.1 |
| 42 | DU | 28 | VAL | 5.1 |
| 19 | CS | 65 | GLU | 5.1 |
| 53 | B5 | 89 | GLU | 5.1 |
| 13 | CM | 79 | ARG | 5.1 |
| 29 | DH | 15 | LEU | 5.1 |
| 7 | CG | 52 | GLN | 5.1 |
| 27 | DF | 26 | MET | 5.1 |
| 53 | B5 | 103 | LYS | 5.1 |
| 1 | AA | 1537 | U | 5.1 |
| 53 | B5 | 159 | ALA | 5.1 |
| 30 | BI | 99 | GLY | 5.1 |
| 10 | CJ | 66 | GLU | 5.1 |
| 42 | DU | 71 | ALA | 5.1 |
| 30 | DI | 43 | ASN | 5.1 |
| 9 | CI | 20 | PHE | 5.1 |
| 53 | B5 | 41 | THR | 5.1 |
| 46 | DY | 21 | LEU | 5.1 |
| 1 | CA | 1031 | C | 5.1 |
| 53 | B5 | 57 | GLN | 5.1 |
| 53 | B5 | 216 | THR | 5.1 |
| 30 | DI | 57 | VAL | 5.0 |
| 53 | B5 | 220 | GLY | 5.0 |
| 27 | DF | 38 | MET | 5.0 |
| 53 | B5 | 154 | ILE | 5.0 |
| 7 | CG | 23 | LEU | 5.0 |
| 19 | AS | 3 | ARG | 5.0 |
| 30 | DI | 17 | MET | 5.0 |
| 42 | DU | 37 | GLU | 5.0 |
| 26 | DE | 164 | LEU | 5.0 |
| 34 | DM | 124 | LEU | 5.0 |
| 26 | DE | 158 | PHE | 5.0 |
| 33 | DL | 3 | LEU | 5.0 |
| 53 | B5 | 105 | LEU | 5.0 |
| 53 | B5 | 93 | ASP | 5.0 |
| 30 | BI | 40 | LYS | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | DU | 48 | PRO | 5.0 |
| 14 | CN | 43 | ASN | 5.0 |
| 25 | DD | 25 | THR | 5.0 |
| 19 | CS | 80 | TYR | 5.0 |
| 43 | DV | 57 | TYR | 5.0 |
| 10 | CJ | 72 | ARG | 5.0 |
| 21 | AU | 4 | ILE | 5.0 |
| 53 | B5 | 222 | SER | 4.9 |
| 42 | DU | 79 | LYS | 4.9 |
| 19 | CS | 25 | SER | 4.9 |
| 36 | DO | 13 | ARG | 4.9 |
| 30 | DI | 49 | ILE | 4.9 |
| 26 | DE | 127 | GLU | 4.9 |
| 53 | B5 | 71 | LYS | 4.9 |
| 25 | DD | 27 | ILE | 4.9 |
| 39 | DR | 27 | ILE | 4.9 |
| 35 | DN | 76 | VAL | 4.9 |
| 30 | DI | 36 | MET | 4.9 |
| 53 | B5 | 152 | GLU | 4.9 |
| 22 | BA | 2180 | U | 4.9 |
| 27 | DF | 36 | LEU | 4.9 |
| 30 | BI | 43 | ASN | 4.9 |
| 41 | DT | 80 | TRP | 4.9 |
| 28 | DG | 52 | PHE | 4.9 |
| 31 | DJ | 142 | ILE | 4.9 |
| 26 | DE | 199 | MET | 4.9 |
| 36 | DO | 90 | VAL | 4.9 |
| 13 | CM | 94 | GLY | 4.9 |
| 41 | DT | 6 | ARG | 4.9 |
| 2 | CB | 164 | ILE | 4.9 |
| 6 | CF | 39 | LEU | 4.9 |
| 53 | B5 | 43 | GLU | 4.8 |
| 53 | B5 | 184 | GLU | 4.8 |
| 27 | DF | 102 | ARG | 4.8 |
| 53 | B5 | 49 | GLY | 4.8 |
| 22 | DA | 546 | U | 4.8 |
| 53 | B5 | 151 | GLY | 4.8 |
| 36 | DO | 64 | TYR | 4.8 |
| 1 | AA | 86 | G | 4.8 |
| 7 | CG | 134 | ALA | 4.8 |
| 30 | BI | 83 | ALA | 4.8 |
| 19 | CS | 61 | PHE | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 53 | B5 | 51 | ASP | 4.8 |
| 19 | CS | 22 | ALA | 4.8 |
| 22 | BA | 2186 | G | 4.8 |
| 37 | DP | 84 | ILE | 4.8 |
| 28 | DG | 20 | ASN | 4.8 |
| 10 | CJ | 98 | VAL | 4.8 |
| 29 | DH | 13 | GLY | 4.8 |
| 30 | BI | 23 | PRO | 4.8 |
| 30 | BI | 100 | LYS | 4.8 |
| 27 | DF | 164 | GLU | 4.8 |
| 22 | BA | 2171 | A | 4.8 |
| 19 | CS | 11 | ILE | 4.8 |
| 25 | DD | 186 | LEU | 4.8 |
| 36 | DO | 58 | ILE | 4.8 |
| 53 | B5 | 56 | ASP | 4.8 |
| 13 | CM | 51 | GLY | 4.8 |
| 42 | DU | 27 | ASN | 4.8 |
| 7 | CG | 80 | VAL | 4.8 |
| 9 | CI | 41 | ARG | 4.8 |
| 33 | DL | 71 | ALA | 4.8 |
| 27 | DF | 106 | ILE | 4.8 |
| 30 | BI | 80 | LEU | 4.7 |
| 13 | CM | 109 | ARG | 4.7 |
| 30 | DI | 112 | THR | 4.7 |
| 2 | CB | 32 | PHE | 4.7 |
| 10 | CJ | 71 | LEU | 4.7 |
| 22 | BA | 2170 | A | 4.7 |
| 53 | B5 | 215 | VAL | 4.7 |
| 20 | CT | 38 | ALA | 4.7 |
| 26 | DE | 172 | ALA | 4.7 |
| 30 | BI | 133 | ALA | 4.7 |
| 46 | DY | 13 | GLU | 4.7 |
| 30 | DI | 45 | LYS | 4.7 |
| 2 | CB | 34 | ALA | 4.7 |
| 12 | CL | 25 | GLU | 4.7 |
| 30 | DI | 56 | PRO | 4.7 |
| 40 | DS | 41 | LYS | 4.7 |
| 2 | CB | 135 | LEU | 4.7 |
| 13 | CM | 40 | ALA | 4.7 |
| 30 | DI | 133 | ALA | 4.7 |
| 27 | DF | 37 | ASN | 4.7 |
| 13 | CM | 111 | GLY | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | DE | 55 | SER | 4.7 |
| 26 | DE | 186 | VAL | 4.7 |
| 14 | CN | 27 | LEU | 4.7 |
| 29 | BH | 124 | THR | 4.7 |
| 44 | DW | 43 | THR | 4.7 |
| 22 | BA | 2146 | C | 4.7 |
| 22 | BA | 2122 | U | 4.7 |
| 9 | CI | 39 | PHE | 4.7 |
| 17 | AQ | 83 | VAL | 4.7 |
| 36 | DO | 106 | LEU | 4.7 |
| 28 | DG | 166 | ASP | 4.7 |
| 45 | DX | 35 | SER | 4.7 |
| 41 | DT | 85 | VAL | 4.6 |
| 20 | CT | 39 | ILE | 4.6 |
| 53 | B5 | 153 | ILE | 4.6 |
| 2 | CB | 9 | MET | 4.6 |
| 19 | CS | 13 | LEU | 4.6 |
| 14 | CN | 44 | ALA | 4.6 |
| 30 | DI | 129 | ILE | 4.6 |
| 42 | DU | 5 | ILE | 4.6 |
| 26 | DE | 124 | PHE | 4.6 |
| 10 | CJ | 94 | ALA | 4.6 |
| 30 | DI | 99 | GLY | 4.6 |
| 18 | AR | 20 | GLU | 4.6 |
| 22 | BA | 2132 | U | 4.6 |
| 30 | DI | 12 | GLN | 4.6 |
| 22 | DA | 1870 | C | 4.6 |
| 44 | DW | 52 | GLY | 4.6 |
| 36 | DO | 99 | TYR | 4.6 |
| 53 | B5 | 88 | GLU | 4.6 |
| 22 | BA | 2108 | A | 4.6 |
| 45 | DX | 11 | ARG | 4.6 |
| 45 | DX | 22 | LEU | 4.6 |
| 24 | DC | 49 | ILE | 4.6 |
| 19 | CS | 17 | LYS | 4.6 |
| 10 | AJ | 89 | ARG | 4.6 |
| 27 | DF | 112 | ARG | 4.6 |
| 22 | BA | 2109 | U | 4.6 |
| 40 | DS | 19 | LEU | 4.6 |
| 40 | DS | 47 | VAL | 4.6 |
| 10 | CJ | 15 | HIS | 4.6 |
| 14 | AN | 22 | ALA | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | DF | 79 | ILE | 4.6 |
| 30 | DI | 38 | PHE | 4.6 |
| 27 | DF | 68 | THR | 4.5 |
| 29 | BH | 137 | GLU | 4.5 |
| 29 | BH | 149 | GLU | 4.5 |
| 30 | DI | 50 | GLU | 4.5 |
| 36 | DO | 61 | GLN | 4.5 |
| 14 | CN | 45 | VAL | 4.5 |
| 28 | DG | 80 | THR | 4.5 |
| 30 | DI | 73 | THR | 4.5 |
| 26 | DE | 104 | ALA | 4.5 |
| 33 | DL | 106 | GLU | 4.5 |
| 53 | B5 | 188 | ASP | 4.5 |
| 2 | CB | 74 | ARG | 4.5 |
| 13 | CM | 64 | VAL | 4.5 |
| 19 | CS | 48 | THR | 4.5 |
| 30 | BI | 59 | ILE | 4.5 |
| 30 | DI | 114 | ALA | 4.5 |
| 3 | CC | 37 | PHE | 4.5 |
| 22 | BA | 2167 | U | 4.5 |
| 39 | DR | 75 | VAL | 4.5 |
| 1 | AA | 1534 | A | 4.5 |
| 19 | CS | 38 | SER | 4.5 |
| 30 | BI | 62 | TYR | 4.5 |
| 27 | DF | 57 | LEU | 4.5 |
| 53 | B5 | 172 | ILE | 4.5 |
| 30 | DI | 96 | ASP | 4.5 |
| 7 | CG | 50 | LEU | 4.5 |
| 17 | CQ | 23 | VAL | 4.5 |
| 26 | DE | 118 | LEU | 4.5 |
| 49 | D1 | 52 | ALA | 4.5 |
| 33 | DL | 57 | LEU | 4.5 |
| 22 | DA | 2126 | A | 4.5 |
| 53 | B5 | 75 | VAL | 4.5 |
| 29 | BH | 64 | ALA | 4.5 |
| 53 | B5 | 38 | PHE | 4.5 |
| 16 | CP | 45 | GLU | 4.5 |
| 29 | DH | 79 | THR | 4.5 |
| 20 | AT | 68 | HIS | 4.5 |
| 30 | DI | 90 | SER | 4.5 |
| 42 | DU | 88 | GLU | 4.4 |
| 28 | DG | 10 | VAL | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 53 | B5 | 176 | VAL | 4.4 |
| 2 | CB | 213 | TYR | 4.4 |
| 40 | DS | 5 | ALA | 4.4 |
| 24 | DC | 26 | LYS | 4.4 |
| 9 | CI | 48 | VAL | 4.4 |
| 41 | DT | 53 | VAL | 4.4 |
| 4 | AD | 28 | ILE | 4.4 |
| 14 | CN | 29 | ALA | 4.4 |
| 36 | DO | 14 | ALA | 4.4 |
| 20 | CT | 3 | ASN | 4.4 |
| 26 | DE | 180 | LEU | 4.4 |
| 7 | CG | 70 | ARG | 4.4 |
| 30 | DI | 28 | LEU | 4.4 |
| 40 | DS | 46 | LEU | 4.4 |
| 42 | DU | 58 | ILE | 4.4 |
| 27 | DF | 116 | GLY | 4.4 |
| 33 | DL | 49 | GLY | 4.4 |
| 27 | DF | 176 | PRO | 4.4 |
| 13 | CM | 89 | LEU | 4.4 |
| 29 | DH | 130 | VAL | 4.4 |
| 25 | DD | 55 | LYS | 4.4 |
| 30 | BI | 97 | LYS | 4.4 |
| 39 | DR | 20 | VAL | 4.4 |
| 22 | BA | 139 | U | 4.4 |
| 22 | DA | 139 | U | 4.4 |
| 34 | DM | 96 | ILE | 4.4 |
| 46 | DY | 36 | GLN | 4.4 |
| 7 | CG | 45 | SER | 4.4 |
| 32 | DK | 14 | SER | 4.4 |
| 13 | CM | 71 | ARG | 4.4 |
| 51 | D3 | 28 | ASN | 4.4 |
| 7 | CG | 86 | GLN | 4.4 |
| 14 | CN | 21 | PHE | 4.4 |
| 21 | CU | 45 | ARG | 4.4 |
| 27 | DF | 153 | ASP | 4.4 |
| 50 | D2 | 18 | PHE | 4.3 |
| 53 | B5 | 90 | ALA | 4.3 |
| 53 | B5 | 191 | ARG | 4.3 |
| 26 | DE | 17 | THR | 4.3 |
| 50 | D2 | 43 | THR | 4.3 |
| 14 | CN | 34 | VAL | 4.3 |
| 52 | D4 | 8 | LYS | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33 | DL | 124 | GLY | 4.3 |
| 29 | BH | 132 | PHE | 4.3 |
| 10 | CJ | 70 | HIS | 4.3 |
| 3 | CC | 144 | LEU | 4.3 |
| 28 | DG | 167 | GLU | 4.3 |
| 30 | DI | 110 | ALA | 4.3 |
| 26 | DE | 191 | ASP | 4.3 |
| 53 | B5 | 185 | LYS | 4.3 |
| 27 | DF | 4 | LEU | 4.3 |
| 27 | DF | 158 | THR | 4.3 |
| 2 | CB | 132 | LYS | 4.3 |
| 53 | B5 | 79 | ALA | 4.3 |
| 2 | CB | 129 | LEU | 4.3 |
| 7 | CG | 85 | TYR | 4.3 |
| 25 | DD | 6 | GLY | 4.3 |
| 30 | DI | 25 | GLY | 4.3 |
| 13 | CM | 52 | GLN | 4.3 |
| 29 | BH | 59 | ALA | 4.3 |
| 20 | CT | 79 | LEU | 4.3 |
| 35 | DN | 63 | ARG | 4.3 |
| 27 | DF | 31 | VAL | 4.3 |
| 48 | D0 | 3 | VAL | 4.3 |
| 32 | DK | 89 | ASN | 4.3 |
| 30 | BI | 96 | ASP | 4.3 |
| 15 | CO | 25 | THR | 4.3 |
| 46 | DY | 33 | ALA | 4.3 |
| 17 | CQ | 8 | LEU | 4.3 |
| 1 | CA | 211 | G | 4.3 |
| 25 | DD | 180 | VAL | 4.3 |
| 41 | DT | 16 | VAL | 4.3 |
| 26 | DE | 148 | ILE | 4.3 |
| 53 | B5 | 22 | THR | 4.3 |
| 9 | CI | 108 | ALA | 4.3 |
| 36 | DO | 66 | GLY | 4.3 |
| 40 | DS | 85 | ILE | 4.3 |
| 15 | CO | 89 | ARG | 4.3 |
| 13 | CM | 106 | ALA | 4.2 |
| 13 | CM | 105 | ASN | 4.2 |
| 26 | DE | 153 | LEU | 4.2 |
| 49 | D1 | 18 | GLY | 4.2 |
| 10 | CJ | 49 | PHE | 4.2 |
| 33 | DL | 122 | VAL | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | DT | 1 | MET | 4.2 |
| 27 | DF | 118 | SER | 4.2 |
| 53 | B5 | 186 | LEU | 4.2 |
| 28 | DG | 104 | ASN | 4.2 |
| 30 | BI | 81 | LYS | 4.2 |
| 7 | CG | 88 | PRO | 4.2 |
| 28 | DG | 58 | TYR | 4.2 |
| 30 | DI | 37 | GLU | 4.2 |
| 40 | DS | 39 | THR | 4.2 |
| 14 | CN | 4 | GLN | 4.2 |
| 27 | DF | 28 | VAL | 4.2 |
| 27 | DF | 40 | VAL | 4.2 |
| 44 | DW | 53 | CYS | 4.2 |
| 30 | DI | 23 | PRO | 4.2 |
| 32 | DK | 2 | ILE | 4.2 |
| 46 | DY | 10 | SER | 4.2 |
| 7 | CG | 49 | THR | 4.2 |
| 11 | AK | 111 | THR | 4.2 |
| 7 | CG | 73 | VAL | 4.2 |
| 14 | CN | 57 | PRO | 4.2 |
| 22 | DA | 1093 | G | 4.2 |
| 22 | DA | 138 | U | 4.2 |
| 53 | B5 | 92 | ALA | 4.2 |
| 13 | CM | 48 | LEU | 4.2 |
| 10 | CJ | 63 | ASP | 4.2 |
| 14 | CN | 32 | SER | 4.2 |
| 22 | BA | 2119 | A | 4.2 |
| 36 | DO | 19 | GLN | 4.2 |
| 9 | AI | 17 | ALA | 4.2 |
| 22 | DA | 2402 | U | 4.2 |
| 26 | DE | 190 | ALA | 4.2 |
| 28 | DG | 86 | LYS | 4.2 |
| 14 | CN | 11 | VAL | 4.2 |
| 36 | DO | 78 | VAL | 4.2 |
| 13 | CM | 75 | MET | 4.2 |
| 30 | DI | 127 | ARG | 4.2 |
| 19 | CS | 72 | GLY | 4.2 |
| 29 | BH | 122 | LEU | 4.2 |
| 29 | BH | 129 | GLU | 4.2 |
| 27 | DF | 120 | LYS | 4.2 |
| 42 | DU | 3 | ALA | 4.1 |
| 51 | D3 | 37 | ALA | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | DO | 39 | VAL | 4.1 |
| 16 | CP | 76 | LYS | 4.1 |
| 1 | AA | 1492 | A | 4.1 |
| 41 | DT | 35 | ALA | 4.1 |
| 33 | DL | 107 | PHE | 4.1 |
| 20 | CT | 85 | LYS | 4.1 |
| 13 | AM | 5 | ALA | 4.1 |
| 7 | CG | 87 | VAL | 4.1 |
| 19 | CS | 68 | GLY | 4.1 |
| 10 | CJ | 16 | ARG | 4.1 |
| 10 | CJ | 86 | ALA | 4.1 |
| 14 | CN | 99 | ALA | 4.1 |
| 13 | CM | 23 | TYR | 4.1 |
| 43 | DV | 56 | PHE | 4.1 |
| 27 | DF | 132 | VAL | 4.1 |
| 39 | DR | 50 | GLY | 4.1 |
| 30 | DI | 19 | ASN | 4.1 |
| 13 | CM | 62 | LYS | 4.1 |
| 14 | CN | 46 | LEU | 4.1 |
| 22 | DA | 1172 | C | 4.1 |
| 29 | BH | 116 | ARG | 4.1 |
| 13 | CM | 10 | PRO | 4.1 |
| 13 | CM | 113 | ARG | 4.1 |
| 53 | B5 | 44 | VAL | 4.1 |
| 7 | CG | 143 | ARG | 4.1 |
| 7 | CG | 83 | SER | 4.1 |
| 19 | CS | 16 | LEU | 4.1 |
| 28 | DG | 50 | LEU | 4.1 |
| 30 | DI | 106 | LEU | 4.1 |
| 36 | DO | 62 | LEU | 4.1 |
| 27 | DF | 172 | ALA | 4.1 |
| 26 | DE | 126 | VAL | 4.1 |
| 53 | B5 | 101 | ILE | 4.1 |
| 39 | DR | 39 | LEU | 4.1 |
| 50 | D2 | 22 | MET | 4.1 |
| 29 | BH | 89 | LYS | 4.1 |
| 9 | CI | 30 | ILE | 4.0 |
| 13 | CM | 77 | ILE | 4.0 |
| 25 | DD | 14 | ILE | 4.0 |
| 7 | CG | 51 | ALA | 4.0 |
| 14 | CN | 26 | GLU | 4.0 |
| 41 | DT | 73 | ARG | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 87 | C | 4.0 |
| 27 | DF | 83 | TYR | 4.0 |
| 30 | BI | 49 | ILE | 4.0 |
| 33 | DL | 100 | ILE | 4.0 |
| 20 | CT | 71 | LYS | 4.0 |
| 30 | DI | 138 | LEU | 4.0 |
| 38 | DQ | 38 | ALA | 4.0 |
| 53 | B5 | 24 | ASP | 4.0 |
| 10 | CJ | 82 | LYS | 4.0 |
| 19 | CS | 51 | VAL | 4.0 |
| 24 | DC | 242 | LYS | 4.0 |
| 7 | CG | 72 | THR | 4.0 |
| 22 | DA | 2174 | C | 4.0 |
| 27 | DF | 95 | ARG | 4.0 |
| 32 | DK | 107 | LEU | 4.0 |
| 30 | DI | 14 | ALA | 4.0 |
| 30 | BI | 47 | ASP | 4.0 |
| 27 | DF | 22 | TYR | 4.0 |
| 30 | BI | 6 | GLN | 4.0 |
| 36 | DO | 57 | ALA | 4.0 |
| 22 | BA | 2106 | U | 4.0 |
| 30 | BI | 34 | ASN | 4.0 |
| 28 | DG | 41 | VAL | 4.0 |
| 39 | DR | 47 | VAL | 4.0 |
| 2 | CB | 133 | GLU | 4.0 |
| 33 | DL | 19 | LEU | 4.0 |
| 28 | DG | 84 | THR | 4.0 |
| 30 | DI | 126 | THR | 4.0 |
| 36 | DO | 63 | LYS | 4.0 |
| 36 | DO | 92 | PHE | 4.0 |
| 10 | CJ | 12 | ALA | 4.0 |
| 53 | B5 | 144 | GLY | 4.0 |
| 13 | CM | 115 | PRO | 4.0 |
| 4 | AD | 25 | VAL | 4.0 |
| 19 | CS | 23 | VAL | 4.0 |
| 36 | DO | 52 | SER | 4.0 |
| 4 | AD | 151 | LYS | 4.0 |
| 33 | DL | 125 | LEU | 4.0 |
| 52 | D4 | 9 | LYS | 4.0 |
| 2 | CB | 139 | ARG | 4.0 |
| 28 | DG | 174 | ALA | 4.0 |
| 53 | B5 | 133 | GLY | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | B5 | 82 | GLU | 4.0 |
| 9 | CI | 4 | ASN | 4.0 |
| 27 | DF | 34 | ILE | 4.0 |
| 43 | DV | 58 | SER | 4.0 |
| 7 | CG | 103 | TRP | 4.0 |
| 28 | DG | 133 | LEU | 4.0 |
| 20 | CT | 72 | ALA | 4.0 |
| 22 | DA | 1535 | A | 4.0 |
| 30 | BI | 120 | ALA | 4.0 |
| 44 | DW | 85 | GLU | 4.0 |
| 10 | CJ | 19 | ASP | 4.0 |
| 48 | D0 | 54 | VAL | 4.0 |
| 53 | B5 | 201 | LYS | 4.0 |
| 19 | AS | 49 | ILE | 4.0 |
| 17 | AQ | 20 | SER | 4.0 |
| 39 | DR | 43 | ASN | 4.0 |
| 29 | BH | 95 | GLY | 4.0 |
| 52 | D4 | 1 | MET | 4.0 |
| 22 | BA | 1925 | C | 3.9 |
| 19 | CS | 76 | PRO | 3.9 |
| 44 | DW | 71 | VAL | 3.9 |
| 35 | DN | 62 | ASN | 3.9 |
| 29 | BH | 139 | PHE | 3.9 |
| 8 | CH | 123 | GLY | 3.9 |
| 30 | DI | 119 | GLY | 3.9 |
| 28 | DG | 40 | ALA | 3.9 |
| 29 | BH | 39 | ALA | 3.9 |
| 22 | DA | 1174 | U | 3.9 |
| 13 | CM | 55 | THR | 3.9 |
| 44 | DW | 55 | ARG | 3.9 |
| 18 | AR | 68 | LEU | 3.9 |
| 13 | CM | 72 | GLU | 3.9 |
| 29 | BH | 83 | LYS | 3.9 |
| 40 | DS | 16 | LYS | 3.9 |
| 26 | DE | 147 | LEU | 3.9 |
| 31 | DJ | 74 | TYR | 3.9 |
| 22 | DA | 1171 | G | 3.9 |
| 53 | B5 | 211 | ARG | 3.9 |
| 11 | CK | 126 | LYS | 3.9 |
| 13 | AM | 115 | PRO | 3.9 |
| 29 | BH | 44 | ILE | 3.9 |
| 52 | D4 | 16 | ILE | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 19 | CS | 64 | ASP | 3.9 |
| 25 | DD | 96 | ILE | 3.9 |
| 30 | BI | 98 | VAL | 3.9 |
| 39 | DR | 52 | PRO | 3.9 |
| 27 | DF | 173 | PHE | 3.9 |
| 16 | CP | 17 | TYR | 3.9 |
| 40 | DS | 94 | ASP | 3.9 |
| 49 | D1 | 24 | THR | 3.9 |
| 30 | BI | 115 | ALA | 3.9 |
| 22 | DA | 613 | A | 3.9 |
| 2 | AB | 221 | VAL | 3.9 |
| 30 | DI | 101 | ILE | 3.9 |
| 2 | AB | 74 | ARG | 3.9 |
| 41 | DT | 50 | LEU | 3.9 |
| 52 | D4 | 15 | LYS | 3.9 |
| 44 | DW | 78 | LYS | 3.9 |
| 14 | AN | 36 | ALA | 3.9 |
| 27 | DF | 55 | ALA | 3.9 |
| 52 | D4 | 6 | SER | 3.9 |
| 27 | DF | 13 | VAL | 3.8 |
| 27 | DF | 149 | VAL | 3.8 |
| 40 | DS | 48 | LYS | 3.8 |
| 44 | DW | 59 | LEU | 3.8 |
| 41 | DT | 41 | ALA | 3.8 |
| 22 | DA | 2172 | U | 3.8 |
| 27 | BF | 116 | GLY | 3.8 |
| 28 | DG | 131 | ILE | 3.8 |
| 29 | BH | 90 | LEU | 3.8 |
| 19 | CS | 59 | PRO | 3.8 |
| 10 | CJ | 11 | LYS | 3.8 |
| 30 | DI | 65 | ARG | 3.8 |
| 33 | DL | 132 | ARG | 3.8 |
| 1 | CA | 1302 | C | 3.8 |
| 19 | CS | 46 | GLY | 3.8 |
| 51 | D3 | 57 | LEU | 3.8 |
| 14 | CN | 53 | ARG | 3.8 |
| 7 | CG | 8 | GLY | 3.8 |
| 27 | DF | 157 | THR | 3.8 |
| 28 | DG | 48 | ASN | 3.8 |
| 30 | DI | 30 | GLN | 3.8 |
| 20 | CT | 34 | LYS | 3.8 |
| 21 | AU | 24 | GLU | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | DK | 98 | ARG | 3.8 |
| 46 | DY | 29 | ARG | 3.8 |
| 25 | DD | 31 | ALA | 3.8 |
| 26 | DE | 201 | ALA | 3.8 |
| 27 | DF | 171 | ALA | 3.8 |
| 43 | DV | 6 | ALA | 3.8 |
| 30 | DI | 16 | GLY | 3.8 |
| 30 | DI | 71 | THR | 3.8 |
| 33 | DL | 87 | GLY | 3.8 |
| 42 | DU | 40 | ASN | 3.8 |
| 44 | BW | 10 | THR | 3.8 |
| 51 | D3 | 58 | VAL | 3.8 |
| 46 | DY | 56 | LEU | 3.8 |
| 1 | CA | 1271 | A | 3.8 |
| 17 | CQ | 21 | ILE | 3.8 |
| 36 | DO | 46 | GLU | 3.8 |
| 36 | DO | 65 | THR | 3.8 |
| 10 | CJ | 89 | ARG | 3.8 |
| 48 | D0 | 39 | LEU | 3.8 |
| 52 | D4 | 12 | ARG | 3.8 |
| 30 | BI | 92 | LYS | 3.8 |
| 3 | CC | 120 | ILE | 3.8 |
| 13 | CM | 43 | VAL | 3.8 |
| 20 | CT | 24 | ARG | 3.8 |
| 22 | BA | 2151 | U | 3.8 |
| 28 | DG | 26 | ILE | 3.8 |
| 46 | DY | 24 | GLU | 3.8 |
| 26 | DE | 157 | LEU | 3.8 |
| 40 | DS | 37 | THR | 3.8 |
| 41 | DT | 49 | LYS | 3.8 |
| 42 | DU | 38 | GLY | 3.8 |
| 35 | DN | 20 | MET | 3.8 |
| 22 | DA | 2125 | G | 3.8 |
| 36 | DO | 85 | LYS | 3.8 |
| 9 | AI | 41 | ARG | 3.8 |
| 27 | DF | 115 | ARG | 3.8 |
| 43 | DV | 74 | ALA | 3.8 |
| 29 | BH | 61 | VAL | 3.8 |
| 27 | DF | 69 | LYS | 3.7 |
| 7 | CG | 148 | ASN | 3.7 |
| 17 | CQ | 53 | CYS | 3.7 |
| 30 | DI | 33 | VAL | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | DQ | 88 | VAL | 3.7 |
| 14 | CN | 33 | ASP | 3.7 |
| 42 | DU | 44 | LYS | 3.7 |
| 35 | DN | 102 | PHE | 3.7 |
| 41 | DT | 87 | LEU | 3.7 |
| 9 | CI | 112 | GLU | 3.7 |
| 14 | CN | 58 | SER | 3.7 |
| 53 | B5 | 175 | PRO | 3.7 |
| 22 | DA | 1046 | A | 3.7 |
| 32 | DK | 112 | PHE | 3.7 |
| 53 | B5 | 124 | VAL | 3.7 |
| 30 | DI | 72 | LYS | 3.7 |
| 30 | BI | 16 | GLY | 3.7 |
| 52 | D4 | 38 | GLY | 3.7 |
| 33 | DL | 15 | ALA | 3.7 |
| 32 | DK | 69 | VAL | 3.7 |
| 3 | CC | 107 | ARG | 3.7 |
| 1 | CA | 82 | G | 3.7 |
| 22 | DA | 1407 | G | 3.7 |
| 27 | DF | 76 | GLY | 3.7 |
| 35 | DN | 73 | ASN | 3.7 |
| 30 | BI | 20 | PRO | 3.7 |
| 9 | CI | 61 | LEU | 3.7 |
| 19 | AS | 15 | LEU | 3.7 |
| 26 | DE | 12 | LEU | 3.7 |
| 22 | DA | 1067 | A | 3.7 |
| 53 | B5 | 91 | GLY | 3.7 |
| 48 | D0 | 38 | HIS | 3.7 |
| 30 | DI | 51 | LYS | 3.7 |
| 33 | DL | 108 | ALA | 3.7 |
| 13 | CM | 108 | THR | 3.7 |
| 26 | DE | 14 | VAL | 3.7 |
| 27 | DF | 24 | SER | 3.7 |
| 28 | DG | 148 | LEU | 3.7 |
| 29 | BH | 4 | ILE | 3.7 |
| 30 | BI | 48 | SER | 3.7 |
| 33 | DL | 77 | ILE | 3.7 |
| 35 | DN | 119 | SER | 3.7 |
| 2 | CB | 65 | GLY | 3.7 |
| 28 | DG | 51 | THR | 3.7 |
| 29 | BH | 5 | LEU | 3.7 |
| 30 | BI | 91 | GLY | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | CJ | 99 | GLN | 3.7 |
| 9 | CI | 103 | PHE | 3.7 |
| 36 | DO | 59 | ALA | 3.7 |
| 9 | AI | 90 | TYR | 3.7 |
| 10 | CJ | 41 | PRO | 3.7 |
| 10 | AJ | 74 | VAL | 3.7 |
| 7 | CG | 133 | THR | 3.7 |
| 22 | DA | 2124 | G | 3.7 |
| 2 | CB | 152 | LYS | 3.6 |
| 35 | DN | 46 | ARG | 3.6 |
| 53 | B5 | 135 | ARG | 3.6 |
| 42 | DU | 75 | ALA | 3.6 |
| 13 | CM | 80 | LEU | 3.6 |
| 36 | DO | 54 | VAL | 3.6 |
| 42 | DU | 13 | VAL | 3.6 |
| 32 | DK | 111 | LYS | 3.6 |
| 10 | CJ | 91 | ASP | 3.6 |
| 53 | B5 | 129 | GLY | 3.6 |
| 53 | B5 | 136 | GLY | 3.6 |
| 36 | DO | 23 | ALA | 3.6 |
| 53 | B5 | 125 | GLY | 3.6 |
| 53 | B5 | 40 | GLU | 3.6 |
| 27 | DF | 100 | PHE | 3.6 |
| 40 | DS | 90 | LYS | 3.6 |
| 29 | BH | 73 | ASN | 3.6 |
| 3 | CC | 42 | TYR | 3.6 |
| 13 | CM | 60 | VAL | 3.6 |
| 51 | D3 | 64 | TYR | 3.6 |
| 42 | DU | 98 | SER | 3.6 |
| 1 | CA | 1305 | G | 3.6 |
| 43 | DV | 94 | ALA | 3.6 |
| 53 | B5 | 74 | ARG | 3.6 |
| 13 | CM | 33 | ILE | 3.6 |
| 27 | DF | 60 | ILE | 3.6 |
| 39 | DR | 96 | VAL | 3.6 |
| 40 | DS | 9 | HIS | 3.6 |
| 27 | DF | 51 | ASP | 3.6 |
| 7 | CG | 26 | PHE | 3.6 |
| 39 | DR | 19 | THR | 3.6 |
| 46 | DY | 16 | THR | 3.6 |
| 30 | BI | 76 | ALA | 3.6 |
| 1 | CA | 1314 | C | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | CN | 48 | LEU | 3.6 |
| 27 | DF | 41 | GLY | 3.6 |
| 10 | AJ | 75 | ASP | 3.6 |
| 27 | DF | 174 | ASP | 3.6 |
| 53 | B5 | 168 | LYS | 3.6 |
| 36 | DO | 109 | ALA | 3.6 |
| 20 | CT | 9 | LYS | 3.6 |
| 36 | DO | 103 | VAL | 3.6 |
| 21 | AU | 21 | ARG | 3.6 |
| 26 | DE | 88 | ARG | 3.6 |
| 9 | AI | 20 | PHE | 3.6 |
| 26 | DE | 179 | SER | 3.6 |
| 53 | B5 | 126 | SER | 3.6 |
| 27 | DF | 107 | ALA | 3.6 |
| 3 | CC | 206 | GLU | 3.6 |
| 7 | CG | 118 | LEU | 3.6 |
| 29 | BH | 142 | VAL | 3.6 |
| 9 | CI | 11 | ARG | 3.6 |
| 31 | DJ | 13 | ARG | 3.6 |
| 27 | DF | 147 | ASP | 3.6 |
| 30 | BI | 82 | LYS | 3.5 |
| 27 | DF | 103 | LEU | 3.5 |
| 7 | CG | 109 | ARG | 3.5 |
| 27 | DF | 105 | THR | 3.5 |
| 34 | DM | 80 | VAL | 3.5 |
| 2 | AB | 88 | ASP | 3.5 |
| 20 | CT | 43 | ASP | 3.5 |
| 29 | DH | 135 | HIS | 3.5 |
| 9 | CI | 7 | TYR | 3.5 |
| 2 | CB | 136 | MET | 3.5 |
| 26 | DE | 1 | MET | 3.5 |
| 13 | CM | 22 | ILE | 3.5 |
| 35 | DN | 29 | VAL | 3.5 |
| 47 | DZ | 48 | ILE | 3.5 |
| 7 | CG | 137 | LYS | 3.5 |
| 14 | CN | 60 | GLN | 3.5 |
| 12 | AL | 25 | GLU | 3.5 |
| 22 | DA | 2903 | U | 3.5 |
| 7 | CG | 144 | MET | 3.5 |
| 25 | DD | 1 | MET | 3.5 |
| 9 | CI | 44 | ALA | 3.5 |
| 10 | AJ | 87 | LEU | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | DO | 115 | LEU | 3.5 |
| 36 | DO | 87 | ILE | 3.5 |
| 19 | CS | 18 | LYS | 3.5 |
| 7 | CG | 41 | SER | 3.5 |
| 30 | BI | 88 | SER | 3.5 |
| 41 | DT | 72 | GLN | 3.5 |
| 26 | DE | 173 | THR | 3.5 |
| 32 | DK | 37 | ASP | 3.5 |
| 32 | DK | 65 | THR | 3.5 |
| 36 | DO | 20 | GLU | 3.5 |
| 47 | DZ | 8 | THR | 3.5 |
| 46 | DY | 7 | ARG | 3.5 |
| 24 | DC | 249 | GLY | 3.5 |
| 39 | DR | 88 | GLY | 3.5 |
| 49 | D1 | 21 | TYR | 3.5 |
| 51 | D3 | 21 | GLY | 3.5 |
| 53 | B5 | 128 | LEU | 3.5 |
| 19 | CS | 62 | VAL | 3.5 |
| 41 | DT | 58 | VAL | 3.5 |
| 29 | BH | 66 | ASN | 3.5 |
| 9 | AI | 63 | LEU | 3.5 |
| 22 | DA | 2112 | G | 3.5 |
| 13 | CM | 101 | ARG | 3.5 |
| 38 | DQ | 22 | LYS | 3.5 |
| 53 | B5 | 60 | ARG | 3.5 |
| 27 | DF | 175 | PHE | 3.5 |
| 52 | D4 | 33 | HIS | 3.5 |
| 2 | AB | 135 | LEU | 3.5 |
| 13 | CM | 73 | ILE | 3.5 |
| 38 | DQ | 21 | ALA | 3.5 |
| 36 | DO | 56 | LYS | 3.5 |
| 42 | DU | 83 | VAL | 3.5 |
| 19 | AS | 21 | LYS | 3.5 |
| 25 | DD | 201 | LEU | 3.5 |
| 26 | DE | 200 | LEU | 3.5 |
| 28 | DG | 6 | LYS | 3.5 |
| 7 | CG | 141 | VAL | 3.5 |
| 10 | CJ | 6 | ILE | 3.5 |
| 24 | DC | 64 | ILE | 3.5 |
| 37 | DP | 95 | ALA | 3.5 |
| 40 | DS | 44 | ALA | 3.5 |
| 10 | CJ | 75 | ASP | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | DQ | 29 | SER | 3.4 |
| 19 | CS | 21 | LYS | 3.4 |
| 9 | AI | 89 | GLU | 3.4 |
| 27 | DF | 90 | THR | 3.4 |
| 40 | DS | 95 | ARG | 3.4 |
| 22 | DA | 2313 | C | 3.4 |
| 7 | CG | 54 | SER | 3.4 |
| 7 | CG | 139 | GLU | 3.4 |
| 20 | AT | 36 | TYR | 3.4 |
| 27 | DF | 64 | LYS | 3.4 |
| 30 | BI | 95 | LYS | 3.4 |
| 14 | CN | 54 | ASP | 3.4 |
| 22 | DA | 1045 | C | 3.4 |
| 38 | DQ | 89 | GLU | 3.4 |
| 9 | CI | 51 | PRO | 3.4 |
| 28 | DG | 106 | SER | 3.4 |
| 2 | CB | 186 | ILE | 3.4 |
| 26 | DE | 150 | THR | 3.4 |
| 27 | DF | 43 | ALA | 3.4 |
| 28 | DG | 132 | VAL | 3.4 |
| 28 | DG | 28 | GLY | 3.4 |
| 30 | BI | 25 | GLY | 3.4 |
| 17 | CQ | 78 | VAL | 3.4 |
| 27 | DF | 143 | TYR | 3.4 |
| 27 | DF | 20 | PHE | 3.4 |
| 9 | CI | 37 | GLN | 3.4 |
| 14 | CN | 31 | ILE | 3.4 |
| 51 | D3 | 49 | MET | 3.4 |
| 32 | DK | 35 | VAL | 3.4 |
| 1 | CA | 1020 | G | 3.4 |
| 1 | CA | 1312 | G | 3.4 |
| 19 | CS | 6 | LYS | 3.4 |
| 46 | DY | 54 | LYS | 3.4 |
| 48 | D0 | 37 | LYS | 3.4 |
| 2 | CB | 182 | PRO | 3.4 |
| 13 | CM | 56 | LEU | 3.4 |
| 22 | DA | 228 | C | 3.4 |
| 19 | CS | 50 | ALA | 3.4 |
| 34 | DM | 6 | ARG | 3.4 |
| 7 | CG | 38 | THR | 3.4 |
| 22 | DA | 896 | A | 3.4 |
| 29 | DH | 40 | THR | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | CJ | 102 | LEU | 3.4 |
| 25 | DD | 84 | LEU | 3.4 |
| 41 | DT | 74 | ILE | 3.4 |
| 3 | CC | 79 | LYS | 3.4 |
| 24 | DC | 27 | GLY | 3.4 |
| 28 | DG | 57 | GLY | 3.4 |
| 7 | CG | 44 | TYR | 3.4 |
| 38 | DQ | 45 | TYR | 3.4 |
| 2 | CB | 130 | THR | 3.4 |
| 2 | CB | 138 | THR | 3.4 |
| 22 | DA | 1095 | A | 3.4 |
| 7 | CG | 79 | ARG | 3.4 |
| 4 | AD | 37 | ALA | 3.4 |
| 26 | DE | 28 | VAL | 3.4 |
| 44 | DW | 23 | VAL | 3.4 |
| 10 | CJ | 22 | THR | 3.4 |
| 25 | DD | 59 | ARG | 3.3 |
| 33 | DL | 78 | ARG | 3.3 |
| 38 | DQ | 37 | GLN | 3.3 |
| 28 | DG | 4 | VAL | 3.3 |
| 48 | D0 | 25 | VAL | 3.3 |
| 36 | DO | 9 | ARG | 3.3 |
| 26 | DE | 144 | GLU | 3.3 |
| 34 | DM | 129 | THR | 3.3 |
| 22 | DA | 1073 | A | 3.3 |
| 9 | AI | 21 | ILE | 3.3 |
| 2 | AB | 9 | MET | 3.3 |
| 2 | AB | 90 | PHE | 3.3 |
| 13 | CM | 97 | VAL | 3.3 |
| 22 | DA | 343 | C | 3.3 |
| 8 | CH | 59 | LEU | 3.3 |
| 10 | CJ | 20 | GLN | 3.3 |
| 22 | DA | 1065 | U | 3.3 |
| 27 | DF | 99 | PHE | 3.3 |
| 42 | DU | 76 | ALA | 3.3 |
| 40 | DS | 6 | LYS | 3.3 |
| 41 | DT | 36 | LYS | 3.3 |
| 10 | CJ | 81 | GLU | 3.3 |
| 27 | DF | 52 | ASN | 3.3 |
| 36 | DO | 108 | ASP | 3.3 |
| 46 | DY | 14 | LEU | 3.3 |
| 2 | CB | 37 | LYS | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | DF | 133 | ARG | 3.3 |
| 28 | DG | 168 | VAL | 3.3 |
| 34 | DM | 136 | MET | 3.3 |
| 35 | DN | 24 | MET | 3.3 |
| 2 | CB | 148 | LEU | 3.3 |
| 4 | CD | 24 | GLY | 3.3 |
| 26 | DE | 183 | PHE | 3.3 |
| 50 | D2 | 1 | MET | 3.3 |
| 1 | AA | 412 | A | 3.3 |
| 22 | DA | 2165 | C | 3.3 |
| 13 | CM | 87 | ARG | 3.3 |
| 2 | AB | 67 | ILE | 3.3 |
| 16 | CP | 57 | ILE | 3.3 |
| 19 | CS | 75 | ALA | 3.3 |
| 41 | DT | 83 | ALA | 3.3 |
| 53 | B5 | 193 | PHE | 3.3 |
| 30 | BI | 125 | MET | 3.3 |
| 53 | B5 | 80 | LYS | 3.3 |
| 3 | CC | 127 | ARG | 3.3 |
| 35 | DN | 38 | LEU | 3.3 |
| 22 | DA | 2797 | U | 3.3 |
| 10 | CJ | 51 | VAL | 3.3 |
| 1 | CA | 79 | G | 3.3 |
| 9 | AI | 27 | LYS | 3.3 |
| 22 | DA | 88 | G | 3.3 |
| 26 | DE | 155 | GLU | 3.3 |
| 35 | DN | 113 | ILE | 3.3 |
| 25 | DD | 5 | VAL | 3.3 |
| 30 | BI | 7 | ALA | 3.3 |
| 7 | CG | 35 | LYS | 3.3 |
| 41 | DT | 33 | LYS | 3.3 |
| 2 | AB | 136 | MET | 3.3 |
| 26 | DE | 21 | ARG | 3.3 |
| 41 | DT | 12 | ARG | 3.3 |
| 7 | CG | 13 | LEU | 3.3 |
| 16 | CP | 60 | TRP | 3.3 |
| 27 | DF | 10 | ASP | 3.3 |
| 26 | DE | 103 | GLY | 3.3 |
| 8 | CH | 75 | ILE | 3.2 |
| 27 | DF | 78 | LYS | 3.2 |
| 34 | DM | 36 | VAL | 3.2 |
| 35 | DN | 25 | ALA | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | DP | 12 | GLN | 3.2 |
| 33 | DL | 45 | GLY | 3.2 |
| 50 | D2 | 37 | LYS | 3.2 |
| 5 | AE | 31 | PHE | 3.2 |
| 22 | BA | 1065 | U | 3.2 |
| 33 | DL | 66 | PHE | 3.2 |
| 13 | CM | 18 | ALA | 3.2 |
| 27 | DF | 25 | VAL | 3.2 |
| 30 | BI | 78 | VAL | 3.2 |
| 30 | DI | 84 | ALA | 3.2 |
| 10 | CJ | 30 | LYS | 3.2 |
| 13 | CM | 38 | GLY | 3.2 |
| 20 | CT | 86 | LEU | 3.2 |
| 25 | DD | 105 | LYS | 3.2 |
| 27 | DF | 50 | LEU | 3.2 |
| 46 | BY | 6 | LEU | 3.2 |
| 49 | B1 | 4 | GLY | 3.2 |
| 53 | B5 | 99 | GLU | 3.2 |
| 7 | CG | 111 | ARG | 3.2 |
| 30 | BI | 21 | SER | 3.2 |
| 22 | DA | 2168 | G | 3.2 |
| 38 | DQ | 23 | GLY | 3.2 |
| 19 | CS | 14 | HIS | 3.2 |
| 33 | DL | 50 | PHE | 3.2 |
| 42 | DU | 95 | PHE | 3.2 |
| 2 | CB | 36 | ASN | 3.2 |
| 30 | BI | 70 | VAL | 3.2 |
| 33 | DL | 85 | VAL | 3.2 |
| 2 | AB | 27 | MET | 3.2 |
| 27 | DF | 142 | ASP | 3.2 |
| 53 | B5 | 137 | LEU | 3.2 |
| 20 | CT | 67 | ILE | 3.2 |
| 41 | DT | 70 | HIS | 3.2 |
| 51 | D3 | 43 | HIS | 3.2 |
| 46 | DY | 35 | GLY | 3.2 |
| 22 | DA | 2157 | G | 3.2 |
| 28 | DG | 127 | THR | 3.2 |
| 44 | DW | 60 | PHE | 3.2 |
| 3 | CC | 62 | LYS | 3.2 |
| 44 | DW | 72 | LYS | 3.2 |
| 9 | AI | 104 | VAL | 3.2 |
| 11 | AK | 53 | ARG | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 44 | DW | 32 | LEU | 3.2 |
| 3 | CC | 192 | THR | 3.2 |
| 31 | DJ | 5 | THR | 3.2 |
| 7 | CG | 69 | VAL | 3.2 |
| 13 | CM | 32 | ALA | 3.2 |
| 32 | DK | 60 | ALA | 3.2 |
| 39 | DR | 103 | ALA | 3.2 |
| 21 | AU | 35 | ARG | 3.2 |
| 25 | DD | 185 | ASN | 3.2 |
| 29 | DH | 18 | GLN | 3.2 |
| 3 | CC | 109 | PRO | 3.2 |
| 31 | DJ | 118 | MET | 3.2 |
| 42 | DU | 14 | LEU | 3.2 |
| 22 | DA | 2300 | C | 3.2 |
| 7 | CG | 123 | GLU | 3.2 |
| 35 | DN | 97 | ILE | 3.2 |
| 22 | DA | 1078 | U | 3.2 |
| 1 | CA | 1022 | A | 3.2 |
| 3 | CC | 91 | VAL | 3.2 |
| 11 | AK | 21 | ALA | 3.2 |
| 27 | DF | 12 | VAL | 3.2 |
| 7 | CG | 77 | SER | 3.2 |
| 10 | CJ | 101 | SER | 3.2 |
| 25 | DD | 97 | SER | 3.2 |
| 7 | CG | 71 | PRO | 3.2 |
| 14 | CN | 6 | MET | 3.2 |
| 3 | CC | 29 | PHE | 3.2 |
| 26 | DE | 122 | GLU | 3.2 |
| 10 | CJ | 32 | THR | 3.1 |
| 25 | DD | 104 | VAL | 3.1 |
| 47 | DZ | 3 | LYS | 3.1 |
| 48 | D0 | 24 | ALA | 3.1 |
| 34 | DM | 88 | ASN | 3.1 |
| 27 | DF | 136 | ILE | 3.1 |
| 30 | BI | 109 | ILE | 3.1 |
| 30 | BI | 122 | ILE | 3.1 |
| 51 | D3 | 16 | LYS | 3.1 |
| 22 | DA | 2109 | U | 3.1 |
| 30 | BI | 84 | ALA | 3.1 |
| 20 | CT | 42 | GLY | 3.1 |
| 27 | DF | 63 | GLN | 3.1 |
| 22 | BA | 1175 | A | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 7 | CG | 116 | MET | 3.1 |
| 9 | CI | 57 | MET | 3.1 |
| 28 | DG | 72 | LEU | 3.1 |
| 42 | DU | 29 | LEU | 3.1 |
| 30 | BI | 26 | PRO | 3.1 |
| 36 | DO | 93 | ASP | 3.1 |
| 39 | DR | 101 | ILE | 3.1 |
| 30 | BI | 104 | ALA | 3.1 |
| 38 | DQ | 2 | ALA | 3.1 |
| 2 | AB | 85 | LEU | 3.1 |
| 26 | DE | 24 | ASN | 3.1 |
| 1 | CA | 1044 | A | 3.1 |
| 6 | CF | 8 | PHE | 3.1 |
| 13 | CM | 114 | LYS | 3.1 |
| 22 | DA | 2147 | A | 3.1 |
| 38 | DQ | 101 | PHE | 3.1 |
| 51 | D3 | 22 | PHE | 3.1 |
| 1 | CA | 1320 | C | 3.1 |
| 24 | DC | 18 | LYS | 3.1 |
| 46 | DY | 37 | LEU | 3.1 |
| 31 | DJ | 119 | PHE | 3.1 |
| 2 | CB | 151 | ILE | 3.1 |
| 20 | CT | 45 | ALA | 3.1 |
| 22 | DA | 2150 | C | 3.1 |
| 16 | CP | 3 | THR | 3.1 |
| 27 | DF | 169 | LEU | 3.1 |
| 28 | DG | 73 | ASN | 3.1 |
| 1 | CA | 1021 | A | 3.1 |
| 11 | AK | 126 | LYS | 3.1 |
| 28 | DG | 78 | GLY | 3.1 |
| 7 | CG | 30 | LEU | 3.1 |
| 22 | BA | 885 | C | 3.1 |
| 24 | DC | 105 | LEU | 3.1 |
| 19 | CS | 10 | PHE | 3.1 |
| 49 | D1 | 23 | THR | 3.1 |
| 45 | DX | 17 | ASN | 3.1 |
| 13 | AM | 4 | ILE | 3.1 |
| 28 | DG | 134 | LYS | 3.1 |
| 10 | CJ | 26 | VAL | 3.1 |
| 22 | DA | 1094 | U | 3.1 |
| 29 | BH | 84 | ALA | 3.1 |
| 40 | DS | 2 | GLU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20 | CT | 8 | LYS | 3.1 |
| 25 | DD | 133 | THR | 3.1 |
| 40 | DS | 82 | MET | 3.1 |
| 7 | CG | 14 | PRO | 3.1 |
| 9 | CI | 31 | ASN | 3.1 |
| 13 | CM | 92 | ARG | 3.1 |
| 20 | AT | 4 | ILE | 3.1 |
| 41 | BT | 2 | ILE | 3.1 |
| 1 | CA | 999 | C | 3.1 |
| 26 | DE | 102 | ARG | 3.1 |
| 30 | BI | 103 | ARG | 3.1 |
| 10 | CJ | 67 | ILE | 3.1 |
| 14 | CN | 52 | PRO | 3.1 |
| 29 | BH | 118 | PRO | 3.1 |
| 36 | DO | 12 | THR | 3.1 |
| 7 | CG | 125 | SER | 3.0 |
| 13 | CM | 65 | VAL | 3.0 |
| 19 | CS | 19 | VAL | 3.0 |
| 30 | BI | 61 | VAL | 3.0 |
| 27 | BF | 72 | LYS | 3.0 |
| 53 | B5 | 37 | LYS | 3.0 |
| 10 | CJ | 90 | LEU | 3.0 |
| 44 | DW | 79 | PHE | 3.0 |
| 40 | DS | 110 | ARG | 3.0 |
| 45 | DX | 74 | ARG | 3.0 |
| 27 | DF | 131 | GLY | 3.0 |
| 30 | DI | 109 | ILE | 3.0 |
| 14 | CN | 50 | THR | 3.0 |
| 1 | AA | 844 | G | 3.0 |
| 32 | DK | 67 | LYS | 3.0 |
| 36 | DO | 73 | ALA | 3.0 |
| 36 | DO | 88 | LYS | 3.0 |
| 9 | AI | 54 | LEU | 3.0 |
| 21 | CU | 47 | ARG | 3.0 |
| 29 | BH | 62 | LEU | 3.0 |
| 2 | CB | 145 | GLU | 3.0 |
| 30 | BI | 121 | ASP | 3.0 |
| 36 | DO | 2 | ASP | 3.0 |
| 44 | DW | 42 | GLY | 3.0 |
| 51 | D3 | 24 | HIS | 3.0 |
| 10 | CJ | 40 | ILE | 3.0 |
| 12 | AL | 15 | LYS | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | DG | 12 | PRO | 3.0 |
| 36 | DO | 3 | LYS | 3.0 |
| 24 | DC | 92 | ALA | 3.0 |
| 27 | DF | 159 | THR | 3.0 |
| 26 | DE | 125 | SER | 3.0 |
| 29 | BH | 63 | ALA | 3.0 |
| 42 | DU | 30 | SER | 3.0 |
| 3 | CC | 157 | LEU | 3.0 |
| 20 | CT | 66 | LEU | 3.0 |
| 41 | DT | 51 | PHE | 3.0 |
| 43 | DV | 91 | PHE | 3.0 |
| 26 | DE | 171 | ASP | 3.0 |
| 2 | CB | 40 | ILE | 3.0 |
| 26 | DE | 188 | MET | 3.0 |
| 30 | DI | 10 | LYS | 3.0 |
| 30 | DI | 86 | ILE | 3.0 |
| 38 | DQ | 74 | ILE | 3.0 |
| 40 | DS | 31 | GLN | 3.0 |
| 25 | DD | 26 | VAL | 3.0 |
| 36 | DO | 53 | THR | 3.0 |
| 37 | DP | 74 | PHE | 3.0 |
| 3 | CC | 197 | GLY | 3.0 |
| 30 | DI | 89 | GLY | 3.0 |
| 30 | DI | 91 | GLY | 3.0 |
| 39 | DR | 66 | HIS | 3.0 |
| 27 | DF | 8 | TYR | 3.0 |
| 7 | CG | 65 | ALA | 3.0 |
| 17 | CQ | 50 | ASN | 3.0 |
| 20 | CT | 41 | ALA | 3.0 |
| 22 | DA | 544 | C | 3.0 |
| 22 | DA | 1176 | U | 3.0 |
| 13 | AM | 114 | LYS | 3.0 |
| 37 | DP | 85 | SER | 3.0 |
| 22 | BA | 2128 | G | 3.0 |
| 26 | DE | 98 | LYS | 3.0 |
| 36 | DO | 50 | ALA | 3.0 |
| 43 | DV | 23 | ALA | 3.0 |
| 46 | DY | 17 | GLU | 3.0 |
| 1 | CA | 1362 | A | 3.0 |
| 10 | AJ | 90 | LEU | 3.0 |
| 22 | DA | 101 | A | 3.0 |
| 29 | DH | 54 | LEU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | CD | 36 | GLN | 3.0 |
| 27 | DF | 80 | ARG | 3.0 |
| 30 | BI | 36 | MET | 3.0 |
| 37 | DP | 13 | MET | 3.0 |
| 1 | AA | 79 | G | 3.0 |
| 22 | DA | 277 | G | 3.0 |
| 27 | DF | 7 | TYR | 3.0 |
| 29 | DH | 139 | PHE | 3.0 |
| 32 | DK | 82 | ASN | 3.0 |
| 25 | DD | 154 | LYS | 3.0 |
| 41 | DT | 40 | LYS | 3.0 |
| 42 | DU | 47 | LYS | 3.0 |
| 22 | DA | 2106 | U | 3.0 |
| 33 | DL | 18 | ARG | 3.0 |
| 44 | DW | 75 | LYS | 3.0 |
| 46 | DY | 40 | SER | 3.0 |
| 17 | CQ | 5 | ILE | 3.0 |
| 26 | DE | 129 | PRO | 2.9 |
| 46 | DY | 32 | ALA | 2.9 |
| 9 | CI | 64 | TYR | 2.9 |
| 33 | DL | 6 | LEU | 2.9 |
| 28 | DG | 53 | GLY | 2.9 |
| 32 | DK | 104 | THR | 2.9 |
| 36 | DO | 74 | VAL | 2.9 |
| 20 | CT | 64 | LYS | 2.9 |
| 36 | DO | 21 | LEU | 2.9 |
| 33 | DL | 58 | TYR | 2.9 |
| 42 | DU | 99 | ASN | 2.9 |
| 1 | CA | 90 | C | 2.9 |
| 3 | CC | 196 | ILE | 2.9 |
| 28 | DG | 49 | THR | 2.9 |
| 41 | DT | 30 | ILE | 2.9 |
| 27 | BF | 80 | ARG | 2.9 |
| 2 | CB | 117 | LEU | 2.9 |
| 3 | CC | 124 | LEU | 2.9 |
| 7 | CG | 152 | ALA | 2.9 |
| 28 | DG | 150 | ALA | 2.9 |
| 25 | DD | 10 | GLY | 2.9 |
| 2 | AB | 213 | TYR | 2.9 |
| 41 | DT | 92 | ASN | 2.9 |
| 6 | CF | 79 | ARG | 2.9 |
| 17 | CQ | 11 | ARG | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | DG | 25 | THR | 2.9 |
| 31 | DJ | 95 | ARG | 2.9 |
| 46 | DY | 60 | LYS | 2.9 |
| 9 | CI | 67 | VAL | 2.9 |
| 40 | DS | 106 | VAL | 2.9 |
| 22 | DA | 549 | G | 2.9 |
| 26 | DE | 23 | PHE | 2.9 |
| 27 | DF | 77 | PHE | 2.9 |
| 36 | DO | 105 | ALA | 2.9 |
| 18 | CR | 20 | GLU | 2.9 |
| 22 | DA | 280 | U | 2.9 |
| 41 | DT | 59 | ASN | 2.9 |
| 25 | DD | 38 | LYS | 2.9 |
| 36 | DO | 76 | LYS | 2.9 |
| 51 | D3 | 52 | LYS | 2.9 |
| 44 | DW | 80 | ILE | 2.9 |
| 26 | DE | 72 | SER | 2.9 |
| 34 | DM | 105 | MET | 2.9 |
| 42 | DU | 49 | VAL | 2.9 |
| 29 | BH | 76 | GLU | 2.9 |
| 22 | DA | 2169 | A | 2.9 |
| 44 | DW | 24 | LYS | 2.9 |
| 47 | DZ | 56 | LYS | 2.9 |
| 41 | BT | 69 | ARG | 2.9 |
| 33 | DL | 81 | ASP | 2.9 |
| 41 | DT | 37 | ASP | 2.9 |
| 26 | DE | 15 | SER | 2.9 |
| 39 | DR | 51 | VAL | 2.9 |
| 9 | CI | 89 | GLU | 2.9 |
| 33 | DL | 28 | GLY | 2.9 |
| 33 | DL | 82 | LEU | 2.9 |
| 13 | CM | 13 | LYS | 2.9 |
| 30 | BI | 72 | LYS | 2.9 |
| 9 | CI | 90 | TYR | 2.9 |
| 53 | B5 | 102 | GLN | 2.9 |
| 22 | DA | 1530 | G | 2.9 |
| 25 | DD | 200 | ASP | 2.9 |
| 10 | CJ | 46 | LYS | 2.9 |
| 13 | CM | 78 | LYS | 2.9 |
| 41 | DT | 88 | LYS | 2.9 |
| 19 | CS | 69 | HIS | 2.9 |
| 27 | DF | 150 | ARG | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 46 | DY | 45 | GLN | 2.9 |
| 22 | DA | 2116 | G | 2.9 |
| 17 | CQ | 46 | VAL | 2.9 |
| 30 | BI | 140 | VAL | 2.9 |
| 30 | DI | 87 | LYS | 2.9 |
| 38 | DQ | 39 | VAL | 2.9 |
| 51 | D3 | 15 | LYS | 2.9 |
| 41 | DT | 75 | GLY | 2.9 |
| 2 | CB | 35 | ARG | 2.9 |
| 34 | DM | 35 | ALA | 2.9 |
| 9 | CI | 9 | THR | 2.9 |
| 9 | CI | 111 | VAL | 2.9 |
| 36 | DO | 114 | GLY | 2.9 |
| 37 | DP | 35 | GLY | 2.9 |
| 40 | DS | 45 | VAL | 2.9 |
| 25 | DD | 95 | SER | 2.8 |
| 22 | DA | 1044 | C | 2.8 |
| 27 | DF | 135 | GLN | 2.8 |
| 33 | DL | 30 | THR | 2.8 |
| 36 | DO | 29 | HIS | 2.8 |
| 17 | AQ | 5 | ILE | 2.8 |
| 27 | DF | 19 | GLU | 2.8 |
| 30 | BI | 119 | GLY | 2.8 |
| 44 | DW | 73 | GLY | 2.8 |
| 13 | CM | 19 | LEU | 2.8 |
| 25 | DD | 75 | ALA | 2.8 |
| 27 | DF | 17 | MET | 2.8 |
| 29 | DH | 100 | ALA | 2.8 |
| 30 | BI | 106 | LEU | 2.8 |
| 36 | DO | 18 | LEU | 2.8 |
| 40 | DS | 54 | ALA | 2.8 |
| 40 | DS | 93 | ALA | 2.8 |
| 12 | AL | 123 | LYS | 2.8 |
| 27 | DF | 29 | PRO | 2.8 |
| 14 | CN | 42 | TRP | 2.8 |
| 44 | DW | 46 | HIS | 2.8 |
| 45 | DX | 20 | HIS | 2.8 |
| 11 | AK | 110 | ILE | 2.8 |
| 14 | CN | 41 | ARG | 2.8 |
| 29 | BH | 94 | ILE | 2.8 |
| 32 | DK | 81 | GLY | 2.8 |
| 1 | CA | 4 | U | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | DF | 121 | SER | 2.8 |
| 28 | BG | 111 | HIS | 2.8 |
| 33 | DL | 142 | ILE | 2.8 |
| 43 | DV | 89 | ILE | 2.8 |
| 14 | CN | 98 | LYS | 2.8 |
| 40 | DS | 20 | VAL | 2.8 |
| 33 | DL | 79 | LEU | 2.8 |
| 37 | DP | 8 | LEU | 2.8 |
| 16 | AP | 22 | ALA | 2.8 |
| 34 | DM | 79 | ALA | 2.8 |
| 22 | DA | 2118 | U | 2.8 |
| 22 | DA | 2173 | A | 2.8 |
| 27 | DF | 178 | ARG | 2.8 |
| 30 | DI | 88 | SER | 2.8 |
| 3 | CC | 207 | ILE | 2.8 |
| 34 | DM | 126 | ILE | 2.8 |
| 2 | CB | 90 | PHE | 2.8 |
| 2 | CB | 162 | PHE | 2.8 |
| 11 | AK | 14 | LYS | 2.8 |
| 22 | DA | 2110 | G | 2.8 |
| 37 | DP | 20 | PHE | 2.8 |
| 6 | CF | 10 | VAL | 2.8 |
| 21 | AU | 23 | CYS | 2.8 |
| 13 | CM | 76 | SER | 2.8 |
| 1 | CA | 1492 | A | 2.8 |
| 26 | DE | 29 | HIS | 2.8 |
| 33 | DL | 5 | THR | 2.8 |
| 7 | CG | 91 | VAL | 2.8 |
| 24 | DC | 94 | VAL | 2.8 |
| 7 | CG | 48 | GLU | 2.8 |
| 28 | DG | 101 | ASN | 2.8 |
| 30 | DI | 104 | ALA | 2.8 |
| 46 | DY | 58 | ASN | 2.8 |
| 22 | DA | 1173 | U | 2.8 |
| 22 | DA | 1224 | U | 2.8 |
| 13 | CM | 4 | ILE | 2.8 |
| 14 | CN | 30 | ILE | 2.8 |
| 35 | DN | 27 | SER | 2.8 |
| 48 | D0 | 42 | HIS | 2.8 |
| 1 | CA | 206 | C | 2.8 |
| 22 | DA | 2164 | C | 2.8 |
| 14 | CN | 19 | LYS | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | DQ | 112 | LYS | 2.8 |
| 39 | DR | 87 | GLN | 2.8 |
| 44 | DW | 61 | ALA | 2.8 |
| 24 | DC | 235 | GLY | 2.8 |
| 19 | AS | 74 | PHE | 2.8 |
| 40 | DS | 108 | SER | 2.8 |
| 10 | CJ | 97 | ASP | 2.8 |
| 3 | CC | 138 | VAL | 2.8 |
| 13 | CM | 29 | ARG | 2.8 |
| 39 | DR | 54 | VAL | 2.8 |
| 22 | DA | 846 | U | 2.8 |
| 22 | DA | 882 | G | 2.8 |
| 27 | DF | 165 | GLU | 2.8 |
| 33 | DL | 13 | LYS | 2.8 |
| 10 | CJ | 42 | LEU | 2.8 |
| 39 | DR | 22 | LEU | 2.8 |
| 19 | AS | 39 | THR | 2.8 |
| 1 | CA | 207 | C | 2.8 |
| 2 | CB | 206 | ALA | 2.8 |
| 2 | CB | 100 | MET | 2.7 |
| 34 | DM | 17 | ASN | 2.7 |
| 40 | DS | 86 | MET | 2.7 |
| 46 | DY | 30 | MET | 2.7 |
| 7 | CG | 78 | ARG | 2.7 |
| 26 | DE | 47 | LYS | 2.7 |
| 41 | DT | 82 | LYS | 2.7 |
| 17 | CQ | 76 | VAL | 2.7 |
| 21 | AU | 32 | VAL | 2.7 |
| 46 | DY | 28 | LEU | 2.7 |
| 20 | CT | 47 | ALA | 2.7 |
| 38 | DQ | 113 | ALA | 2.7 |
| 39 | DR | 29 | THR | 2.7 |
| 41 | DT | 60 | THR | 2.7 |
| 14 | CN | 95 | GLY | 2.7 |
| 22 | DA | 1085 | A | 2.7 |
| 28 | DG | 149 | ARG | 2.7 |
| 36 | DO | 43 | ASN | 2.7 |
| 7 | CG | 27 | VAL | 2.7 |
| 26 | DE | 138 | LEU | 2.7 |
| 37 | BP | 2 | SER | 2.7 |
| 39 | DR | 38 | VAL | 2.7 |
| 3 | CC | 180 | ALA | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 50 | D2 | 36 | ALA | 2.7 |
| 27 | DF | 9 | LYS | 2.7 |
| 27 | DF | 88 | LYS | 2.7 |
| 31 | DJ | 92 | MET | 2.7 |
| 22 | DA | 1058 | U | 2.7 |
| 50 | D2 | 13 | ASN | 2.7 |
| 9 | CI | 72 | ILE | 2.7 |
| 14 | AN | 52 | PRO | 2.7 |
| 40 | DS | 7 | HIS | 2.7 |
| 25 | DD | 41 | ALA | 2.7 |
| 51 | D3 | 47 | LYS | 2.7 |
| 36 | DO | 84 | GLU | 2.7 |
| 2 | AB | 69 | PHE | 2.7 |
| 13 | CM | 9 | ILE | 2.7 |
| 2 | CB | 217 | VAL | 2.7 |
| 3 | CC | 108 | LYS | 2.7 |
| 26 | DE | 32 | VAL | 2.7 |
| 40 | DS | 105 | VAL | 2.7 |
| 41 | DT | 47 | VAL | 2.7 |
| 30 | BI | 15 | ALA | 2.7 |
| 11 | AK | 19 | GLY | 2.7 |
| 13 | AM | 47 | GLU | 2.7 |
| 28 | BG | 24 | ILE | 2.7 |
| 3 | CC | 33 | LEU | 2.7 |
| 9 | CI | 32 | GLN | 2.7 |
| 13 | CM | 57 | ARG | 2.7 |
| 14 | CN | 63 | ARG | 2.7 |
| 20 | CT | 25 | ARG | 2.7 |
| 2 | CB | 83 | ALA | 2.7 |
| 3 | CC | 155 | GLY | 2.7 |
| 9 | CI | 86 | ALA | 2.7 |
| 32 | DK | 110 | GLU | 2.7 |
| 1 | CA | 1321 | U | 2.7 |
| 19 | AS | 41 | PHE | 2.7 |
| 16 | AP | 4 | ILE | 2.7 |
| 40 | DS | 103 | ILE | 2.7 |
| 44 | DW | 44 | LYS | 2.7 |
| 2 | AB | 139 | ARG | 2.7 |
| 19 | CS | 58 | VAL | 2.7 |
| 29 | BH | 65 | ALA | 2.7 |
| 33 | DL | 83 | ALA | 2.7 |
| 13 | CM | 81 | MET | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | DA | 1066 | U | 2.7 |
| 45 | DX | 50 | ARG | 2.7 |
| 13 | CM | 16 | VAL | 2.7 |
| 22 | DA | 1170 | C | 2.7 |
| 26 | DE | 178 | VAL | 2.7 |
| 30 | BI | 30 | GLN | 2.7 |
| 30 | BI | 33 | VAL | 2.7 |
| 35 | DN | 120 | GLU | 2.7 |
| 41 | DT | 31 | VAL | 2.7 |
| 22 | DA | 1057 | A | 2.7 |
| 28 | DG | 130 | GLU | 2.7 |
| 36 | DO | 80 | GLU | 2.7 |
| 44 | DW | 83 | GLU | 2.7 |
| 4 | CD | 151 | LYS | 2.7 |
| 40 | DS | 73 | LYS | 2.7 |
| 42 | DU | 93 | VAL | 2.7 |
| 50 | D2 | 2 | LYS | 2.7 |
| 28 | DG | 61 | GLY | 2.7 |
| 3 | CC | 71 | ALA | 2.7 |
| 2 | CB | 18 | HIS | 2.7 |
| 34 | DM | 40 | ARG | 2.7 |
| 14 | AN | 55 | SER | 2.6 |
| 25 | DD | 188 | LEU | 2.6 |
| 33 | DL | 14 | LYS | 2.6 |
| 27 | DF | 56 | ASP | 2.6 |
| 42 | BU | 52 | LEU | 2.6 |
| 28 | DG | 7 | ALA | 2.6 |
| 41 | DT | 77 | ARG | 2.6 |
| 45 | DX | 18 | ARG | 2.6 |
| 31 | DJ | 15 | TRP | 2.6 |
| 48 | D0 | 34 | SER | 2.6 |
| 34 | DM | 103 | TYR | 2.6 |
| 52 | D4 | 26 | ILE | 2.6 |
| 1 | AA | 81 | A | 2.6 |
| 13 | AM | 19 | LEU | 2.6 |
| 19 | AS | 71 | LEU | 2.6 |
| 20 | CT | 82 | GLN | 2.6 |
| 22 | DA | 1048 | A | 2.6 |
| 10 | CJ | 80 | THR | 2.6 |
| 10 | AJ | 34 | ALA | 2.6 |
| 22 | DA | 1606 | C | 2.6 |
| 24 | DC | 106 | ALA | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | DD | 101 | PHE | 2.6 |
| 7 | CG | 60 | GLU | 2.6 |
| 30 | DI | 100 | LYS | 2.6 |
| 53 | B5 | 163 | GLU | 2.6 |
| 44 | DW | 82 | ILE | 2.6 |
| 26 | DE | 41 | GLN | 2.6 |
| 33 | DL | 27 | LEU | 2.6 |
| 40 | DS | 69 | LEU | 2.6 |
| 49 | D1 | 34 | LEU | 2.6 |
| 1 | CA | 80 | A | 2.6 |
| 1 | CA | 1441 | A | 2.6 |
| 2 | AB | 187 | VAL | 2.6 |
| 3 | CC | 158 | GLY | 2.6 |
| 22 | DA | 344 | A | 2.6 |
| 25 | DD | 9 | VAL | 2.6 |
| 28 | DG | 56 | ASP | 2.6 |
| 35 | DN | 26 | GLY | 2.6 |
| 29 | DH | 149 | GLU | 2.6 |
| 6 | CF | 36 | ILE | 2.6 |
| 9 | CI | 79 | ILE | 2.6 |
| 33 | DL | 103 | ILE | 2.6 |
| 1 | CA | 1025 | U | 2.6 |
| 38 | DQ | 44 | GLN | 2.6 |
| 2 | AB | 35 | ARG | 2.6 |
| 37 | DP | 31 | TRP | 2.6 |
| 3 | CC | 85 | GLU | 2.6 |
| 7 | CG | 63 | GLU | 2.6 |
| 27 | DF | 160 | ALA | 2.6 |
| 40 | DS | 43 | ALA | 2.6 |
| 14 | CN | 49 | GLN | 2.6 |
| 27 | DF | 111 | ILE | 2.6 |
| 36 | DO | 16 | ARG | 2.6 |
| 36 | DO | 38 | GLN | 2.6 |
| 44 | DW | 57 | HIS | 2.6 |
| 9 | CI | 98 | LEU | 2.6 |
| 26 | DE | 20 | GLY | 2.6 |
| 29 | DH | 147 | VAL | 2.6 |
| 38 | DQ | 15 | LYS | 2.6 |
| 42 | DU | 81 | ASP | 2.6 |
| 45 | DX | 4 | VAL | 2.6 |
| 48 | D0 | 57 | LYS | 2.6 |
| 3 | CC | 146 | ALA | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | DD | 23 | PRO | 2.6 |
| 36 | DO | 113 | ALA | 2.6 |
| 22 | DA | 2120 | G | 2.6 |
| 22 | DA | 2127 | G | 2.6 |
| 28 | DG | 129 | THR | 2.6 |
| 19 | CS | 3 | ARG | 2.6 |
| 28 | DG | 77 | ILE | 2.6 |
| 28 | DG | 141 | ILE | 2.6 |
| 52 | D4 | 24 | ARG | 2.6 |
| 22 | DA | 183 | C | 2.6 |
| 1 | AA | 842 | U | 2.6 |
| 3 | AC | 175 | LEU | 2.6 |
| 22 | DA | 653 | U | 2.6 |
| 29 | BH | 13 | GLY | 2.6 |
| 30 | BI | 138 | LEU | 2.6 |
| 41 | DT | 93 | LEU | 2.6 |
| 53 | B5 | 83 | LYS | 2.6 |
| 2 | AB | 196 | VAL | 2.6 |
| 41 | DT | 78 | SER | 2.6 |
| 4 | CD | 27 | ALA | 2.6 |
| 53 | B5 | 187 | ALA | 2.6 |
| 28 | DG | 153 | ARG | 2.6 |
| 36 | DO | 81 | ARG | 2.6 |
| 42 | DU | 6 | ARG | 2.6 |
| 46 | BY | 23 | ARG | 2.6 |
| 22 | DA | 1084 | A | 2.6 |
| 22 | DA | 1103 | A | 2.6 |
| 3 | AC | 55 | ILE | 2.6 |
| 27 | DF | 27 | GLN | 2.6 |
| 2 | AB | 18 | HIS | 2.6 |
| 7 | CG | 90 | GLU | 2.6 |
| 8 | CH | 25 | VAL | 2.6 |
| 26 | DE | 169 | VAL | 2.6 |
| 33 | DL | 143 | GLU | 2.6 |
| 35 | DN | 60 | VAL | 2.6 |
| 35 | DN | 21 | PHE | 2.6 |
| 37 | DP | 115 | ASN | 2.6 |
| 44 | DW | 47 | ALA | 2.6 |
| 25 | DD | 8 | LYS | 2.6 |
| 3 | CC | 70 | THR | 2.6 |
| 27 | DF | 44 | ILE | 2.6 |
| 10 | CJ | 92 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | DC | 205 | LEU | 2.6 |
| 51 | D3 | 62 | LEU | 2.6 |
| 17 | CQ | 59 | VAL | 2.6 |
| 14 | AN | 20 | TYR | 2.6 |
| 25 | DD | 77 | ARG | 2.6 |
| 49 | D1 | 14 | SER | 2.6 |
| 27 | DF | 53 | ALA | 2.6 |
| 29 | DH | 74 | ALA | 2.6 |
| 30 | DI | 95 | LYS | 2.6 |
| 37 | DP | 38 | LYS | 2.6 |
| 9 | AI | 4 | ASN | 2.6 |
| 26 | DE | 89 | PRO | 2.6 |
| 52 | D4 | 37 | GLN | 2.5 |
| 22 | DA | 2181 | U | 2.5 |
| 46 | DY | 22 | LEU | 2.5 |
| 22 | DA | 2309 | A | 2.5 |
| 26 | DE | 187 | VAL | 2.5 |
| 1 | CA | 1454 | G | 2.5 |
| 28 | DG | 74 | SER | 2.5 |
| 26 | DE | 161 | ALA | 2.5 |
| 28 | DG | 5 | ALA | 2.5 |
| 29 | BH | 111 | ALA | 2.5 |
| 41 | DT | 45 | ALA | 2.5 |
| 20 | CT | 84 | ASN | 2.5 |
| 42 | BU | 53 | ASN | 2.5 |
| 28 | DG | 66 | GLY | 2.5 |
| 36 | DO | 22 | GLY | 2.5 |
| 10 | CJ | 7 | ARG | 2.5 |
| 40 | DS | 98 | LYS | 2.5 |
| 53 | B5 | 19 | LYS | 2.5 |
| 30 | DI | 142 | ASP | 2.5 |
| 31 | DJ | 48 | VAL | 2.5 |
| 33 | DL | 90 | VAL | 2.5 |
| 39 | DR | 63 | VAL | 2.5 |
| 22 | DA | 2129 | C | 2.5 |
| 22 | DA | 2163 | A | 2.5 |
| 40 | DS | 34 | ASP | 2.5 |
| 39 | DR | 35 | PHE | 2.5 |
| 22 | BA | 2133 | G | 2.5 |
| 25 | DD | 125 | TRP | 2.5 |
| 30 | DI | 81 | LYS | 2.5 |
| 44 | DW | 68 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | AN | 24 | ARG | 2.5 |
| 19 | AS | 24 | GLU | 2.5 |
| 19 | CS | 9 | PRO | 2.5 |
| 19 | CS | 70 | LYS | 2.5 |
| 42 | DU | 33 | LYS | 2.5 |
| 33 | DL | 4 | ASN | 2.5 |
| 15 | AO | 57 | LEU | 2.5 |
| 16 | CP | 52 | LEU | 2.5 |
| 48 | D0 | 28 | LEU | 2.5 |
| 1 | CA | 1224 | U | 2.5 |
| 22 | DA | 2167 | U | 2.5 |
| 13 | CM | 61 | ALA | 2.5 |
| 37 | DP | 9 | GLU | 2.5 |
| 41 | DT | 13 | ALA | 2.5 |
| 44 | BW | 85 | GLU | 2.5 |
| 22 | BA | 1847 | A | 2.5 |
| 22 | DA | 866 | A | 2.5 |
| 9 | CI | 83 | ILE | 2.5 |
| 29 | DH | 119 | ASN | 2.5 |
| 32 | DK | 38 | ILE | 2.5 |
| 50 | D2 | 7 | PRO | 2.5 |
| 3 | CC | 173 | VAL | 2.5 |
| 7 | CG | 11 | LYS | 2.5 |
| 41 | DT | 79 | ASP | 2.5 |
| 13 | CM | 37 | ALA | 2.5 |
| 28 | DG | 170 | ARG | 2.5 |
| 42 | DU | 72 | ILE | 2.5 |
| 29 | BH | 145 | ASN | 2.5 |
| 47 | DZ | 29 | LEU | 2.5 |
| 53 | B5 | 189 | ASN | 2.5 |
| 3 | CC | 153 | VAL | 2.5 |
| 5 | CE | 152 | MET | 2.5 |
| 10 | CJ | 27 | GLU | 2.5 |
| 23 | DB | 117 | G | 2.5 |
| 44 | DW | 26 | PHE | 2.5 |
| 18 | AR | 74 | HIS | 2.5 |
| 27 | DF | 110 | ARG | 2.5 |
| 13 | CM | 2 | ALA | 2.5 |
| 32 | DK | 83 | ALA | 2.5 |
| 44 | DW | 34 | GLY | 2.5 |
| 28 | DG | 112 | PRO | 2.5 |
| 33 | DL | 8 | PRO | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 20 | CT | 19 | LYS | 2.5 |
| 43 | DV | 38 | LEU | 2.5 |
| 22 | DA | 2111 | U | 2.5 |
| 37 | DP | 17 | VAL | 2.5 |
| 39 | DR | 90 | ARG | 2.5 |
| 49 | D1 | 19 | HIS | 2.5 |
| 1 | AA | 82 | G | 2.5 |
| 35 | DN | 101 | GLY | 2.5 |
| 46 | DY | 25 | GLN | 2.5 |
| 7 | CG | 110 | LYS | 2.5 |
| 24 | DC | 93 | LEU | 2.5 |
| 30 | BI | 86 | ILE | 2.5 |
| 29 | DH | 123 | ARG | 2.5 |
| 35 | DN | 45 | ARG | 2.5 |
| 36 | DO | 102 | ARG | 2.5 |
| 41 | DT | 89 | GLU | 2.5 |
| 4 | AD | 177 | LYS | 2.5 |
| 27 | DF | 33 | LYS | 2.5 |
| 28 | DG | 29 | LYS | 2.5 |
| 28 | DG | 97 | ALA | 2.5 |
| 39 | DR | 24 | LYS | 2.5 |
| 14 | AN | 26 | GLU | 2.4 |
| 22 | BA | 1926 | U | 2.4 |
| 29 | BH | 11 | ASN | 2.4 |
| 30 | BI | 42 | PHE | 2.4 |
| 50 | D2 | 30 | VAL | 2.4 |
| 3 | CC | 150 | LYS | 2.4 |
| 26 | DE | 168 | ASP | 2.4 |
| 7 | CG | 81 | GLY | 2.4 |
| 22 | DA | 2158 | A | 2.4 |
| 43 | DV | 34 | LYS | 2.4 |
| 28 | DG | 128 | GLN | 2.4 |
| 9 | CI | 84 | THR | 2.4 |
| 10 | CJ | 31 | ARG | 2.4 |
| 33 | DL | 126 | ARG | 2.4 |
| 22 | DA | 883 | G | 2.4 |
| 22 | DA | 1068 | G | 2.4 |
| 23 | DB | 18 | G | 2.4 |
| 37 | DP | 19 | SER | 2.4 |
| 21 | AU | 25 | LYS | 2.4 |
| 22 | BA | 1094 | U | 2.4 |
| 27 | DF | 96 | MET | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | DF | 151 | GLY | 2.4 |
| 25 | DD | 132 | ALA | 2.4 |
| 22 | BA | 613 | A | 2.4 |
| 11 | AK | 13 | ARG | 2.4 |
| 29 | BH | 125 | THR | 2.4 |
| 39 | DR | 49 | ILE | 2.4 |
| 29 | DH | 35 | LYS | 2.4 |
| 22 | BA | 1100 | C | 2.4 |
| 22 | BA | 2402 | U | 2.4 |
| 22 | DA | 2175 | C | 2.4 |
| 44 | DW | 64 | ASP | 2.4 |
| 29 | DH | 140 | ALA | 2.4 |
| 30 | BI | 63 | ALA | 2.4 |
| 17 | CQ | 63 | GLU | 2.4 |
| 34 | DM | 78 | LEU | 2.4 |
| 45 | DX | 71 | LEU | 2.4 |
| 28 | DG | 157 | TYR | 2.4 |
| 30 | BI | 56 | PRO | 2.4 |
| 29 | BH | 147 | VAL | 2.4 |
| 2 | AB | 226 | SER | 2.4 |
| 7 | CG | 37 | SER | 2.4 |
| 22 | BA | 2192 | U | 2.4 |
| 22 | DA | 2796 | U | 2.4 |
| 30 | DI | 128 | SER | 2.4 |
| 9 | CI | 62 | ASP | 2.4 |
| 9 | CI | 17 | ALA | 2.4 |
| 36 | DO | 82 | ALA | 2.4 |
| 36 | DO | 4 | LYS | 2.4 |
| 28 | BG | 26 | ILE | 2.4 |
| 29 | DH | 58 | LEU | 2.4 |
| 22 | DA | 279 | A | 2.4 |
| 32 | DK | 10 | VAL | 2.4 |
| 1 | AA | 85 | U | 2.4 |
| 1 | CA | 208 | U | 2.4 |
| 18 | CR | 43 | ARG | 2.4 |
| 22 | DA | 931 | U | 2.4 |
| 29 | BH | 17 | ASP | 2.4 |
| 30 | BI | 64 | ASP | 2.4 |
| 30 | DI | 117 | MET | 2.4 |
| 14 | AN | 23 | LYS | 2.4 |
| 28 | DG | 42 | GLU | 2.4 |
| 48 | D0 | 53 | LYS | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | CC | 77 | ILE | 2.4 |
| 7 | CG | 47 | LEU | 2.4 |
| 11 | AK | 42 | LEU | 2.4 |
| 26 | DE | 133 | LEU | 2.4 |
| 19 | AS | 32 | ARG | 2.4 |
| 26 | DE | 121 | VAL | 2.4 |
| 34 | DM | 130 | PHE | 2.4 |
| 38 | DQ | 106 | PHE | 2.4 |
| 53 | B5 | 21 | TYR | 2.4 |
| 1 | CA | 1313 | U | 2.4 |
| 26 | DE | 2 | GLU | 2.4 |
| 42 | DU | 9 | ASP | 2.4 |
| 53 | B5 | 25 | GLU | 2.4 |
| 7 | CG | 130 | ASN | 2.4 |
| 7 | CG | 46 | ALA | 2.4 |
| 20 | CT | 87 | ALA | 2.4 |
| 28 | DG | 136 | ALA | 2.4 |
| 1 | CA | 1317 | C | 2.4 |
| 2 | CB | 22 | TYR | 2.4 |
| 3 | CC | 195 | VAL | 2.4 |
| 9 | AI | 19 | VAL | 2.4 |
| 24 | DC | 103 | TYR | 2.4 |
| 42 | DU | 43 | LYS | 2.4 |
| 33 | DL | 31 | GLY | 2.4 |
| 22 | DA | 2119 | A | 2.4 |
| 11 | CK | 42 | LEU | 2.4 |
| 38 | DQ | 83 | LEU | 2.4 |
| 42 | DU | 41 | LEU | 2.4 |
| 3 | CC | 172 | ARG | 2.4 |
| 30 | DI | 40 | LYS | 2.4 |
| 7 | AG | 151 | PHE | 2.4 |
| 13 | CM | 112 | PRO | 2.4 |
| 29 | DH | 108 | VAL | 2.4 |
| 30 | BI | 89 | GLY | 2.4 |
| 32 | DK | 103 | VAL | 2.4 |
| 36 | DO | 49 | VAL | 2.4 |
| 1 | CA | 1043 | G | 2.4 |
| 1 | CA | 1235 | U | 2.4 |
| 19 | CS | 27 | ASP | 2.4 |
| 30 | BI | 117 | MET | 2.4 |
| 30 | DI | 125 | MET | 2.4 |
| 31 | DJ | 14 | ASP | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | DG | 46 | ALA | 2.4 |
| 25 | DD | 56 | LYS | 2.4 |
| 40 | DS | 83 | LYS | 2.4 |
| 50 | D2 | 21 | ARG | 2.4 |
| 51 | D3 | 44 | LEU | 2.4 |
| 22 | DA | 275 | C | 2.4 |
| 18 | CR | 74 | HIS | 2.3 |
| 29 | DH | 132 | PHE | 2.3 |
| 3 | AC | 39 | VAL | 2.3 |
| 29 | DH | 21 | VAL | 2.3 |
| 39 | DR | 33 | VAL | 2.3 |
| 43 | DV | 60 | VAL | 2.3 |
| 33 | DL | 62 | PRO | 2.3 |
| 33 | DL | 104 | GLN | 2.3 |
| 25 | DD | 176 | ASP | 2.3 |
| 26 | DE | 154 | ASP | 2.3 |
| 2 | AB | 134 | ALA | 2.3 |
| 2 | AB | 152 | LYS | 2.3 |
| 28 | DG | 27 | LYS | 2.3 |
| 48 | D0 | 23 | THR | 2.3 |
| 36 | DO | 37 | ALA | 2.3 |
| 3 | CC | 14 | ILE | 2.3 |
| 3 | CC | 94 | ILE | 2.3 |
| 9 | CI | 35 | LEU | 2.3 |
| 13 | AM | 80 | LEU | 2.3 |
| 30 | BI | 102 | SER | 2.3 |
| 22 | DA | 345 | A | 2.3 |
| 3 | CC | 78 | GLY | 2.3 |
| 41 | DT | 67 | VAL | 2.3 |
| 42 | DU | 4 | LYS | 2.3 |
| 51 | D3 | 23 | LYS | 2.3 |
| 2 | CB | 225 | ARG | 2.3 |
| 24 | DC | 48 | ARG | 2.3 |
| 26 | DE | 170 | ARG | 2.3 |
| 33 | DL | 69 | ARG | 2.3 |
| 37 | DP | 91 | ALA | 2.3 |
| 6 | AF | 61 | LEU | 2.3 |
| 9 | AI | 128 | SER | 2.3 |
| 22 | DA | 1408 | G | 2.3 |
| 41 | BT | 92 | ASN | 2.3 |
| 33 | DL | 114 | GLY | 2.3 |
| 1 | AA | 1031 | C | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | DA | 1100 | C | 2.3 |
| 30 | DI | 9 | VAL | 2.3 |
| 53 | B5 | 178 | LYS | 2.3 |
| 1 | CA | 121 | U | 2.3 |
| 17 | CQ | 66 | PRO | 2.3 |
| 42 | DU | 86 | ARG | 2.3 |
| 3 | AC | 168 | TYR | 2.3 |
| 35 | DN | 112 | TYR | 2.3 |
| 43 | DV | 22 | ALA | 2.3 |
| 9 | CI | 53 | GLU | 2.3 |
| 25 | DD | 4 | LEU | 2.3 |
| 31 | DJ | 54 | ILE | 2.3 |
| 34 | DM | 102 | LEU | 2.3 |
| 2 | CB | 215 | GLY | 2.3 |
| 28 | DG | 31 | GLY | 2.3 |
| 22 | BA | 2885 | G | 2.3 |
| 22 | DA | 356 | G | 2.3 |
| 2 | CB | 210 | VAL | 2.3 |
| 16 | AP | 14 | ARG | 2.3 |
| 24 | DC | 172 | VAL | 2.3 |
| 28 | DG | 17 | VAL | 2.3 |
| 32 | DK | 61 | VAL | 2.3 |
| 44 | DW | 51 | VAL | 2.3 |
| 50 | D2 | 41 | ARG | 2.3 |
| 40 | DS | 38 | TYR | 2.3 |
| 43 | DV | 43 | ASP | 2.3 |
| 41 | DT | 56 | GLU | 2.3 |
| 43 | DV | 1 | MET | 2.3 |
| 3 | AC | 157 | LEU | 2.3 |
| 4 | AD | 21 | LEU | 2.3 |
| 40 | DS | 33 | LEU | 2.3 |
| 20 | CT | 51 | PHE | 2.3 |
| 45 | DX | 75 | GLY | 2.3 |
| 26 | DE | 120 | VAL | 2.3 |
| 52 | D4 | 35 | GLN | 2.3 |
| 1 | CA | 81 | A | 2.3 |
| 28 | DG | 54 | PRO | 2.3 |
| 3 | CC | 43 | LEU | 2.3 |
| 3 | CC | 111 | LEU | 2.3 |
| 17 | CQ | 82 | ALA | 2.3 |
| 51 | D3 | 48 | ALA | 2.3 |
| 7 | CG | 84 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | DL | 20 | GLY | 2.3 |
| 28 | DG | 11 | VAL | 2.3 |
| 7 | CG | 56 | LYS | 2.3 |
| 22 | DA | 1460 | U | 2.3 |
| 30 | DI | 141 | GLU | 2.3 |
| 9 | AI | 6 | TYR | 2.3 |
| 10 | CJ | 52 | LEU | 2.3 |
| 17 | CQ | 24 | ALA | 2.3 |
| 26 | DE | 11 | ALA | 2.3 |
| 26 | DE | 141 | MET | 2.3 |
| 12 | AL | 14 | ARG | 2.3 |
| 29 | BH | 99 | ILE | 2.3 |
| 34 | DM | 99 | GLY | 2.3 |
| 30 | BI | 112 | THR | 2.3 |
| 30 | DI | 105 | GLN | 2.3 |
| 33 | DL | 93 | ASN | 2.3 |
| 36 | DO | 116 | GLN | 2.3 |
| 42 | DU | 70 | VAL | 2.3 |
| 7 | CG | 40 | GLU | 2.3 |
| 29 | DH | 137 | GLU | 2.3 |
| 30 | DI | 113 | LYS | 2.3 |
| 42 | DU | 17 | LYS | 2.3 |
| 46 | DY | 4 | LYS | 2.3 |
| 1 | CA | 1228 | C | 2.3 |
| 5 | AE | 115 | LEU | 2.3 |
| 6 | CF | 54 | LEU | 2.3 |
| 24 | DC | 101 | ARG | 2.3 |
| 29 | BH | 12 | LEU | 2.3 |
| 36 | DO | 11 | ALA | 2.3 |
| 2 | AB | 151 | ILE | 2.3 |
| 28 | DG | 24 | ILE | 2.3 |
| 22 | DA | 117 | G | 2.3 |
| 22 | DA | 1529 | G | 2.3 |
| 22 | DA | 2128 | G | 2.3 |
| 53 | B5 | 177 | GLY | 2.3 |
| 9 | CI | 110 | GLN | 2.3 |
| 6 | CF | 96 | VAL | 2.3 |
| 14 | CN | 35 | ASN | 2.3 |
| 49 | D1 | 22 | THR | 2.3 |
| 7 | CG | 5 | ARG | 2.3 |
| 17 | CQ | 65 | ARG | 2.3 |
| 20 | CT | 68 | HIS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | BA | 846 | U | 2.3 |
| 4 | AD | 27 | ALA | 2.3 |
| 30 | BI | 44 | ALA | 2.3 |
| 38 | DQ | 32 | TYR | 2.3 |
| 53 | B5 | 23 | ILE | 2.3 |
| 30 | BI | 45 | LYS | 2.3 |
| 34 | DM | 8 | LYS | 2.3 |
| 2 | CB | 122 | GLN | 2.3 |
| 11 | AK | 113 | VAL | 2.2 |
| 21 | AU | 9 | ASN | 2.2 |
| 24 | DC | 216 | VAL | 2.2 |
| 29 | DH | 110 | VAL | 2.2 |
| 22 | DA | 2833 | U | 2.2 |
| 30 | BI | 116 | ASP | 2.2 |
| 10 | CJ | 23 | ALA | 2.2 |
| 14 | CN | 16 | LEU | 2.2 |
| 14 | CN | 94 | PRO | 2.2 |
| 24 | DC | 99 | GLY | 2.2 |
| 27 | DF | 75 | ALA | 2.2 |
| 28 | DG | 8 | PRO | 2.2 |
| 28 | DG | 44 | LYS | 2.2 |
| 37 | DP | 63 | LYS | 2.2 |
| 1 | CA | 1325 | C | 2.2 |
| 34 | DM | 9 | PHE | 2.2 |
| 21 | AU | 36 | GLU | 2.2 |
| 3 | CC | 39 | VAL | 2.2 |
| 35 | DN | 17 | ARG | 2.2 |
| 49 | D1 | 13 | SER | 2.2 |
| 44 | DW | 56 | ASP | 2.2 |
| 26 | DE | 34 | ALA | 2.2 |
| 27 | DF | 109 | PRO | 2.2 |
| 6 | CF | 80 | PHE | 2.2 |
| 15 | CO | 15 | PHE | 2.2 |
| 39 | DR | 45 | GLU | 2.2 |
| 47 | DZ | 39 | GLU | 2.2 |
| 22 | DA | 1064 | C | 2.2 |
| 32 | DK | 3 | GLN | 2.2 |
| 27 | DF | 108 | VAL | 2.2 |
| 50 | D2 | 34 | ARG | 2.2 |
| 30 | BI | 94 | ASN | 2.2 |
| 30 | BI | 73 | THR | 2.2 |
| 46 | DY | 55 | THR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 1455 | G | 2.2 |
| 2 | AB | 57 | LEU | 2.2 |
| 24 | DC | 232 | HIS | 2.2 |
| 41 | DT | 90 | GLY | 2.2 |
| 51 | D3 | 26 | HIS | 2.2 |
| 3 | AC | 64 | ILE | 2.2 |
| 29 | DH | 4 | ILE | 2.2 |
| 27 | DF | 161 | LYS | 2.2 |
| 43 | DV | 92 | VAL | 2.2 |
| 37 | DP | 3 | ASN | 2.2 |
| 7 | CG | 61 | ALA | 2.2 |
| 21 | CU | 37 | PHE | 2.2 |
| 44 | DW | 36 | ILE | 2.2 |
| 44 | DW | 69 | PHE | 2.2 |
| 22 | BA | 549 | G | 2.2 |
| 22 | DA | 1107 | G | 2.2 |
| 40 | DS | 49 | LYS | 2.2 |
| 23 | DB | 118 | C | 2.2 |
| 24 | DC | 220 | VAL | 2.2 |
| 22 | DA | 2180 | U | 2.2 |
| 27 | DF | 6 | ASP | 2.2 |
| 39 | DR | 25 | LEU | 2.2 |
| 42 | DU | 18 | ASP | 2.2 |
| 43 | DV | 32 | GLY | 2.2 |
| 3 | CC | 149 | ILE | 2.2 |
| 8 | CH | 36 | ILE | 2.2 |
| 30 | DI | 122 | ILE | 2.2 |
| 35 | DN | 52 | ILE | 2.2 |
| 53 | B5 | 26 | ALA | 2.2 |
| 44 | DW | 62 | LYS | 2.2 |
| 1 | CA | 1018 | G | 2.2 |
| 28 | DG | 164 | TYR | 2.2 |
| 24 | DC | 47 | GLY | 2.2 |
| 9 | AI | 39 | PHE | 2.2 |
| 17 | CQ | 4 | LYS | 2.2 |
| 17 | CQ | 6 | ARG | 2.2 |
| 42 | DU | 53 | ASN | 2.2 |
| 2 | CB | 69 | PHE | 2.2 |
| 20 | CT | 62 | ALA | 2.2 |
| 46 | DY | 9 | LYS | 2.2 |
| 26 | DE | 73 | ILE | 2.2 |
| 29 | BH | 82 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 39 | DR | 7 | SER | 2.2 |
| 40 | DS | 74 | ILE | 2.2 |
| 48 | D0 | 55 | ILE | 2.2 |
| 26 | DE | 30 | GLN | 2.2 |
| 51 | D3 | 6 | THR | 2.2 |
| 1 | CA | 1242 | G | 2.2 |
| 2 | AB | 222 | ARG | 2.2 |
| 2 | CB | 137 | ARG | 2.2 |
| 14 | CN | 61 | ARG | 2.2 |
| 22 | DA | 143 | C | 2.2 |
| 33 | DL | 91 | ASP | 2.2 |
| 7 | CG | 12 | ILE | 2.2 |
| 10 | CJ | 25 | ILE | 2.2 |
| 27 | DF | 104 | ILE | 2.2 |
| 30 | BI | 27 | ALA | 2.2 |
| 22 | DA | 1614 | A | 2.2 |
| 24 | DC | 28 | LYS | 2.2 |
| 28 | DG | 169 | VAL | 2.2 |
| 33 | DL | 140 | GLY | 2.2 |
| 34 | DM | 29 | GLY | 2.2 |
| 3 | CC | 87 | LEU | 2.2 |
| 9 | CI | 63 | LEU | 2.2 |
| 22 | DA | 2107 | G | 2.2 |
| 51 | D3 | 55 | LEU | 2.2 |
| 10 | CJ | 34 | ALA | 2.2 |
| 25 | DD | 22 | ILE | 2.2 |
| 13 | AM | 85 | CYS | 2.2 |
| 13 | CM | 30 | SER | 2.2 |
| 20 | AT | 20 | HIS | 2.2 |
| 20 | CT | 80 | THR | 2.2 |
| 24 | DC | 51 | THR | 2.2 |
| 33 | DL | 117 | THR | 2.2 |
| 14 | CN | 23 | LYS | 2.2 |
| 26 | DE | 113 | VAL | 2.2 |
| 27 | BF | 83 | TYR | 2.2 |
| 32 | DK | 101 | GLY | 2.1 |
| 2 | AB | 30 | PHE | 2.1 |
| 1 | CA | 210 | C | 2.1 |
| 19 | AS | 56 | GLN | 2.1 |
| 32 | DK | 33 | ALA | 2.1 |
| 51 | D3 | 41 | LYS | 2.1 |
| 13 | AM | 92 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | DD | 128 | ARG | 2.1 |
| 37 | DP | 102 | GLU | 2.1 |
| 41 | DT | 4 | GLU | 2.1 |
| 52 | D4 | 36 | ARG | 2.1 |
| 26 | DE | 193 | VAL | 2.1 |
| 3 | CC | 36 | ASP | 2.1 |
| 28 | DG | 60 | ASP | 2.1 |
| 33 | DL | 61 | LEU | 2.1 |
| 7 | CG | 117 | ALA | 2.1 |
| 33 | DL | 38 | GLN | 2.1 |
| 34 | DM | 100 | LYS | 2.1 |
| 38 | DQ | 118 | ALA | 2.1 |
| 13 | CM | 3 | ARG | 2.1 |
| 22 | DA | 1043 | C | 2.1 |
| 43 | DV | 48 | MET | 2.1 |
| 1 | CA | 86 | G | 2.1 |
| 22 | DA | 289 | G | 2.1 |
| 2 | CB | 149 | GLY | 2.1 |
| 9 | AI | 58 | VAL | 2.1 |
| 35 | DN | 116 | VAL | 2.1 |
| 37 | DP | 28 | VAL | 2.1 |
| 40 | DS | 17 | VAL | 2.1 |
| 40 | DS | 26 | GLY | 2.1 |
| 48 | D0 | 30 | VAL | 2.1 |
| 12 | AL | 44 | LYS | 2.1 |
| 16 | CP | 54 | LEU | 2.1 |
| 24 | DC | 98 | ASP | 2.1 |
| 25 | DD | 116 | LYS | 2.1 |
| 39 | DR | 26 | ASP | 2.1 |
| 3 | AC | 101 | ILE | 2.1 |
| 19 | AS | 55 | ARG | 2.1 |
| 28 | DG | 116 | GLN | 2.1 |
| 32 | DK | 77 | ILE | 2.1 |
| 37 | DP | 110 | ILE | 2.1 |
| 50 | D2 | 39 | ARG | 2.1 |
| 9 | AI | 48 | VAL | 2.1 |
| 38 | DQ | 31 | VAL | 2.1 |
| 9 | AI | 22 | LYS | 2.1 |
| 12 | CL | 123 | LYS | 2.1 |
| 22 | DA | 548 | G | 2.1 |
| 49 | D1 | 38 | LYS | 2.1 |
| 8 | CH | 61 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 15 | AO | 31 | LEU | 2.1 |
| 18 | CR | 51 | TYR | 2.1 |
| 19 | CS | 32 | ARG | 2.1 |
| 8 | CH | 130 | ALA | 2.1 |
| 22 | DA | 12 | U | 2.1 |
| 22 | DA | 102 | U | 2.1 |
| 22 | DA | 1872 | A | 2.1 |
| 28 | DG | 13 | ALA | 2.1 |
| 28 | DG | 38 | ASN | 2.1 |
| 28 | DG | 126 | PRO | 2.1 |
| 3 | CC | 5 | VAL | 2.1 |
| 13 | CM | 14 | HIS | 2.1 |
| 34 | DM | 26 | VAL | 2.1 |
| 40 | DS | 71 | VAL | 2.1 |
| 9 | CI | 66 | THR | 2.1 |
| 2 | AB | 91 | PHE | 2.1 |
| 3 | CC | 203 | PHE | 2.1 |
| 8 | CH | 49 | PHE | 2.1 |
| 36 | DO | 111 | ARG | 2.1 |
| 50 | D2 | 35 | ARG | 2.1 |
| 22 | BA | 1171 | G | 2.1 |
| 26 | DE | 152 | GLU | 2.1 |
| 43 | DV | 55 | GLU | 2.1 |
| 39 | DR | 18 | GLN | 2.1 |
| 1 | CA | 843 | U | 2.1 |
| 7 | CG | 24 | ALA | 2.1 |
| 51 | D3 | 27 | ALA | 2.1 |
| 1 | AA | 1493 | A | 2.1 |
| 14 | AN | 12 | LYS | 2.1 |
| 23 | DB | 119 | A | 2.1 |
| 44 | DW | 50 | ASN | 2.1 |
| 29 | DH | 144 | VAL | 2.1 |
| 37 | DP | 92 | VAL | 2.1 |
| 53 | B5 | 120 | VAL | 2.1 |
| 30 | DI | 134 | ARG | 2.1 |
| 19 | AS | 31 | LEU | 2.1 |
| 21 | CU | 44 | GLU | 2.1 |
| 37 | DP | 68 | GLU | 2.1 |
| 13 | CM | 82 | ASP | 2.1 |
| 52 | D4 | 20 | ASP | 2.1 |
| 2 | AB | 131 | LYS | 2.1 |
| 20 | CT | 63 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | DA | 1468 | U | 2.1 |
| 27 | DF | 137 | ILE | 2.1 |
| 51 | D3 | 65 | ALA | 2.1 |
| 3 | CC | 142 | MET | 2.1 |
| 3 | CC | 126 | ARG | 2.1 |
| 32 | DK | 108 | ARG | 2.1 |
| 39 | DR | 58 | VAL | 2.1 |
| 42 | DU | 22 | ARG | 2.1 |
| 1 | AA | 841 | C | 2.1 |
| 24 | BC | 272 | SER | 2.1 |
| 28 | DG | 124 | GLU | 2.1 |
| 37 | DP | 43 | PHE | 2.1 |
| 41 | DT | 11 | LEU | 2.1 |
| 10 | CJ | 28 | THR | 2.1 |
| 13 | CM | 11 | ASP | 2.1 |
| 13 | CM | 54 | ASP | 2.1 |
| 30 | BI | 35 | ILE | 2.1 |
| 36 | DO | 89 | ASP | 2.1 |
| 38 | DQ | 71 | GLN | 2.1 |
| 1 | CA | 85 | U | 2.1 |
| 22 | DA | 884 | U | 2.1 |
| 2 | AB | 180 | GLY | 2.1 |
| 9 | AI | 40 | GLY | 2.1 |
| 10 | CJ | 38 | GLY | 2.1 |
| 6 | CF | 62 | MET | 2.1 |
| 10 | CJ | 96 | VAL | 2.1 |
| 21 | AU | 28 | VAL | 2.1 |
| 24 | DC | 225 | MET | 2.1 |
| 28 | DG | 76 | VAL | 2.1 |
| 49 | D1 | 7 | GLU | 2.1 |
| 2 | CB | 104 | TRP | 2.1 |
| 3 | AC | 43 | LEU | 2.1 |
| 22 | DA | 1117 | C | 2.1 |
| 28 | DG | 87 | LEU | 2.1 |
| 30 | DI | 102 | SER | 2.1 |
| 34 | DM | 62 | LYS | 2.1 |
| 42 | DU | 96 | PHE | 2.1 |
| 3 | CC | 183 | ASP | 2.1 |
| 24 | DC | 246 | THR | 2.1 |
| 25 | DD | 54 | ALA | 2.1 |
| 25 | DD | 87 | GLY | 2.1 |
| 27 | DF | 82 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 52 | D4 | 19 | ARG | 2.1 |
| 7 | AG | 80 | VAL | 2.1 |
| 7 | CG | 94 | VAL | 2.1 |
| 28 | DG | 79 | VAL | 2.1 |
| 38 | DQ | 100 | VAL | 2.1 |
| 41 | DT | 5 | GLU | 2.1 |
| 41 | DT | 54 | GLU | 2.1 |
| 10 | CJ | 13 | PHE | 2.1 |
| 22 | DA | 359 | G | 2.1 |
| 22 | DA | 1452 | G | 2.1 |
| 37 | DP | 97 | LEU | 2.0 |
| 27 | DF | 162 | SER | 2.0 |
| 33 | DL | 7 | SER | 2.0 |
| 31 | DJ | 16 | TYR | 2.0 |
| 31 | DJ | 37 | ARG | 2.0 |
| 33 | DL | 23 | ILE | 2.0 |
| 37 | DP | 109 | ARG | 2.0 |
| 45 | DX | 64 | ILE | 2.0 |
| 10 | CJ | 69 | THR | 2.0 |
| 22 | BA | 1729 | U | 2.0 |
| 22 | DA | 1729 | U | 2.0 |
| 27 | DF | 47 | LYS | 2.0 |
| 16 | AP | 36 | VAL | 2.0 |
| 24 | DC | 132 | MET | 2.0 |
| 31 | DJ | 97 | PRO | 2.0 |
| 3 | AC | 47 | LEU | 2.0 |
| 19 | CS | 5 | LEU | 2.0 |
| 35 | DN | 98 | LEU | 2.0 |
| 39 | DR | 53 | PHE | 2.0 |
| 40 | DS | 75 | PHE | 2.0 |
| 45 | DX | 30 | LEU | 2.0 |
| 46 | DY | 41 | HIS | 2.0 |
| 1 | AA | 1032 | G | 2.0 |
| 7 | CG | 20 | SER | 2.0 |
| 22 | DA | 1303 | G | 2.0 |
| 22 | DA | 1311 | G | 2.0 |
| 17 | CQ | 61 | ILE | 2.0 |
| 26 | DE | 40 | ARG | 2.0 |
| 29 | BH | 143 | ILE | 2.0 |
| 40 | DS | 67 | ASP | 2.0 |
| 3 | CC | 148 | GLY | 2.0 |
| 22 | DA | 2376 | A | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 20 | CT | 76 | LYS | 2.0 |
| 22 | DA | 1083 | U | 2.0 |
| 44 | DW | 84 | ALA | 2.0 |
| 36 | DO | 112 | GLU | 2.0 |
| 43 | DV | 69 | GLU | 2.0 |
| 26 | DE | 33 | VAL | 2.0 |
| 34 | DM | 131 | VAL | 2.0 |
| 27 | DF | 177 | PHE | 2.0 |
| 43 | DV | 42 | LEU | 2.0 |
| 3 | AC | 107 | ARG | 2.0 |
| 24 | DC | 214 | ARG | 2.0 |
| 36 | DO | 30 | ARG | 2.0 |
| 9 | CI | 91 | ASP | 2.0 |
| 24 | DC | 36 | LYS | 2.0 |
| 36 | DO | 96 | GLY | 2.0 |
| 37 | DP | 65 | SER | 2.0 |
| 40 | DS | 66 | ILE | 2.0 |
| 1 | CA | 1024 | G | 2.0 |
| 22 | DA | 290 | U | 2.0 |
| 22 | DA | 795 | C | 2.0 |
| 26 | DE | 50 | ALA | 2.0 |
| 42 | DU | 100 | SER | 2.0 |
| 22 | DA | 1347 | A | 2.0 |
| 22 | DA | 2121 | G | 2.0 |
| 45 | DX | 7 | VAL | 2.0 |
| 8 | AH | 38 | ASN | 2.0 |
| 8 | CH | 63 | LEU | 2.0 |
| 21 | AU | 47 | ARG | 2.0 |
| 24 | DC | 238 | ARG | 2.0 |
| 46 | DY | 26 | PHE | 2.0 |
| 50 | D2 | 5 | PHE | 2.0 |
| 7 | CG | 58 | GLU | 2.0 |
| 14 | CN | 10 | GLU | 2.0 |
| 32 | DK | 115 | ILE | 2.0 |
| 39 | DR | 59 | ILE | 2.0 |
| 42 | DU | 101 | GLU | 2.0 |
| 2 | CB | 191 | SER | 2.0 |
| 29 | BH | 131 | SER | 2.0 |
| 38 | DQ | 96 | ALA | 2.0 |
| 22 | DA | 2143 | C | 2.0 |
| 22 | DA | 141 | G | 2.0 |
| 30 | BI | 65 | ARG | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30 | BI | 118 | THR | 2.0 |
| 7 | CG | 68 | ASN | 2.0 |
| 13 | AM | 8 | ASN | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 54 | MHW | D6 | 1 | 9/10 | 0.87 | 0.20 | 40,52,59,59 | 0 |
| 54 | DBB | D6 | 3 | 6/7 | 0.91 | 0.30 | 36,38,47,51 | 0 |
| 54 | MHU | D6 | 5 | 15/16 | 0.92 | 0.32 | 44,54,60,61 | 0 |
| 54 | MHW | B6 | 1 | 9/10 | 0.94 | 0.18 | 0,0,2,9 | 0 |
| 54 | MHV | D6 | 6 | 9/10 | 0.94 | 0.14 | 45,51,58,60 | 0 |
| 54 | 004 | D6 | 7 | 10/11 | 0.94 | 0.21 | 42,47,58,59 | 0 |
| 54 | MHU | B6 | 5 | 15/16 | 0.96 | 0.20 | 0,0,1,2 | 0 |
| 54 | DBB | B6 | 3 | 6/7 | 0.96 | 0.19 | 0,1,1,2 | 0 |
| 54 | 004 | B6 | 7 | 10/11 | 0.97 | 0.23 | 0,0,2,3 | 0 |
| 54 | MHV | B6 | 6 | 9/10 | 0.97 | 0.16 | 0,0,1,1 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides 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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55 | MG | DA | 3111 | 1/1 | 0.18 | 0.32 | 107,107,107,107 | 0 |
| 55 | MG | DA | 3048 | 1/1 | 0.20 | 0.44 | 127,127,127,127 | 0 |
| 55 | MG | DA | 3135 | 1/1 | 0.24 | 0.32 | 101,101,101,101 | 0 |
| 55 | MG | DA | 3084 | 1/1 | 0.35 | 0.23 | 105,105,105,105 | 0 |
| 55 | MG | DA | 3100 | 1/1 | 0.36 | 0.20 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3041 | 1/1 | 0.38 | 0.42 | 68,68,68,68 | 0 |
| 55 | MG | DA | 3017 | 1/1 | 0.38 | 0.25 | 98,98,98,98 | 0 |
| 55 | MG | DA | 3026 | 1/1 | 0.43 | 0.48 | 101,101,101,101 | 0 |
| 55 | MG | DA | 3093 | 1/1 | 0.46 | 0.11 | 86,86,86,86 | 0 |
| 55 | MG | BA | 3134 | 1/1 | 0.46 | 0.42 | 54,54,54,54 | 0 |
| 55 | MG | CA | 1630 | 1/1 | 0.48 | 0.36 | 120,120,120,120 | 0 |
| 55 | MG | AA | 1619 | 1/1 | 0.50 | 0.31 | 73,73,73,73 | 0 |
| 55 | MG | DA | 3062 | 1/1 | 0.51 | 0.61 | 82,82,82,82 | 0 |
| 55 | MG | CA | 1636 | 1/1 | 0.51 | 0.14 | 126,126,126,126 | 0 |
| 55 | MG | DA | 3148 | 1/1 | 0.51 | 0.29 | 65,65,65,65 | 0 |
| 55 | MG | DA | 3113 | 1/1 | 0.52 | 0.29 | 66,66,66,66 | 0 |
| 55 | MG | DA | 3144 | 1/1 | 0.52 | 0.10 | 68,68,68,68 | 0 |
| 55 | MG | DA | 3133 | 1/1 | 0.52 | 0.78 | 100,100,100,100 | 0 |
| 55 | MG | DA | 3045 | 1/1 | 0.53 | 0.12 | 94,94,94,94 | 0 |
| 55 | MG | DA | 3042 | 1/1 | 0.54 | 0.19 | 87,87,87,87 | 0 |
| 55 | MG | DA | 3057 | 1/1 | 0.54 | 0.29 | 95,95,95,95 | 0 |
| 55 | MG | CA | 1635 | 1/1 | 0.54 | 0.13 | 124,124,124,124 | 0 |
| 55 | MG | BA | 3090 | 1/1 | 0.55 | 0.10 | 19,19,19,19 | 0 |
| 55 | MG | DA | 3099 | 1/1 | 0.57 | 0.38 | 86,86,86,86 | 0 |
| 55 | MG | DA | 3075 | 1/1 | 0.57 | 0.16 | 91,91,91,91 | 0 |
| 55 | MG | DA | 3067 | 1/1 | 0.59 | 0.13 | 58,58,58,58 | 0 |
| 55 | MG | DA | 3029 | 1/1 | 0.59 | 0.22 | 73,73,73,73 | 0 |
| 55 | MG | BA | 3100 | 1/1 | 0.60 | 0.28 | 52,52,52,52 | 0 |
| 55 | MG | DA | 3028 | 1/1 | 0.61 | 0.87 | 103,103,103,103 | 0 |
| 55 | MG | CA | 1627 | 1/1 | 0.61 | 0.20 | 89,89,89,89 | 0 |
| 55 | MG | AA | 1614 | 1/1 | 0.61 | 0.22 | 69,69,69,69 | 0 |
| 55 | MG | CA | 1608 | 1/1 | 0.61 | 0.22 | 84,84,84,84 | 0 |
| 55 | MG | DA | 3027 | 1/1 | 0.62 | 0.17 | 91,91,91,91 | 0 |
| 55 | MG | DA | 3071 | 1/1 | 0.63 | 0.49 | 92,92,92,92 | 0 |
| 55 | MG | CA | 1606 | 1/1 | 0.64 | 0.19 | 89,89,89,89 | 0 |
| 55 | MG | DA | 3002 | 1/1 | 0.64 | 0.10 | 78,78,78,78 | 0 |
| 55 | MG | DA | 3127 | 1/1 | 0.64 | 0.15 | 71,71,71,71 | 0 |
| 55 | MG | DA | 3131 | 1/1 | 0.64 | 1.04 | 99,99,99,99 | 0 |
| 55 | MG | DA | 3090 | 1/1 | 0.65 | 0.14 | 90,90,90,90 | 0 |
| 55 | MG | DA | 3070 | 1/1 | 0.65 | 0.17 | 108,108,108,108 | 0 |
| 55 | MG | DA | 3010 | 1/1 | 0.65 | 0.12 | 80,80,80,80 | 0 |
| 55 | MG | D2 | 101 | 1/1 | 0.65 | 0.15 | 83,83,83,83 | 0 |
| 55 | MG | CA | 1629 | 1/1 | 0.66 | 0.12 | 91,91,91,91 | 0 |
| 55 | MG | DA | 3126 | 1/1 | 0.67 | 0.23 | 80,80,80,80 | 0 |
| 55 | MG | AA | 1658 | 1/1 | 0.67 | 0.35 | 62,62,62,62 | 0 |
| 55 | MG | AA | 1665 | 1/1 | 0.67 | 0.40 | 37,37,37,37 | 0 |
| 55 | MG | AA | 1639 | 1/1 | 0.67 | 0.07 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3078 | 1/1 | 0.68 | 0.14 | 106,106,106,106 | 0 |
| 55 | MG | CA | 1632 | 1/1 | 0.69 | 0.12 | 73,73,73,73 | 0 |
| 55 | MG | DA | 3077 | 1/1 | 0.69 | 0.70 | 113,113,113,113 | 0 |
| 55 | MG | DA | 3019 | 1/1 | 0.69 | 0.18 | 107,107,107,107 | 0 |
| 55 | MG | DA | 3034 | 1/1 | 0.69 | 0.16 | 69,69,69,69 | 0 |
| 55 | MG | DQ | 201 | 1/1 | 0.69 | 0.30 | 45,45,45,45 | 0 |
| 55 | MG | DA | 3103 | 1/1 | 0.69 | 0.24 | 73,73,73,73 | 0 |
| 55 | MG | DA | 3044 | 1/1 | 0.70 | 0.40 | 112,112,112,112 | 0 |
| 55 | MG | DA | 3155 | 1/1 | 0.71 | 0.45 | 62,62,62,62 | 0 |
| 55 | MG | CA | 1602 | 1/1 | 0.72 | 0.11 | 88,88,88,88 | 0 |
| 55 | MG | DA | 3088 | 1/1 | 0.72 | 0.10 | 74,74,74,74 | 0 |
| 55 | MG | DA | 3060 | 1/1 | 0.72 | 0.31 | 77,77,77,77 | 0 |
| 55 | MG | DA | 3012 | 1/1 | 0.72 | 0.10 | 73,73,73,73 | 0 |
| 55 | MG | DA | 3098 | 1/1 | 0.72 | 0.16 | 66,66,66,66 | 0 |
| 55 | MG | AA | 1620 | 1/1 | 0.73 | 0.12 | 69,69,69,69 | 0 |
| 55 | MG | DA | 3134 | 1/1 | 0.73 | 0.14 | 58,58,58,58 | 0 |
| 55 | MG | DB | 201 | 1/1 | 0.73 | 0.06 | 116,116,116,116 | 0 |
| 55 | MG | DA | 3064 | 1/1 | 0.73 | 0.20 | 48,48,48,48 | 0 |
| 55 | MG | DA | 3013 | 1/1 | 0.73 | 0.16 | 44,44,44,44 | 0 |
| 55 | MG | AA | 1648 | 1/1 | 0.74 | 0.20 | 47,47,47,47 | 0 |
| 55 | MG | CA | 1631 | 1/1 | 0.74 | 0.13 | 95,95,95,95 | 0 |
| 55 | MG | DA | 3136 | 1/1 | 0.74 | 0.16 | 91,91,91,91 | 0 |
| 55 | MG | BA | 3050 | 1/1 | 0.74 | 0.07 | 27,27,27,27 | 0 |
| 55 | MG | DA | 3147 | 1/1 | 0.74 | 0.39 | 54,54,54,54 | 0 |
| 55 | MG | DA | 3005 | 1/1 | 0.75 | 0.43 | 102,102,102,102 | 0 |
| 55 | MG | BA | 3186 | 1/1 | 0.75 | 0.30 | 29,29,29,29 | 0 |
| 55 | MG | CA | 1617 | 1/1 | 0.76 | 0.12 | 39,39,39,39 | 0 |
| 55 | MG | BA | 3093 | 1/1 | 0.76 | 0.09 | 58,58,58,58 | 0 |
| 55 | MG | DA | 3037 | 1/1 | 0.76 | 0.08 | 93,93,93,93 | 0 |
| 55 | MG | AA | 1651 | 1/1 | 0.76 | 0.32 | 61,61,61,61 | 0 |
| 55 | MG | CA | 1605 | 1/1 | 0.76 | 0.19 | 86,86,86,86 | 0 |
| 55 | MG | BA | 3049 | 1/1 | 0.76 | 0.13 | 44,44,44,44 | 0 |
| 55 | MG | BA | 3153 | 1/1 | 0.76 | 0.23 | 31,31,31,31 | 0 |
| 55 | MG | DA | 3046 | 1/1 | 0.76 | 0.16 | 62,62,62,62 | 0 |
| 55 | MG | DA | 3072 | 1/1 | 0.76 | 0.52 | 90,90,90,90 | 0 |
| 55 | MG | DA | 3163 | 1/1 | 0.77 | 0.32 | 54,54,54,54 | 0 |
| 55 | MG | DA | 3125 | 1/1 | 0.77 | 0.22 | 62,62,62,62 | 0 |
| 55 | MG | AA | 1626 | 1/1 | 0.77 | 0.17 | 23,23,23,23 | 0 |
| 55 | MG | BA | 3038 | 1/1 | 0.77 | 0.16 | 42,42,42,42 | 0 |
| 55 | MG | DA | 3107 | 1/1 | 0.78 | 0.16 | 75,75,75,75 | 0 |
| 55 | MG | BA | 3167 | 1/1 | 0.78 | 0.18 | 25,25,25,25 | 0 |
| 55 | MG | DA | 3056 | 1/1 | 0.78 | 0.41 | 93,93,93,93 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DB | 203 | 1/1 | 0.78 | 0.08 | 85,85,85,85 | 0 |
| 55 | MG | DA | 3121 | 1/1 | 0.78 | 0.10 | 52,52,52,52 | 0 |
| 55 | MG | AA | 1659 | 1/1 | 0.78 | 0.76 | 50,50,50,50 | 0 |
| 55 | MG | AM | 201 | 1/1 | 0.79 | 0.86 | 62,62,62,62 | 0 |
| 55 | MG | AA | 1652 | 1/1 | 0.79 | 0.19 | 49,49,49,49 | 0 |
| 55 | MG | AA | 1635 | 1/1 | 0.79 | 0.17 | 66,66,66,66 | 0 |
| 55 | MG | AA | 1667 | 1/1 | 0.79 | 0.19 | 49,49,49,49 | 0 |
| 55 | MG | BA | 3057 | 1/1 | 0.79 | 0.35 | 73,73,73,73 | 0 |
| 55 | MG | BA | 3058 | 1/1 | 0.79 | 0.29 | 15,15,15,15 | 0 |
| 55 | MG | DA | 3108 | 1/1 | 0.79 | 0.17 | 59,59,59,59 | 0 |
| 55 | MG | DA | 3003 | 1/1 | 0.79 | 0.47 | 99,99,99,99 | 0 |
| 55 | MG | BA | 3077 | 1/1 | 0.79 | 0.17 | 8,8,8,8 | 0 |
| 55 | MG | AA | 1657 | 1/1 | 0.80 | 0.63 | 64,64,64,64 | 0 |
| 55 | MG | DA | 3152 | 1/1 | 0.80 | 0.29 | 52,52,52,52 | 0 |
| 55 | MG | CA | 1621 | 1/1 | 0.80 | 0.09 | 64,64,64,64 | 0 |
| 55 | MG | DA | 3115 | 1/1 | 0.80 | 0.19 | 111,111,111,111 | 0 |
| 55 | MG | DA | 3006 | 1/1 | 0.80 | 0.13 | 93,93,93,93 | 0 |
| 55 | MG | AA | 1662 | 1/1 | 0.80 | 0.38 | 57,57,57,57 | 0 |
| 55 | MG | BA | 3059 | 1/1 | 0.80 | 0.25 | 38,38,38,38 | 0 |
| 55 | MG | CA | 1609 | 1/1 | 0.80 | 0.15 | 89,89,89,89 | 0 |
| 55 | MG | DA | 3073 | 1/1 | 0.81 | 0.11 | 60,60,60,60 | 0 |
| 55 | MG | DA | 3097 | 1/1 | 0.81 | 0.25 | 91,91,91,91 | 0 |
| 55 | MG | CA | 1638 | 1/1 | 0.81 | 0.10 | 76,76,76,76 | 0 |
| 55 | MG | DA | 3149 | 1/1 | 0.81 | 0.29 | 35,35,35,35 | 0 |
| 55 | MG | DA | 3009 | 1/1 | 0.81 | 0.37 | 90,90,90,90 | 0 |
| 55 | MG | DA | 3022 | 1/1 | 0.81 | 0.10 | 52,52,52,52 | 0 |
| 55 | MG | BA | 3137 | 1/1 | 0.81 | 0.42 | 49,49,49,49 | 0 |
| 55 | MG | BA | 3103 | 1/1 | 0.81 | 0.17 | 0,0,0,0 | 0 |
| 55 | MG | DA | 3089 | 1/1 | 0.81 | 0.33 | 83,83,83,83 | 0 |
| 55 | MG | AA | 1601 | 1/1 | 0.81 | 0.09 | 58,58,58,58 | 0 |
| 55 | MG | DA | 3092 | 1/1 | 0.81 | 0.58 | 113,113,113,113 | 0 |
| 55 | MG | BA | 3075 | 1/1 | 0.82 | 0.16 | 29,29,29,29 | 0 |
| 55 | MG | CA | 1646 | 1/1 | 0.82 | 0.24 | 92,92,92,92 | 0 |
| 55 | MG | BA | 3119 | 1/1 | 0.82 | 0.07 | 20,20,20,20 | 0 |
| 55 | MG | BA | 3180 | 1/1 | 0.82 | 0.19 | 32,32,32,32 | 0 |
| 55 | MG | BA | 3146 | 1/1 | 0.82 | 0.19 | 30,30,30,30 | 0 |
| 55 | MG | BA | 3189 | 1/1 | 0.82 | 0.24 | 45,45,45,45 | 0 |
| 55 | MG | DA | 3120 | 1/1 | 0.82 | 0.11 | 79,79,79,79 | 0 |
| 55 | MG | BA | 3151 | 1/1 | 0.82 | 0.27 | 12,12,12,12 | 0 |
| 55 | MG | CA | 1626 | 1/1 | 0.82 | 0.08 | 48,48,48,48 | 0 |
| 55 | MG | DA | 3033 | 1/1 | 0.83 | 0.10 | 71,71,71,71 | 0 |
| 55 | MG | DA | 3129 | 1/1 | 0.83 | 0.18 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | CA | 1637 | 1/1 | 0.83 | 0.10 | 64,64,64,64 | 0 |
| 55 | MG | DA | 3114 | 1/1 | 0.83 | 0.14 | 65,65,65,65 | 0 |
| 55 | MG | BA | 3021 | 1/1 | 0.83 | 0.19 | 1,1,1,1 | 0 |
| 55 | MG | DA | 3038 | 1/1 | 0.83 | 0.13 | 63,63,63,63 | 0 |
| 55 | MG | DA | 3091 | 1/1 | 0.83 | 0.09 | 77,77,77,77 | 0 |
| 55 | MG | DA | 3040 | 1/1 | 0.83 | 0.18 | 83,83,83,83 | 0 |
| 55 | MG | AA | 1628 | 1/1 | 0.83 | 0.10 | 48,48,48,48 | 0 |
| 55 | MG | BA | 3054 | 1/1 | 0.84 | 0.09 | 9,9,9,9 | 0 |
| 55 | MG | BA | 3089 | 1/1 | 0.84 | 0.07 | 33,33,33,33 | 0 |
| 55 | MG | CA | 1655 | 1/1 | 0.84 | 0.10 | 44,44,44,44 | 0 |
| 55 | MG | DA | 3016 | 1/1 | 0.84 | 0.14 | 62,62,62,62 | 0 |
| 55 | MG | DA | 3153 | 1/1 | 0.84 | 0.26 | 53,53,53,53 | 0 |
| 55 | MG | AA | 1644 | 1/1 | 0.84 | 0.39 | 44,44,44,44 | 0 |
| 55 | MG | BA | 3046 | 1/1 | 0.84 | 0.09 | 17,17,17,17 | 0 |
| 55 | MG | DA | 3094 | 1/1 | 0.84 | 0.18 | 84,84,84,84 | 0 |
| 55 | MG | AA | 1638 | 1/1 | 0.84 | 0.10 | 87,87,87,87 | 0 |
| 55 | MG | CA | 1603 | 1/1 | 0.84 | 0.15 | 44,44,44,44 | 0 |
| 55 | MG | AA | 1623 | 1/1 | 0.84 | 0.05 | 46,46,46,46 | 0 |
| 55 | MG | DA | 3047 | 1/1 | 0.85 | 0.13 | 73,73,73,73 | 0 |
| 55 | MG | BA | 3170 | 1/1 | 0.85 | 0.35 | 38,38,38,38 | 0 |
| 55 | MG | BA | 3016 | 1/1 | 0.85 | 0.43 | 58,58,58,58 | 0 |
| 55 | MG | DA | 3145 | 1/1 | 0.85 | 0.17 | 71,71,71,71 | 0 |
| 55 | MG | DA | 3119 | 1/1 | 0.85 | 0.44 | 106,106,106,106 | 0 |
| 55 | MG | AA | 1631 | 1/1 | 0.85 | 0.10 | 46,46,46,46 | 0 |
| 55 | MG | BA | 3069 | 1/1 | 0.85 | 0.15 | 4,4,4,4 | 0 |
| 55 | MG | DA | 3151 | 1/1 | 0.85 | 0.52 | 59,59,59,59 | 0 |
| 55 | MG | DA | 3124 | 1/1 | 0.85 | 0.23 | 89,89,89,89 | 0 |
| 55 | MG | DA | 3080 | 1/1 | 0.85 | 0.15 | 95,95,95,95 | 0 |
| 55 | MG | DA | 3154 | 1/1 | 0.85 | 0.17 | 40,40,40,40 | 0 |
| 55 | MG | CA | 1601 | 1/1 | 0.85 | 0.09 | 39,39,39,39 | 0 |
| 55 | MG | BA | 3120 | 1/1 | 0.85 | 0.20 | 37,37,37,37 | 0 |
| 55 | MG | DA | 3104 | 1/1 | 0.85 | 0.08 | 79,79,79,79 | 0 |
| 55 | MG | CA | 1624 | 1/1 | 0.85 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | BA | 3027 | 1/1 | 0.85 | 0.34 | 46,46,46,46 | 0 |
| 55 | MG | CA | 1604 | 1/1 | 0.85 | 0.13 | 95,95,95,95 | 0 |
| 55 | MG | CA | 1654 | 1/1 | 0.86 | 0.36 | 56,56,56,56 | 0 |
| 55 | MG | BA | 3104 | 1/1 | 0.86 | 0.17 | 17,17,17,17 | 0 |
| 55 | MG | BA | 3178 | 1/1 | 0.86 | 0.68 | 30,30,30,30 | 0 |
| 55 | MG | AA | 1605 | 1/1 | 0.86 | 0.22 | 23,23,23,23 | 0 |
| 55 | MG | CA | 1615 | 1/1 | 0.86 | 0.30 | 58,58,58,58 | 0 |
| 55 | MG | DA | 3039 | 1/1 | 0.86 | 0.18 | 57,57,57,57 | 0 |
| 55 | MG | BA | 3154 | 1/1 | 0.86 | 0.33 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3157 | 1/1 | 0.86 | 0.30 | 58,58,58,58 | 0 |
| 55 | MG | DA | 3061 | 1/1 | 0.86 | 1.12 | 96,96,96,96 | 0 |
| 55 | MG | DA | 3143 | 1/1 | 0.86 | 0.24 | 60,60,60,60 | 0 |
| 55 | MG | DA | 3008 | 1/1 | 0.86 | 0.26 | 100,100,100,100 | 0 |
| 55 | MG | AA | 1612 | 1/1 | 0.86 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | CA | 1651 | 1/1 | 0.86 | 0.30 | 44,44,44,44 | 0 |
| 55 | MG | DA | 3024 | 1/1 | 0.87 | 0.17 | 46,46,46,46 | 0 |
| 55 | MG | DA | 3025 | 1/1 | 0.87 | 0.26 | 69,69,69,69 | 0 |
| 55 | MG | BB | 202 | 1/1 | 0.87 | 0.10 | 16,16,16,16 | 0 |
| 55 | MG | AA | 1661 | 1/1 | 0.87 | 0.29 | 29,29,29,29 | 0 |
| 55 | MG | DA | 3081 | 1/1 | 0.87 | 0.10 | 60,60,60,60 | 0 |
| 55 | MG | CA | 1656 | 1/1 | 0.87 | 0.37 | 54,54,54,54 | 0 |
| 55 | MG | AA | 1613 | 1/1 | 0.87 | 0.09 | 24,24,24,24 | 0 |
| 55 | MG | DA | 3165 | 1/1 | 0.87 | 0.22 | 42,42,42,42 | 0 |
| 55 | MG | CA | 1628 | 1/1 | 0.87 | 0.18 | 98,98,98,98 | 0 |
| 55 | MG | DB | 202 | 1/1 | 0.87 | 0.11 | 66,66,66,66 | 0 |
| 55 | MG | BA | 3125 | 1/1 | 0.87 | 0.54 | 37,37,37,37 | 0 |
| 55 | MG | AA | 1671 | 1/1 | 0.87 | 0.52 | 59,59,59,59 | 0 |
| 55 | MG | AA | 1664 | 1/1 | 0.87 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | DA | 3112 | 1/1 | 0.88 | 1.38 | 104,104,104,104 | 0 |
| 55 | MG | AA | 1650 | 1/1 | 0.88 | 0.32 | 36,36,36,36 | 0 |
| 55 | MG | DA | 3036 | 1/1 | 0.88 | 0.15 | 62,62,62,62 | 0 |
| 55 | MG | AA | 1670 | 1/1 | 0.88 | 0.29 | 33,33,33,33 | 0 |
| 55 | MG | BA | 3102 | 1/1 | 0.88 | 0.10 | 7,7,7,7 | 0 |
| 55 | MG | AA | 1634 | 1/1 | 0.88 | 0.13 | 35,35,35,35 | 0 |
| 55 | MG | AA | 1643 | 1/1 | 0.88 | 0.14 | 28,28,28,28 | 0 |
| 55 | MG | BA | 3004 | 1/1 | 0.88 | 0.11 | 26,26,26,26 | 0 |
| 55 | MG | BA | 3082 | 1/1 | 0.88 | 0.11 | 6,6,6,6 | 0 |
| 55 | MG | BA | 3179 | 1/1 | 0.88 | 0.33 | 26,26,26,26 | 0 |
| 55 | MG | AA | 1609 | 1/1 | 0.88 | 0.08 | 36,36,36,36 | 0 |
| 55 | MG | AA | 1632 | 1/1 | 0.88 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | DA | 3160 | 1/1 | 0.88 | 0.24 | 43,43,43,43 | 0 |
| 55 | MG | BA | 3092 | 1/1 | 0.88 | 0.10 | 19,19,19,19 | 0 |
| 55 | MG | DA | 3132 | 1/1 | 0.88 | 0.18 | 54,54,54,54 | 0 |
| 55 | MG | DA | 3031 | 1/1 | 0.88 | 0.08 | 69,69,69,69 | 0 |
| 55 | MG | DA | 3049 | 1/1 | 0.88 | 0.25 | 84,84,84,84 | 0 |
| 55 | MG | DA | 3052 | 1/1 | 0.88 | 0.07 | 56,56,56,56 | 0 |
| 55 | MG | BA | 3141 | 1/1 | 0.88 | 0.15 | 17,17,17,17 | 0 |
| 55 | MG | DA | 3138 | 1/1 | 0.88 | 0.35 | 40,40,40,40 | 0 |
| 56 | DOL | DA | 3001 | 48/48 | 0.88 | 0.26 | 26,45,58,63 | 0 |
| 55 | MG | DA | 3020 | 1/1 | 0.89 | 0.15 | 54,54,54,54 | 0 |
| 55 | MG | DA | 3117 | 1/1 | 0.89 | 0.09 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1630 | 1/1 | 0.89 | 0.18 | 73,73,73,73 | 0 |
| 55 | MG | BA | 3064 | 1/1 | 0.89 | 0.19 | 5,5,5,5 | 0 |
| 55 | MG | BA | 3114 | 1/1 | 0.89 | 0.17 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3157 | 1/1 | 0.89 | 0.19 | 24,24,24,24 | 0 |
| 55 | MG | AA | 1637 | 1/1 | 0.89 | 0.10 | 15,15,15,15 | 0 |
| 55 | MG | DA | 3074 | 1/1 | 0.89 | 0.33 | 77,77,77,77 | 0 |
| 55 | MG | BA | 3191 | 1/1 | 0.89 | 0.23 | 12,12,12,12 | 0 |
| 55 | MG | CA | 1649 | 1/1 | 0.89 | 0.18 | 52,52,52,52 | 0 |
| 55 | MG | DA | 3011 | 1/1 | 0.89 | 0.08 | 75,75,75,75 | 0 |
| 55 | MG | CA | 1650 | 1/1 | 0.89 | 0.22 | 35,35,35,35 | 0 |
| 55 | MG | BA | 3040 | 1/1 | 0.89 | 0.15 | 0,0,0,0 | 0 |
| 55 | MG | DA | 3110 | 1/1 | 0.89 | 0.23 | 33,33,33,33 | 0 |
| 55 | MG | DA | 3014 | 1/1 | 0.89 | 0.14 | 73,73,73,73 | 0 |
| 55 | MG | BB | 204 | 1/1 | 0.89 | 0.37 | 16,16,16,16 | 0 |
| 55 | MG | DA | 3137 | 1/1 | 0.89 | 0.42 | 47,47,47,47 | 0 |
| 55 | MG | CA | 1610 | 1/1 | 0.89 | 0.10 | 63,63,63,63 | 0 |
| 55 | MG | DA | 3141 | 1/1 | 0.89 | 0.27 | 40,40,40,40 | 0 |
| 55 | MG | CA | 1613 | 1/1 | 0.89 | 0.14 | 19,19,19,19 | 0 |
| 55 | MG | AA | 1660 | 1/1 | 0.90 | 0.22 | 51,51,51,51 | 0 |
| 55 | MG | BA | 3002 | 1/1 | 0.90 | 0.06 | 18,18,18,18 | 0 |
| 55 | MG | DA | 3146 | 1/1 | 0.90 | 0.10 | 43,43,43,43 | 0 |
| 55 | MG | BA | 3169 | 1/1 | 0.90 | 0.16 | 35,35,35,35 | 0 |
| 55 | MG | DA | 3066 | 1/1 | 0.90 | 0.07 | 47,47,47,47 | 0 |
| 55 | MG | BA | 3112 | 1/1 | 0.90 | 0.08 | 20,20,20,20 | 0 |
| 55 | MG | DA | 3069 | 1/1 | 0.90 | 0.09 | 79,79,79,79 | 0 |
| 55 | MG | DA | 3096 | 1/1 | 0.90 | 0.08 | 57,57,57,57 | 0 |
| 55 | MG | BA | 3171 | 1/1 | 0.90 | 0.20 | 24,24,24,24 | 0 |
| 55 | MG | BA | 3076 | 1/1 | 0.90 | 0.07 | 14,14,14,14 | 0 |
| 55 | MG | DA | 3007 | 1/1 | 0.90 | 0.44 | 121,121,121,121 | 0 |
| 55 | MG | CA | 1640 | 1/1 | 0.90 | 0.14 | 26,26,26,26 | 0 |
| 55 | MG | BA | 3051 | 1/1 | 0.90 | 0.17 | 6,6,6,6 | 0 |
| 55 | MG | CA | 1647 | 1/1 | 0.90 | 0.11 | 41,41,41,41 | 0 |
| 55 | MG | CA | 1648 | 1/1 | 0.90 | 0.20 | 22,22,22,22 | 0 |
| 55 | MG | AA | 1602 | 1/1 | 0.90 | 0.13 | 46,46,46,46 | 0 |
| 55 | MG | BA | 3182 | 1/1 | 0.90 | 0.25 | 33,33,33,33 | 0 |
| 55 | MG | BA | 3087 | 1/1 | 0.90 | 0.13 | 4,4,4,4 | 0 |
| 55 | MG | DA | 3058 | 1/1 | 0.90 | 1.10 | 109,109,109,109 | 0 |
| 55 | MG | DA | 3085 | 1/1 | 0.90 | 0.12 | 67,67,67,67 | 0 |
| 55 | MG | BA | 3156 | 1/1 | 0.90 | 0.28 | 19,19,19,19 | 0 |
| 55 | MG | BA | 3116 | 1/1 | 0.91 | 0.26 | 34,34,34,34 | 0 |
| 55 | MG | DA | 3065 | 1/1 | 0.91 | 0.12 | 36,36,36,36 | 0 |
| 55 | MG | CA | 1616 | 1/1 | 0.91 | 0.10 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3193 | 1/1 | 0.91 | 0.15 | 38,38,38,38 | 0 |
| 55 | MG | DA | 3068 | 1/1 | 0.91 | 0.13 | 65,65,65,65 | 0 |
| 55 | MG | BA | 3195 | 1/1 | 0.91 | 0.56 | 23,23,23,23 | 0 |
| 55 | MG | DA | 3015 | 1/1 | 0.91 | 0.06 | 55,55,55,55 | 0 |
| 55 | MG | DA | 3105 | 1/1 | 0.91 | 0.18 | 80,80,80,80 | 0 |
| 55 | MG | DA | 3106 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 55 | MG | BA | 3006 | 1/1 | 0.91 | 0.14 | 50,50,50,50 | 0 |
| 55 | MG | BA | 3008 | 1/1 | 0.91 | 0.14 | 37,37,37,37 | 0 |
| 55 | MG | BA | 3168 | 1/1 | 0.91 | 0.12 | 35,35,35,35 | 0 |
| 55 | MG | BA | 3015 | 1/1 | 0.91 | 0.07 | 2,2,2,2 | 0 |
| 55 | MG | DA | 3021 | 1/1 | 0.91 | 0.18 | 63,63,63,63 | 0 |
| 55 | MG | DA | 3150 | 1/1 | 0.91 | 0.20 | 56,56,56,56 | 0 |
| 55 | MG | BA | 3132 | 1/1 | 0.91 | 0.09 | 23,23,23,23 | 0 |
| 55 | MG | AA | 1629 | 1/1 | 0.91 | 0.14 | 61,61,61,61 | 0 |
| 55 | MG | BA | 3003 | 1/1 | 0.91 | 0.06 | 17,17,17,17 | 0 |
| 55 | MG | AA | 1641 | 1/1 | 0.91 | 0.15 | 19,19,19,19 | 0 |
| 55 | MG | DA | 3050 | 1/1 | 0.91 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | BA | 3078 | 1/1 | 0.91 | 0.72 | 79,79,79,79 | 0 |
| 55 | MG | DA | 3159 | 1/1 | 0.91 | 0.30 | 43,43,43,43 | 0 |
| 55 | MG | DA | 3087 | 1/1 | 0.91 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | DA | 3123 | 1/1 | 0.91 | 0.12 | 57,57,57,57 | 0 |
| 55 | MG | DA | 3164 | 1/1 | 0.91 | 0.18 | 57,57,57,57 | 0 |
| 55 | MG | DA | 3054 | 1/1 | 0.91 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | BA | 3081 | 1/1 | 0.91 | 0.12 | 24,24,24,24 | 0 |
| 55 | MG | BA | 3033 | 1/1 | 0.91 | 0.12 | 11,11,11,11 | 0 |
| 55 | MG | DA | 3030 | 1/1 | 0.91 | 0.24 | 60,60,60,60 | 0 |
| 55 | MG | BA | 3005 | 1/1 | 0.91 | 0.07 | 34,34,34,34 | 0 |
| 55 | MG | DA | 3032 | 1/1 | 0.91 | 0.26 | 68,68,68,68 | 0 |
| 55 | MG | CA | 1614 | 1/1 | 0.91 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | CA | 1622 | 1/1 | 0.92 | 0.13 | 51,51,51,51 | 0 |
| 55 | MG | DA | 3004 | 1/1 | 0.92 | 0.11 | 76,76,76,76 | 0 |
| 55 | MG | BA | 3071 | 1/1 | 0.92 | 0.07 | 60,60,60,60 | 0 |
| 55 | MG | BA | 3098 | 1/1 | 0.92 | 0.12 | 2,2,2,2 | 0 |
| 55 | MG | AA | 1654 | 1/1 | 0.92 | 0.14 | 43,43,43,43 | 0 |
| 55 | MG | AA | 1625 | 1/1 | 0.92 | 0.07 | 47,47,47,47 | 0 |
| 55 | MG | BA | 3152 | 1/1 | 0.92 | 0.19 | 6,6,6,6 | 0 |
| 55 | MG | AA | 1606 | 1/1 | 0.92 | 0.11 | 44,44,44,44 | 0 |
| 55 | MG | AA | 1603 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 55 | MG | BA | 3042 | 1/1 | 0.92 | 0.38 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3113 | 1/1 | 0.92 | 0.17 | 22,22,22,22 | 0 |
| 55 | MG | AA | 1666 | 1/1 | 0.92 | 0.19 | 46,46,46,46 | 0 |
| 55 | MG | BA | 3086 | 1/1 | 0.92 | 0.07 | 14,14,14,14 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3063 | 1/1 | 0.92 | 0.45 | 31,31,31,31 | 0 |
| 55 | MG | CA | 1639 | 1/1 | 0.92 | 0.10 | 43,43,43,43 | 0 |
| 55 | MG | DA | 3116 | 1/1 | 0.92 | 0.36 | 76,76,76,76 | 0 |
| 55 | MG | DA | 3082 | 1/1 | 0.92 | 0.13 | 60,60,60,60 | 0 |
| 55 | MG | CA | 1607 | 1/1 | 0.92 | 0.08 | 54,54,54,54 | 0 |
| 55 | MG | BA | 3047 | 1/1 | 0.92 | 0.10 | 4,4,4,4 | 0 |
| 55 | MG | DA | 3158 | 1/1 | 0.92 | 0.19 | 70,70,70,70 | 0 |
| 55 | MG | BA | 3066 | 1/1 | 0.92 | 0.15 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3174 | 1/1 | 0.92 | 0.12 | 12,12,12,12 | 0 |
| 55 | MG | DA | 3023 | 1/1 | 0.92 | 0.05 | 69,69,69,69 | 0 |
| 55 | MG | BA | 3127 | 1/1 | 0.92 | 0.12 | 9,9,9,9 | 0 |
| 55 | MG | BA | 3131 | 1/1 | 0.92 | 0.18 | 1,1,1,1 | 0 |
| 55 | MG | BA | 3091 | 1/1 | 0.92 | 0.09 | 3,3,3,3 | 0 |
| 55 | MG | BA | 3133 | 1/1 | 0.92 | 0.10 | 32,32,32,32 | 0 |
| 55 | MG | AA | 1646 | 1/1 | 0.92 | 0.20 | 49,49,49,49 | 0 |
| 55 | MG | DA | 3095 | 1/1 | 0.92 | 0.41 | 91,91,91,91 | 0 |
| 55 | MG | CA | 1620 | 1/1 | 0.92 | 0.06 | 61,61,61,61 | 0 |
| 55 | MG | BA | 3187 | 1/1 | 0.92 | 0.06 | 33,33,33,33 | 0 |
| 55 | MG | DA | 3101 | 1/1 | 0.93 | 0.09 | 57,57,57,57 | 0 |
| 55 | MG | BA | 3155 | 1/1 | 0.93 | 0.21 | 20,20,20,20 | 0 |
| 55 | MG | AA | 1669 | 1/1 | 0.93 | 0.42 | 51,51,51,51 | 0 |
| 55 | MG | DA | 3140 | 1/1 | 0.93 | 0.43 | 43,43,43,43 | 0 |
| 55 | MG | BA | 3121 | 1/1 | 0.93 | 0.12 | 3,3,3,3 | 0 |
| 55 | MG | DA | 3142 | 1/1 | 0.93 | 0.26 | 33,33,33,33 | 0 |
| 55 | MG | BA | 3166 | 1/1 | 0.93 | 0.17 | 19,19,19,19 | 0 |
| 55 | MG | CA | 1633 | 1/1 | 0.93 | 0.32 | 64,64,64,64 | 0 |
| 55 | MG | AA | 1663 | 1/1 | 0.93 | 0.22 | 48,48,48,48 | 0 |
| 55 | MG | BA | 3126 | 1/1 | 0.93 | 0.12 | 6,6,6,6 | 0 |
| 55 | MG | BA | 3030 | 1/1 | 0.93 | 0.14 | 9,9,9,9 | 0 |
| 55 | MG | BA | 3031 | 1/1 | 0.93 | 0.07 | 14,14,14,14 | 0 |
| 55 | MG | AA | 1610 | 1/1 | 0.93 | 0.23 | 65,65,65,65 | 0 |
| 55 | MG | BA | 3173 | 1/1 | 0.93 | 0.14 | 27,27,27,27 | 0 |
| 55 | MG | CA | 1643 | 1/1 | 0.93 | 0.24 | 50,50,50,50 | 0 |
| 55 | MG | BA | 3056 | 1/1 | 0.93 | 0.08 | 5,5,5,5 | 0 |
| 55 | MG | BA | 3034 | 1/1 | 0.93 | 0.10 | 6,6,6,6 | 0 |
| 55 | MG | BA | 3136 | 1/1 | 0.93 | 0.12 | 21,21,21,21 | 0 |
| 55 | MG | DA | 3053 | 1/1 | 0.93 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | BA | 3079 | 1/1 | 0.93 | 0.09 | 22,22,22,22 | 0 |
| 55 | MG | BA | 3181 | 1/1 | 0.93 | 0.20 | 24,24,24,24 | 0 |
| 55 | MG | AA | 1617 | 1/1 | 0.93 | 0.12 | 52,52,52,52 | 0 |
| 55 | MG | CA | 1652 | 1/1 | 0.93 | 0.11 | 83,83,83,83 | 0 |
| 55 | MG | DA | 3161 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3185 | 1/1 | 0.93 | 0.30 | 16,16,16,16 | 0 |
| 55 | MG | BA | 3013 | 1/1 | 0.93 | 0.21 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3149 | 1/1 | 0.93 | 0.12 | 38,38,38,38 | 0 |
| 55 | MG | DA | 3130 | 1/1 | 0.93 | 0.10 | 81,81,81,81 | 0 |
| 55 | MG | BA | 3085 | 1/1 | 0.93 | 0.22 | 27,27,27,27 | 0 |
| 55 | MG | BA | 3190 | 1/1 | 0.93 | 0.10 | 31,31,31,31 | 0 |
| 55 | MG | AA | 1627 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | AA | 1618 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | BA | 3065 | 1/1 | 0.93 | 0.14 | 0,0,0,0 | 0 |
| 55 | MG | AA | 1616 | 1/1 | 0.94 | 0.12 | 50,50,50,50 | 0 |
| 55 | MG | BA | 3140 | 1/1 | 0.94 | 0.39 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3043 | 1/1 | 0.94 | 0.13 | 16,16,16,16 | 0 |
| 55 | MG | DA | 3079 | 1/1 | 0.94 | 0.13 | 96,96,96,96 | 0 |
| 55 | MG | BA | 3084 | 1/1 | 0.94 | 0.05 | 6,6,6,6 | 0 |
| 55 | MG | CA | 1625 | 1/1 | 0.94 | 0.15 | 22,22,22,22 | 0 |
| 55 | MG | AA | 1607 | 1/1 | 0.94 | 0.09 | 44,44,44,44 | 0 |
| 55 | MG | CA | 1653 | 1/1 | 0.94 | 0.09 | 52,52,52,52 | 0 |
| 55 | MG | BA | 3150 | 1/1 | 0.94 | 0.20 | 37,37,37,37 | 0 |
| 55 | MG | BA | 3025 | 1/1 | 0.94 | 0.10 | 2,2,2,2 | 0 |
| 55 | MG | DA | 3055 | 1/1 | 0.94 | 0.13 | 72,72,72,72 | 0 |
| 55 | MG | AA | 1649 | 1/1 | 0.94 | 0.14 | 32,32,32,32 | 0 |
| 55 | MG | BA | 3130 | 1/1 | 0.94 | 0.12 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3039 | 1/1 | 0.94 | 0.27 | 0,0,0,0 | 0 |
| 55 | MG | AA | 1668 | 1/1 | 0.94 | 0.13 | 29,29,29,29 | 0 |
| 55 | MG | BA | 3053 | 1/1 | 0.94 | 0.14 | 2,2,2,2 | 0 |
| 55 | MG | BA | 3115 | 1/1 | 0.94 | 0.12 | 20,20,20,20 | 0 |
| 55 | MG | BA | 3159 | 1/1 | 0.94 | 0.22 | 14,14,14,14 | 0 |
| 55 | MG | BA | 3160 | 1/1 | 0.94 | 0.10 | 10,10,10,10 | 0 |
| 55 | MG | DA | 3035 | 1/1 | 0.94 | 0.09 | 79,79,79,79 | 0 |
| 55 | MG | BA | 3164 | 1/1 | 0.94 | 0.14 | 4,4,4,4 | 0 |
| 55 | MG | BA | 3165 | 1/1 | 0.94 | 0.30 | 43,43,43,43 | 0 |
| 55 | MG | BA | 3080 | 1/1 | 0.94 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | DA | 3167 | 1/1 | 0.94 | 0.29 | 100,100,100,100 | 0 |
| 55 | MG | CA | 1641 | 1/1 | 0.94 | 0.68 | 73,73,73,73 | 0 |
| 55 | MG | DA | 3102 | 1/1 | 0.94 | 0.22 | 62,62,62,62 | 0 |
| 55 | MG | CA | 1642 | 1/1 | 0.94 | 0.25 | 25,25,25,25 | 0 |
| 55 | MG | BA | 3192 | 1/1 | 0.94 | 0.21 | 22,22,22,22 | 0 |
| 55 | MG | CA | 1645 | 1/1 | 0.94 | 0.20 | 32,32,32,32 | 0 |
| 55 | MG | CA | 1619 | 1/1 | 0.94 | 0.10 | 33,33,33,33 | 0 |
| 55 | MG | AA | 1608 | 1/1 | 0.95 | 0.14 | 17,17,17,17 | 0 |
| 55 | MG | AA | 1653 | 1/1 | 0.95 | 0.17 | 28,28,28,28 | 0 |
| 55 | MG | AA | 1640 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3094 | 1/1 | 0.95 | 0.05 | 31,31,31,31 | 0 |
| 55 | MG | BA | 3045 | 1/1 | 0.95 | 0.08 | 9,9,9,9 | 0 |
| 55 | MG | BA | 3061 | 1/1 | 0.95 | 0.35 | 30,30,30,30 | 0 |
| 55 | MG | DA | 3118 | 1/1 | 0.95 | 0.08 | 60,60,60,60 | 0 |
| 55 | MG | CA | 1611 | 1/1 | 0.95 | 0.29 | 90,90,90,90 | 0 |
| 55 | MG | BA | 3062 | 1/1 | 0.95 | 0.36 | 50,50,50,50 | 0 |
| 55 | MG | AA | 1655 | 1/1 | 0.95 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | AA | 1624 | 1/1 | 0.95 | 0.04 | 41,41,41,41 | 0 |
| 55 | MG | BA | 3188 | 1/1 | 0.95 | 0.14 | 10,10,10,10 | 0 |
| 55 | MG | BA | 3017 | 1/1 | 0.95 | 0.06 | 2,2,2,2 | 0 |
| 55 | MG | BA | 3161 | 1/1 | 0.95 | 0.17 | 31,31,31,31 | 0 |
| 55 | MG | BA | 3035 | 1/1 | 0.95 | 0.18 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3036 | 1/1 | 0.95 | 0.12 | 11,11,11,11 | 0 |
| 55 | MG | DA | 3043 | 1/1 | 0.95 | 0.13 | 66,66,66,66 | 0 |
| 55 | MG | BA | 3138 | 1/1 | 0.95 | 0.45 | 1,1,1,1 | 0 |
| 55 | MG | BA | 3088 | 1/1 | 0.95 | 0.23 | 2,2,2,2 | 0 |
| 55 | MG | BA | 3020 | 1/1 | 0.95 | 0.09 | 22,22,22,22 | 0 |
| 55 | MG | BB | 203 | 1/1 | 0.95 | 0.06 | 7,7,7,7 | 0 |
| 55 | MG | DA | 3166 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 55 | MG | BA | 3145 | 1/1 | 0.95 | 0.29 | 28,28,28,28 | 0 |
| 55 | MG | BA | 3118 | 1/1 | 0.95 | 0.12 | 1,1,1,1 | 0 |
| 55 | MG | BA | 3148 | 1/1 | 0.95 | 0.12 | 29,29,29,29 | 0 |
| 55 | MG | DA | 3051 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 55 | MG | DA | 3109 | 1/1 | 0.95 | 0.22 | 42,42,42,42 | 0 |
| 55 | MG | BA | 3172 | 1/1 | 0.95 | 0.17 | 31,31,31,31 | 0 |
| 55 | MG | AA | 1647 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 55 | MG | CA | 1612 | 1/1 | 0.96 | 0.05 | 40,40,40,40 | 0 |
| 55 | MG | BA | 3135 | 1/1 | 0.96 | 0.14 | 2,2,2,2 | 0 |
| 55 | MG | BA | 3023 | 1/1 | 0.96 | 0.14 | 1,1,1,1 | 0 |
| 55 | MG | BA | 3024 | 1/1 | 0.96 | 0.17 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3012 | 1/1 | 0.96 | 0.05 | 14,14,14,14 | 0 |
| 55 | MG | CA | 1644 | 1/1 | 0.96 | 0.15 | 42,42,42,42 | 0 |
| 55 | MG | DA | 3018 | 1/1 | 0.96 | 0.12 | 60,60,60,60 | 0 |
| 55 | MG | BA | 3026 | 1/1 | 0.96 | 0.15 | 3,3,3,3 | 0 |
| 55 | MG | CA | 1618 | 1/1 | 0.96 | 0.11 | 37,37,37,37 | 0 |
| 55 | MG | AA | 1633 | 1/1 | 0.96 | 0.12 | 30,30,30,30 | 0 |
| 55 | MG | DA | 3083 | 1/1 | 0.96 | 0.10 | 69,69,69,69 | 0 |
| 55 | MG | BA | 3029 | 1/1 | 0.96 | 0.08 | 21,21,21,21 | 0 |
| 55 | MG | BA | 3095 | 1/1 | 0.96 | 0.09 | 21,21,21,21 | 0 |
| 55 | MG | BB | 201 | 1/1 | 0.96 | 0.10 | 20,20,20,20 | 0 |
| 55 | MG | CA | 1623 | 1/1 | 0.96 | 0.16 | 50,50,50,50 | 0 |
| 55 | MG | BA | 3147 | 1/1 | 0.96 | 0.31 | 9,9,9,9 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3014 | 1/1 | 0.96 | 0.18 | 0,0,0,0 | 0 |
| 55 | MG | DA | 3122 | 1/1 | 0.96 | 0.15 | 41,41,41,41 | 0 |
| 55 | MG | BA | 3122 | 1/1 | 0.96 | 0.04 | 18,18,18,18 | 0 |
| 55 | MG | BA | 3124 | 1/1 | 0.96 | 0.09 | 11,11,11,11 | 0 |
| 55 | MG | DA | 3059 | 1/1 | 0.96 | 0.10 | 51,51,51,51 | 0 |
| 55 | MG | BA | 3009 | 1/1 | 0.96 | 0.09 | 4,4,4,4 | 0 |
| 55 | MG | BA | 3175 | 1/1 | 0.96 | 0.11 | 27,27,27,27 | 0 |
| 55 | MG | DA | 3128 | 1/1 | 0.96 | 0.08 | 80,80,80,80 | 0 |
| 55 | MG | BA | 3176 | 1/1 | 0.96 | 0.10 | 20,20,20,20 | 0 |
| 55 | MG | BA | 3101 | 1/1 | 0.96 | 0.07 | 1,1,1,1 | 0 |
| 55 | MG | BA | 3070 | 1/1 | 0.96 | 0.21 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3044 | 1/1 | 0.96 | 0.14 | 3,3,3,3 | 0 |
| 55 | MG | CA | 1634 | 1/1 | 0.96 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | BA | 3074 | 1/1 | 0.96 | 0.18 | 1,1,1,1 | 0 |
| 55 | MG | BA | 3108 | 1/1 | 0.96 | 0.24 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3110 | 1/1 | 0.96 | 0.20 | 3,3,3,3 | 0 |
| 56 | DOL | BA | 3001 | 48/48 | 0.96 | 0.21 | 0,3,25,36 | 0 |
| 55 | MG | BA | 3022 | 1/1 | 0.96 | 0.08 | 2,2,2,2 | 0 |
| 55 | MG | BA | 3111 | 1/1 | 0.97 | 0.20 | 6,6,6,6 | 0 |
| 55 | MG | DA | 3086 | 1/1 | 0.97 | 0.10 | 76,76,76,76 | 0 |
| 55 | MG | BA | 3072 | 1/1 | 0.97 | 0.08 | 3,3,3,3 | 0 |
| 55 | MG | BA | 3183 | 1/1 | 0.97 | 0.21 | 12,12,12,12 | 0 |
| 55 | MG | BA | 3184 | 1/1 | 0.97 | 0.20 | 6,6,6,6 | 0 |
| 55 | MG | BA | 3158 | 1/1 | 0.97 | 0.12 | 19,19,19,19 | 0 |
| 55 | MG | BA | 3073 | 1/1 | 0.97 | 0.07 | 7,7,7,7 | 0 |
| 55 | MG | DA | 3063 | 1/1 | 0.97 | 0.22 | 54,54,54,54 | 0 |
| 55 | MG | BA | 3037 | 1/1 | 0.97 | 0.17 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3060 | 1/1 | 0.97 | 0.06 | 15,15,15,15 | 0 |
| 55 | MG | BA | 3163 | 1/1 | 0.97 | 0.33 | 15,15,15,15 | 0 |
| 55 | MG | AA | 1615 | 1/1 | 0.97 | 0.06 | 47,47,47,47 | 0 |
| 55 | MG | DA | 3156 | 1/1 | 0.97 | 0.19 | 41,41,41,41 | 0 |
| 55 | MG | BA | 3117 | 1/1 | 0.97 | 0.17 | 1,1,1,1 | 0 |
| 55 | MG | BA | 3007 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 55 | MG | AA | 1611 | 1/1 | 0.97 | 0.09 | 21,21,21,21 | 0 |
| 55 | MG | BA | 3142 | 1/1 | 0.97 | 0.43 | 2,2,2,2 | 0 |
| 55 | MG | BA | 3052 | 1/1 | 0.97 | 0.06 | 11,11,11,11 | 0 |
| 55 | MG | BA | 3032 | 1/1 | 0.97 | 0.16 | 4,4,4,4 | 0 |
| 55 | MG | AA | 1604 | 1/1 | 0.97 | 0.06 | 48,48,48,48 | 0 |
| 55 | MG | BA | 3123 | 1/1 | 0.97 | 0.16 | 0,0,0,0 | 0 |
| 55 | MG | DA | 3076 | 1/1 | 0.97 | 0.12 | 69,69,69,69 | 0 |
| 55 | MG | BQ | 201 | 1/1 | 0.97 | 0.20 | 3,3,3,3 | 0 |
| 55 | MG | BA | 3067 | 1/1 | 0.97 | 0.17 | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3083 | 1/1 | 0.97 | 0.17 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3068 | 1/1 | 0.97 | 0.17 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3010 | 1/1 | 0.97 | 0.11 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3129 | 1/1 | 0.97 | 0.19 | 4,4,4,4 | 0 |
| 55 | MG | BA | 3018 | 1/1 | 0.97 | 0.20 | 0,0,0,0 | 0 |
| 55 | MG | AA | 1642 | 1/1 | 0.97 | 0.15 | 23,23,23,23 | 0 |
| 55 | MG | BA | 3109 | 1/1 | 0.98 | 0.19 | 12,12,12,12 | 0 |
| 55 | MG | AA | 1636 | 1/1 | 0.98 | 0.08 | 27,27,27,27 | 0 |
| 55 | MG | BA | 3041 | 1/1 | 0.98 | 0.18 | 6,6,6,6 | 0 |
| 55 | MG | BA | 3128 | 1/1 | 0.98 | 0.10 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3096 | 1/1 | 0.98 | 0.07 | 11,11,11,11 | 0 |
| 55 | MG | BA | 3097 | 1/1 | 0.98 | 0.07 | 4,4,4,4 | 0 |
| 55 | MG | AA | 1622 | 1/1 | 0.98 | 0.20 | 16,16,16,16 | 0 |
| 55 | MG | BA | 3099 | 1/1 | 0.98 | 0.12 | 4,4,4,4 | 0 |
| 55 | MG | BA | 3194 | 1/1 | 0.98 | 0.07 | 8,8,8,8 | 0 |
| 55 | MG | BA | 3028 | 1/1 | 0.98 | 0.08 | 5,5,5,5 | 0 |
| 55 | MG | DA | 3162 | 1/1 | 0.98 | 0.21 | 38,38,38,38 | 0 |
| 55 | MG | AA | 1656 | 1/1 | 0.98 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | AA | 1621 | 1/1 | 0.98 | 0.08 | 39,39,39,39 | 0 |
| 55 | MG | BA | 3055 | 1/1 | 0.98 | 0.17 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3177 | 1/1 | 0.98 | 0.17 | 17,17,17,17 | 0 |
| 55 | MG | AA | 1645 | 1/1 | 0.98 | 0.12 | 42,42,42,42 | 0 |
| 55 | MG | BA | 3105 | 1/1 | 0.98 | 0.10 | 4,4,4,4 | 0 |
| 55 | MG | BA | 3139 | 1/1 | 0.98 | 0.37 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3106 | 1/1 | 0.98 | 0.20 | 16,16,16,16 | 0 |
| 55 | MG | BA | 3107 | 1/1 | 0.98 | 0.19 | 0,0,0,0 | 0 |
| 55 | MG | BA | 3162 | 1/1 | 0.98 | 0.07 | 36,36,36,36 | 0 |
| 55 | MG | BA | 3019 | 1/1 | 0.98 | 0.12 | 11,11,11,11 | 0 |
| 55 | MG | BA | 3144 | 1/1 | 0.98 | 0.26 | 15,15,15,15 | 0 |
| 57 | ZN | B4 | 101 | 1/1 | 0.98 | 0.10 | 33,33,33,33 | 0 |
| 57 | ZN | D4 | 101 | 1/1 | 0.98 | 0.10 | 87,87,87,87 | 0 |
| 55 | MG | BA | 3143 | 1/1 | 0.99 | 0.36 | 12,12,12,12 | 0 |
| 55 | MG | BA | 3011 | 1/1 | 0.99 | 0.15 | 1,1,1,1 | 0 |
| 55 | MG | DA | 3139 | 1/1 | 0.99 | 0.33 | 30,30,30,30 | 0 |
| 55 | MG | BA | 3048 | 1/1 | 0.99 | 0.15 | 8,8,8,8 | 0 |

6.5 Other polymers

There are no such residues in this entry.